Peculiarities of using classification indicators of the coal metamorphism degree for predicting the hazardous coal seams properties

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Abstract. Currently, there is no reliable regulatory framework for determining the hazardous properties of coal seams, including the propensity of coal for spontaneous combustion. Under relatively identical mining engineering and geological conditions for mining coal seams, the probability of emergency situations is determined to a large extent by the genetic properties of coal. The research methodology is based on the classical definition of metamorphism, which characterizes the change in the composition and properties of coal. The analysis involves indicators that directly or indirectly characterize the elemental composition of organic and mineral mass, chemical activity and physico-mechanical properties. This will allow to establish a specific composition and properties that contribute to the manifestation of certain hazardous properties of coal seams during mining operations. It is shown that the modern industrial classification does not take into account the change in the organic and mineral constituents of coal, which does not make it possible to use it unchanged to predict the hazardous properties of coal seams.

1 Introduction

Hazardous properties of coal seams are the gas content of coal, its tendency to gas-dynamic phenomena, spontaneous combustion, dust-forming ability and explosive power of coal dust [1]. This is not an exhaustive list of the hazardous properties of coal seams that accompany mining operations and can lead to underground accidents with tragic consequences [2].

Under relatively identical mining-engineering and geological conditions for mining the coal seams, the probability of emergency situations is determined to a large extent by the genetic properties of coal. Their appearance is due to metamorphic transformations of the source material. The conditions for the formation of metamorphic rocks in general [3] and fossil coals in particular [4 – 7] practically do not differ from each other. It is assumed that the processes of metamorphism occurred in past geological periods at a temperature of 200 – 650ºC at a depth of 10 – 40 km [8, 9].

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In general, metamorphism refers to a variety of endogenous processes, which are associated with changes in the structure, mineral and chemical composition of rocks. When converting coal, they are reduced to the enrichment of organic matter with carbon and depletion of its other components [3 – 6]. Metamorphism is part of the process of coal formation; it does not include the transition of peat to brown coals, which is determined by diagenesis.

Based on the classical definition of the degree of metamorphism concept, it follows that when forecasting the hazardous properties of coal seams by genetic characteristics, it is necessary to take into account changes in the composition and structure of coal that have occurred as a result of geological transformations.

In the regulatory framework of Ukraine [10 – 13], which provides for the safe development of coal seams, only certain classification indicators are used. They only indirectly characterize the composition and structure of coals in the process of their metamorphic transformations. Their limited number includes the mass yield of volatiles during the thermal decomposition of coal without access of air (V^{daf}), volumetric yield of volatiles (V_v^{daf}), the logarithm of the electrical resistivity of anthracites ($\lg\rho$) and the thickness of the plastic layer (y). Each of these indicators or some combination of them characterizes different aspects of the degree of metamorphism of coals and anthracites.

The methods for determining the degree of metamorphism by the parameters of the indicators (V^{daf}, V_v^{daf}, $\lg\rho$, y) are based on completely different coal properties. The indicators (V^{daf} and V_v^{daf}) characterize [14] the amount of released gases (H_2, CH_4, CO, CO_2), according to which there is no immediate opportunity to establish changes in the elemental composition or structure of coal. The logarithm of the electrical resistivity of anthracites ($\lg\rho$) characterizes the dielectric properties of anthracites only. The connection of this indicator with changes in chemical composition and structure has been little studied.

The thickness of the coal layer (y) is a product of dry coal distillation and characterizes the output of coal tar. The value of this indicator is used to establish the coking ability of coal. From a comparison of the properties characterizing the indicators (V^{daf}, V_v^{daf}, $\lg\rho$, y), it follows that they reflect different aspects of coal conversion in the process of metamorphism.

According to the methods for determining the parameters V^{daf}, V_v^{daf}, $\lg\rho$ and y, it is clearly impossible to establish what hazardous properties of coal seams they characterize. The V^{daf} and V_v^{daf} indicators conditionally determine the overall degree of metamorphism and in most cases are used in industrial classifications to establish the brand of coal. In the thermal decomposition of coal without access to air, hydrogen (H_2), methane (CH_4), and carbon oxides (CO, CO_2) are released in different proportions [14].

At different stages of metamorphism, ambiguous changes in the elemental composition of organic matter took place. Changes are found in carbon (C^o), nitrogen (N^o), sulphur (S^o) and oxygen (O^o). In parallel with these processes, the formation of volatile products at each stage of metamorphism was observed. As a result of the implementation of certain stages of metamorphic processes, volatile products appeared that could be removed from the system. These include H_2O, CO_2, CH_4, H_2S and NH_3 [15].

The above features of the formation of volatile substances during thermal decomposition of coal [14] and in the process of metamorphic transformations [15] are not taken into account by regulatory documents [10 – 13]. This indicates the incomplete compliance of the applied V^{daf} and V_v^{daf} indicators and to establish the degree of coal metamorphism and the manifestation of the hazardous properties of coal seams during mining operations.

The logarithm of the electrical resistivity of anthracites (lgρ) by its nature only indirectly reflects a change in the internal structure of anthracites in the process of metamorphic transformations.

The thickness of the coal layer (y) characterizes the yield of coal tar and in almost all known industrial classifications serves to establish the coking ability of coal [16]. Without sufficient scientific justification, in combination with V^{daf} it is used to establish the outburst hazard of coal seams [10].

The manifestation of hazardous properties of coal seams is determined by a wide range of factors. Apart from metamorphism, these include tectonic structures and mining conditions of field development, which lead to significant changes in gas content, gas pressure, stress-strain state of the seams, physical and mechanical and reservoir properties of coal [17].

In turn, most of these factors (gas content, gas pressure, physical, mechanical and reservoir properties, etc.) are largely associated with metamorphic transformations of coal.

The indicators used [10 – 13] (V^{daf}, V_v^{daf}, lgρ, y) by their nature and methods for their determination cannot, fully and unambiguously, characterize the manifestation of the hazardous properties of coal seams. This indicates the need to improve the regulatory framework [10 – 13] and the relevance of work aimed at ensuring trouble-free operation of coal deposits.

2 Methods of research

Historically, the primary choice of classification indicators of the degree of coal metamorphism was due to the need to establish their consumer properties. In most cases, the possibility of obtaining coke for the metallurgical industry or raw materials for energy production is determined. The classification indicators used should correspond to these two tasks.

The research methodology is based on the classical definition of metamorphism, which characterizes the change in the composition and properties of coal. The analysis involves indicators that directly or indirectly can characterize the elemental composition of organic and mineral mass, chemical activity and physico-mechanical properties. This will allow to establish a specific composition and properties that contribute to the manifestation of certain hazardous properties of coal seams during mining operations.

3 Results and discussion

The degree of metamorphism was established by their different combination. In some cases [15], it was initially determined by the value of coke yield as a percentage of organic matter and moisture content. In others [14, 18, 19] – the release of volatiles and the carbon content of the conventional organic matter. According to the carbon content, with a high degree of probability, a relationship has been established with the specific heat of combustion [14, 19], which is important for the classification of energy coals.

For non-sintering coals and anthracites, the specific gravity (K_d) and the mechanical strength of the copra are accepted as indicators of the degree of metamorphism [14]. One of the direct indicators of coal metamorphism, according to the authors of [17, 19], is the true density of the organic mass (γ). When developing industrial classifications, indicators were selected, first of all, to characterize the consumer properties of coal [14, 15, 19].

Some of them, without sufficient scientific justification, were used to characterize the entire complex of hazardous properties of coal seams [10 – 13, 18], which reflected on the quality of regulatory documents. For example, as an assessment of the degree of metamorphism, in some cases, the brand name of coals was used, which was formed by artificially selecting ranges of changes in auxiliary indicators to obtain certain consumer properties. Thus, significant errors were made in assessing the hazardous properties of coal seams.

The principles for constructing industrial classifications made it possible, if necessary, to experimentally select indicators for the fine gradation of coals according to their technological properties. For example, at the time, new quantitative indicators RI (the Roh index) and specific heat of combustion were introduced, the limit of the weight yield of volatile substances was changed to establish the grades of coal, etc. [21]. This indicates that, in order to establish technological properties, the ranking of coals by the natural degree of their metamorphic transformations was not always maintained.

A similar approach to determining the degree of metamorphism was retained when developing a modern classification of coal by genetic and technological parameters [22]. The average reflection of vitrinite (R_r) is taken as the main indicator of the degree of metamorphism. The ranges of the remaining nine auxiliary indicators, in turn, are selected for dividing into types, classes, categories, types and subtypes in order to establish the brand of coals. For this reason, coal brands cannot serve as a criterion for assessing the manifestation of the hazardous properties of coal seams, as is customary in regulatory documents [10 – 13]. In addition, the classification [22] does not consider changes in the organic and mineral components in the process of geological transformations of coal.

The above facts indicate that in order to forecast the manifestation of the hazardous properties of coal seams by the degree of coal metamorphism, it is necessary to use other evaluation criteria compared to industrial classifications. First of all, this concerns the scientific justification of the selection of classification indicators for establishing specific hazardous properties of coal seams. At the same time, a complex manifestation of dangers is possible, in which several factors are realized: gas, dust, sudden emissions of coal and gas, fires [23]. The authors of the scientific work [20] came to the conclusion that there is a genetic relationship between the outburst and fire hazard of coal seams, dictated by the geomechanical-geodynamic and thermochemical conditions for the formation of coal deposits in the past tectonic-magmatic eras of the Earth's development. This indicates the need for a more detailed analysis of the known indicators of the degree of coal metamorphism and the establishment of their role in the formation of the hazardous properties of coal seams. Each indicator reflects only one side of the metamorphic transformation of coal. Along with this, in some cases, close correlation relationships have been established between the classification indicators [18, 19, 24], which do not give grounds for mutual replacement of classification indicators, which is due to the nonlinear nature of some dependencies. The nonlinearity of the dependences was established for the volumetric yield of volatile substances (V_v^{daf}), the thickness of the plastic layer (y), mechanical strength, mechanical resistance, grindability, specific gravity (K_d), gas content for the thermal decomposition of coals (H_2, CH_4, CO, CO_2) depending on the mass the release of volatile substances [14]. In turn, the change in V^{daf} is described by a nonlinear equation depending on the reflection of vitrinite (R_o) [20].

Inversely proportional, almost functional, dependence is characterized by the total content of oxygen, hydrogen and nitrogen from increasing carbon [25]. This is evidenced by the high value of the correlation coefficient ($r = -0.99$). In parallel with this, the oxygen and hydrogen contents, depending on the presence of carbon, are characterized by non-linear laws.

The logarithm of the electrical resistivity of anthracites ($\lg\rho$) by its determination method reflects a certain side of the change in the internal structure of coal in the process of metamorphism. A close direct proportional relationship was established ($r = -0.91$) $\lg\rho$ and

V_v^{daf} [26], i.e. the dependence of the internal structure on the volumetric output of the sum of gases from a sample of coal during its thermal decomposition. The maximum relative deviation of individual values of experimental data from the averaging line reaches more than 200%. The given example shows that even with a directly proportional relationship between classification indicators, their mutual replacement is not always possible. In the case under consideration, a significant scatter in the experimental data is obviously caused by the fact that the output of individual gases during thermal decomposition of coals is not taken into account.

The mass yield of volatile substances (V^{daf}) is currently the most studied and easy to determine, which was a reason for its use in establishing almost all the hazardous properties of coal seams [10 – 12]. The indicator allows us to differentiate coals by the degree of their metamorphic transformations. Along with this, a low accuracy of its determination is noted [18]. There are discrepancies between parallel laboratory determinations of more than 9 times. When determining V^{daf} by the standard method, the mineral part gives up its volatiles. In particular, when coal is heated to a temperature exceeding 102 ºC, hydrated water is allocated from mineral substances, which is referred to as combustible mass. Volatile substances released from coal are not classified as organic, but as a fictitious ashless mass. More correctly, it is necessary to attribute volatile substances not to ashless, but to conditionally organic mass. When coal is heated in laboratory conditions, sulfur compounds undergo complex changes and hydrogen sulfide is formed, which is part of the volatile mass. Inclusion of this component, as well as hydrated water, in the total V^{daf} yield is unduly. The mineral part is mainly random inclusions that are not related to the degree of metamorphism. At the stage of seam formation in reconstructive environment, the process of conversion of organic substances is more complicated than when heating coals [18]. Coal metamorphism and their thermal decomposition are different forms of organic mass transformation. The resulting chemical compounds differ significantly in qualitative and quantitative compositions [25].

There are also difficulties in determining the true density, which is associated with the inability to completely separate mineral impurities always present in coal from the organic mass [18].

The restraining factor of reliable prediction of hazardous properties of coal seams of various nature is the use of one classification indicator that is not directly related to the properties and phenomena under consideration. For example, the reference to the degree of metamorphism is the brand of coals when determining the mechanical properties [27], dust-forming ability [28] and the tendency to spontaneous combustion [29]. It was previously established that ranking a number of coal by brand composition does not correspond to the degree of metamorphic transformations due to the artificial selection of auxiliary indicators for combining coal into technological groups for industrial use. It should also be recognized as unsuccessful and the experience of determining gas content using grades of coal and several auxiliary indicators [30, 31], which do not directly reflect the essence of the property in question. The present gas content of coal seams is determined by the amount of methane that has been preserved depending on their gas consumption and the geological conditions for the degassing of deposits after the completion of gas formation processes during coal metamorphism. In both cases [30, 31], gas content is assigned to the ranked number of coal by brand. Along with this, the totality of auxiliary indicators used is somewhat different from each other. Their reliable determination is difficult for the whole series of fossil coals because of the significant errors obtained for individual stages of geological transformations. In [30], using auxiliary V^{daf}, V_v^{daf}, lgρ, γ and maximum reflection of vitrinite in the air (A_r), gas content was characterized only in separate ranges of the ranked series, compiled according to the vintage character.

A slightly different set of auxiliary indicators (V^{daf}, V_v^{daf}, lg*ρ*, lgV^{daf}) was used in the second case [31]. The graphs of gas content [30, 31] reflect only its averaged directivity during coal metamorphism, which does not allow the use of these dependencies due to large errors in engineering calculations. This is confirmed by the statistical processing [26] of the experimental data [12, 32 – 35] and the gas content of the Donbas mine beds depending on V^{daf} and lg*ρ*. For example, with V^{daf} = 5.0%, the gas content varies from 0 to its maximum value (45 m^3/t). The processing results [26] made it possible to establish only the ranges of gas content for fossil fuels and anthracites, as well as for fossil fuels having intermediate properties between them. The results indicate the need for a completely different methodological approach to forecasting the gas content of coal seams. The use of a significant number of auxiliary indicators, which inherently do not reflect the nature of the phenomena under consideration, cannot provide high reliability of the results obtained.

Indicative in this regard is the study of the relationship between the structure and moisture of coal with their gas content [17]. An indisputable fact is the dependence of the dynamic and gas-dynamic hazard of the formations on these factors. The maximum hygroscopic and natural humidity are determined by the mechanical properties and sorption methane consumption of coal. It is proved that in small intervals of changes in the classification indicators of the degree of metamorphism, significant fluctuations in gas content and phase-physical properties of coal occur. They correspond to the genetic nature of metamorphic changes in coal and anthracite layers, determined by physicochemical transformations, gas formation, or their complete degassing. On the example of the Donetsk basin, it is shown that the critical transition for fossil fuels occurs at V^{daf} = 35÷36%, and for anthracites at lg*ρ* = 3.5. It should be noted that for lg*ρ* ≤ 2, the gas content is 0 [26] and for such cases there is no need to consider the manifestations of the hazardous properties of coal seams due to gas content.

The logarithm of electrical resistivity indirectly reflects changes in the chemical composition and structural rearrangement of organic matter and the combination of molecules into crystalline aggregates [14]. It does not functionally determine (r = 0.84) the gas content of anthracites [26], which indicates the need to use indicators that directly determine the formation of hazardous properties by the gas factor. For similar reasons, the V^{daf} index cannot fully characterize all sides of coal metamorphic transformations, including the formation of gas content in coal seams. It should be noted that the stages of metamorphism according to [17] were determined by the values of V^{daf} and the brand of coals, which are not directly related to the assessment of the gas content of coal seams. This explains the significant fluctuations in gas content and sorption ability, established by the release of volatile substances.

When considering the laws of change in the phase-physical properties of coal [17], the question arises of determining their residual gas content ($X_{r.g}$), which characterizes the stability of the structure and bond strength in the gas-coal system. The establishment of this indicator is necessary for forecasting gas release during mining operations. According to the normative document [11], the value of $X_{r.g.}$ for fossil fuels and highly metamorphosed anthracites, it is calculated depending on V^{daf} and V_v^{daf} :

$$X_{r.g} = 18.3 \cdot (V^{daf})^{-0,6}, \text{ m}^3/\text{t}; \quad (1)$$

$$X_{r.g} = x_1 = 0.15 \cdot V^{daf} - 13.6, \text{ m}^3/\text{t}, \quad (2)$$

where x_1 is the residual methane content of highly metamorphosed anthracites located outside the excavation site.

According to equation (1), the residual gas content of fossil fuels and anthracites is determined at V_v^{daf} > 165 см^3/г и V^{daf} = 2÷5% for immovable exposed formation surfaces during the preparation of the workings, the pillars of coal left in the mined space and coal, the close-together underworked and worked-out layers. In all these cases, the residual gas content is determined by various mining factors, which are not related, even theoretical, to the V^{daf} index.

Equation (2) establishes a relationship between the residual gas content of highly metamorphosed anthracites issued outside the excavation site. This dependence does not take into account the fact that the vast majority of anthracite formations (more than 70%) are not gas-bearing, and on the other hand, there are formations with a maximum (45 m^3/t) gas content. This situation is not taken into account by the V_v^{daf} classification indicator. In addition, the definition of $X_{r.g}$ (x_1) according to equation (2) loses its meaning if $V_v^{daf} \leq 90.7$ cm^3/g, since in this case the parameters of residual gas content take negative values. For this reason, using equation (2), it is possible to determine the residual gas content of highly metamorphosed anthracites only when changing in a narrow range of 90.7÷165 cm^3/g. According to [11], coal, as well as anthracite, includes coal with V^{daf} = 2÷8%, the residual methane content of which is 12.1 – 5.3 m^3/t.

In this regard, it is not possible to identify fossil fuels by additional features with V^{daf} = 2÷8%, which belong to the category of highly metamorphosed anthracites.

The inappropriateness of determining the gas content of anthracites, using indicators that indirectly determine its values, is confirmed by the statistical processing of experimental data and the absence of dependences close to functional [26]. The highest correlations between the gas content of anthracites were found with lgρ (r = 0.84), V_v^{daf} (r = 0.79), γ (r = 0.73), hydrogen (r = 0.76) and carbon (r= -0.51).

With the remaining indicators used in industrial classifications, correlation relationships have not been established. The correlation coefficients were less than 0.50. For V^{daf} they were 0.45, calorific value 0.49, reflectivity in air – 0.39, melting point of ash 0.16, phosphorus content – 0.12, sulfur content 0.03, formation ash 0.04 etc. The above facts additionally indicate the need to take into account the peculiarities of the appearance of the hazardous properties of coal seams in comparison with methods for determining the technological suitability of coal.

The establishment of a role in the occurrence of sudden emissions of coal, rock and gas, fire hazard situations in coal mines is proposed to study the issues associated with the presence of higher hydrocarbons [23], which is not reflected in regulatory documents.

To establish the role of the organic component in the occurrence of sudden emissions of coal, rock and gas, fire hazard situations in coal mines, it is proposed to study issues related to the presence of higher hydrocarbons [23], which is not reflected in regulatory documents.

4 Conclusions

Studies of the usage of classification indicators of the degree of coal metamorphism made it possible to establish some of their features necessary for predicting the hazardous properties of coal seams. They are as follows:

– each classification indicator characterizes only typical aspect of the manifestation of the degree of coal metamorphism;

– in the general case, it is almost impossible to fully replace some indicators with others. This is due to different methods and techniques for their determination, which causes discrepancies in the accuracy of the results obtained and excludes the functionality of the dependencies. In many cases, the interdependence of indicators is non-linear;

– in different historical periods, more than 20 indicators were used to characterize the technological properties of coal, which were selected on the basis of industrial use experience. In the modern international classification, 10 indicators are used that cannot directly characterize the hazardous properties of coal seams;

– in the regulatory framework of Ukraine for forecasting the hazardous properties of coal seams, a limited number of indirect indicators are used, which, by the method of their determination, cannot reliably characterize the whole variety of these properties;

– the use of a significant number of indirect indicators does not guarantee reliability of the results, but on the other hand, one indicator cannot characterize all aspects of the metamorphic transformations of coal;

– gaseous and liquid products of metamorphism, due to the peculiarities of their physical state, are mostly removed and only solid residual products are almost completely preserved. The balance of the total amount of substances and the characteristics of the retreating fluids can be obtained only indirectly;

– brands of coal, their consumer properties and ranking on this basis do not correspond, according to isolated indicators, to the degree of metamorphic transformations in geological processes;

– the manifestation of certain hazardous properties of coal seams is sometimes interconnected, to some extent, among themselves;

– the regulatory documents on safe mining operations do not reflect to the necessary extent the properties acquired in the process of metamorphism and characterizing mechanical strength, the composition of the organic and mineral components, humidity, changes in the internal structure, sorption capacity of coals, etc. This does not allow reliable prediction of the hazardous properties of coal seams during mining operations.

To successfully improve the regulatory framework and ensure trouble-free operation of coal deposits, it is necessary to study the manifestations of the hazardous properties of coal seams depending on the following factors:

– a change in the ratio of the content in the process of metamorphic transformations of coals of the main elements of the organic mass (C^0, O^0, H^0, N^0) and mineral impurities;

– the content of all types of moisture at different stages of the geological transformation of coal;

– composition and content of higher hydrocarbons;

– change in the internal structure, mechanical strength and sorption abilities of coals;

– approximate balance of the formation of initial and final products at each stage of coal metamorphism.

The studies conducted allowed us to assess the validity of the use of individual indicators of the degree of metamorphic coal transformations for predicting the manifestation of hazardous properties of mine plastics and draw the following conclusions:

– based on the definition of coal metamorphism, it is necessary to control the increase in carbon content and the reduction of other components with a parallel change in the physico-mechanical properties and structural structure of the converted substance;

– each individual classification indicator reflects, as a rule, one side of metamorphic coal transformations;

– in most cases, when determining the hazardous properties of coal seams, researchers used one or two indicators that characterize the variety of coal metamorphic transformations one-sided and served as a general measure of the degree of metamorphism. In particular, such properties of indicators, without sufficient scientific justification, were attributed to the release of volatile substances during thermal decomposition without access of coal air and their brand name;

– ranking of coal properties by brand does not coincide with the degree of their metamorphic transformations in past geological periods;

– different methods, techniques and accuracy of determining classification indicators do not allow their full interchangeability in determining the hazardous properties of coal seams;

– the modern industrial classification does not take into account the change in the organic and mineral constituents of coal, which makes it impossible to use it unchanged to predict the hazardous properties of coal seams.

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