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ASSESSMENT OF THE INFLUENCE OF THE SURFACE LAYER OF COALS ON GAS-DYNAMIC PHENOMENA IN THE COAL SEAM

Purpose. Development of physical and mathematical model linking nanostructured surface layer of coal substance with geodynamic phenomena of coal seam, through adhesion energy of different layers and coal grades, melting temperature of the nanolayer, determination of the role of stress-strain state of the seam in the formation of fine coal and methane at their emissions into the mine workings.

Methodology. Mathematical and experimental studies of the regular change in the surface layer of coal substance depending on the grade of coals for different formations of the Karaganda basin; assessment of the influence of the surface layer of coal on the adhesion energy, which determines the stress-strain state of the coal seam. Physical methods for studying the decomposition temperature of methane-bearing coal seams, changes in its concentration, reaction rate of methane release from coals.

Findings. A regular decrease in the thickness of the surface nanolayer of coal substance in different coal grades and formations in the metamorphic series of coals is shown. It has been found that this decrease is accompanied by an increase in surface energy and adhesion energy. The connection of gas-dynamic phenomena with stress-strain state of coal seam, which forms fine-dispersed structure of coal, forms of methane location, activation energy of solid coal-methane solution, rate of thermal decomposition reaction, critical stresses determining development of cracks in coal substance is shown.

Originality. For the first time, a physical model for calculating the thickness of the surface nanolayer and its surface energy for coals of different grades of the Karaganda basin has been developed; the relationship between the thickness of the nanolayer and the melting temperature, adhesion energy, linking the stress-strain state of the coal bed in the zone of gas-dynamic phenomena and the concentration of methane has been established. The value of internal stresses in the surface layer of coals of different grades has been found to be a constant value. Connection of activation energy of decomposition of solid coal-methane solution from Gibbs energy and methane concentration, which explains its significant amount in gas-dynamic phenomena, has been established.

Practical value. The physical and mathematical model describes the influence of surface coal on the processes occurring in the zone of gas-dynamic phenomena and the regularities of their changes depending on the thickness of the surface nanolayer determining such parameters as: stress-strain state, dispersion of coals, as well as the release of a large amount of methane at the sudden release of coal gas into the mine workings.

Keywords: *gas-dynamic phenomenon, coal grades, adhesion, Gibbs energy, methane, cracks, temperature*

Introduction. Gas-dynamic phenomena in the form of self-sustained methane and coal emissions occur in the world's coal fields, which are associated with the stress-strain state (SSS) of the coal-rock mass, tectonic disturbances, and plication. Currently, there are a large number of theories that make attempts to explain the causes of gas-dynamic phenomena (GDPH) [1]. They can be grouped into three groups according to the main role of factors in the processes of GDPH.

In the hypotheses of the first group, the main role is played by coal seam gas. The analysis of the theories of this group showed that they do not fully explain the process of GDPH in the coal seam.

In the second group, the main cause of GDPH is considered to be exclusively the SSS of the coal seam, without considering the gas component, which was later not properly confirmed.

The third group includes hypotheses in which the main factors determining GDPH are: geological conditions of coal seam occurrence, its structure and thickness; rock pressure; tectonics of the coal-rock mass [2].

The analysis of materials devoted to the study of the causes of GDPH in coal mines gives cause to group by the main operating factors:

- under the action of mining pressure, the resulting SSS in the coal seam leads to the growth of cracks, and then to the squeezing of coal into the mine workings, at the same time, there is a strength decline of the coal seam and a change in its gas content; thus, the mining pressure together with the gas pressure provides conditions for the sudden release of coal into the mine workings and for the immediate distribution of heat in a large volume of gas, mainly methane;

- the coal gas factor is an additional reason for the movement of large coal masses during sudden emissions, it is determined by such parameters as porosity and structure of the coal seam, the rate at which gas is released.

In works [3, 4] the connection between gas emission of coal seams and geophysical parameters such as specific electrical resistance, secondary gamma intensity, velocity of longitudinal and cross acoustic waves was established.

Coal seams of the Karaganda basin are characterized by the degree of metamorphism, thickness, moisture content, ash content, gas content and other factors.

One of the most effective methods for predicting GDPH is the detection of geological heterogeneity. These are tectonic disturbances, flexure bend, sudden change in the thickness of the coal seam structure, and gas-bearing capacity. Geostatic pressure forms a system of cracks, and tectonic shear deformations, form zones of highly dispersed coal, while changing the composition of coal substance, its micro-pore structure, gas bearing capacity. This process is accompanied by acoustic and electromagnetic impulses [4]. 3D modeling, on the basis of the exploration and ventilation well intersection base, is the most effective way to delineate these zones. Major disturbances are identified during the exploration phase. Low amplitude tectonic disturbances are difficult to establish due to the sparse drilling mains.

Geophysical methods are used for their detection: seismic survey, in CDP version [5] and duplex wave measurement (Marmalevsky N. Ya., Kostyukevich A. S., Antsiferov A. V., UkrNDMT NAS Ukraine); electrical correlation of coal seams, (Shafarenko V. A., Vorotnikov V. M., 1976) [6].

To detect geologic inhomogeneities of the coal seam the following methods are used: methods of mine geophysics (Seismic exploration, Antsiferov A. V., 2020, Donetsk, Ukraine); three-part measurements of seismic and electromagnetic emission, as well as an analytical method for predicting coal seam faults (Khodjaev R. R., Gabaidullin R. I., 2013).

Studies of coal nanostructures are being intensively developed in China, Australia, Iran and many other countries due to their influence on its physical properties.

Highly dispersed coals possessing anomalous values of a number of physical parameters and responsible for GDPH are of interest in terms of their prediction. Thus, in [7] the electrical conductivity of coal nanoparticles from outburst zones was investigated. It was established that the coal from the outburst pack is characterized by fine grain size and surface structure defectiveness. These patterns were obtained for the lower layer of the D6 seam of the Karaganda coal basin [8, 9].

The purpose of the work is to develop a physical and mathematical model linking coal nanostructure with gas-dynamic phenomena of the seam, based on the established regularities of changes in its physical characteristics.

The research objective is *to* determine regularities of formation of nanostructures of coals of different grades of Karaganda basin, their connection with adhesion, porosity and formation of cracks.

Research methods. For development of the physical and mathematical model it is necessary: to establish regularities of change in thickness of a surface nanolayer of a coal substance of various marks of coals of the Karaganda basin; to reveal regularities of change in a nanolayer of surface energy and energy of adhesion, and to estimate a role of nanostructures in destruction of coal and activation of methane-bearing coal solution.

It is essential to study the surface tension of coals and the processes associated with the participation of interfaces; estimate the free energy (work) that must be expended to form a unit of surface area or interface.

Methods. The thickness of the surface layer (surface energy) of the coal substance was measured by X-ray fluorescence method in the Research Center "Ion-plasma technologies and modern instrumentation" of Karaganda Buketov University. Methods of measurements and partially the results of research are published in the work [10]. The intensity of these X-ray luminescence was determined by the standard photoelectric method. Grain size was determined using a metallographic microscope of MIM-8 type.

The melting temperature of the coal nanolayer of different thickness, depending on its grade, was determined using Galen's constant [11] and experimental data of the melting temperature of a massive coal sample (laboratory of the research center "Ugol", Karaganda).

Results and discussions. ***Thickness of the surface layer of coals.*** In [9], a generalized model determining the thickness of the surface layer of atomically smooth metals, which consists of two layers R(I) and R(II), is given.

The thickness of the first layer $h = R(\mathrm{I}) = d$, and the thickness of the second layer $h \approx 9R(\mathrm{I})$. The lower interface, at $h \approx 10\,R(\mathrm{I})$, is a layer of atomically smooth material.

At $h = R(\mathrm{I})$ phase transition occurs in the surface layer, and at $h \approx 10R(\mathrm{I})$ the size dependence of physical properties of materials begins to appear [9], including hard coals.

To determine the thickness of the surface layer in [10] a relation is obtained

$$R(\mathrm{I}) = 0.17 \cdot 10^{-9}\upsilon. \qquad (1)$$

It follows from equation (1) that $R(I)$ is determined by the molar (atomic) volume of the element ($\upsilon = M/\rho$; M – molar mass of coal; ρ – its density). M_{100} molecular weight of coal, reflects the degree of metamorphism, its composition and structure (Moskalenko T. V., et al., 2018).

$$M_{100} = 130.385C \cdot 1{,}941 \cdot O - 14{,}042 \cdot f_e + 461.909 \cdot N, \qquad (2)$$

where M_{100} is molecular weight per 100 carbon atoms; C, O – bon and oxygen content; f_e – an indicator of the degree of aromaticity of the organic mass of coal; N – the number of paramagnetic centers.

According to formula (2) in [9, 12] the thickness of the surface layer of coal of different grades and formations of the Karaganda basin was calculated (Table 2), where $T(h)$, K is melting temperature of the coal nanolayer. From the data in the table, it is marked that $R(\mathrm{I})$ and $R(\mathrm{II})$ decrease with increasing coal metamorphism.

Let us calculate the thickness of the nanolayer of higher fullerenes. Thus, for fullerene $C_{96} = R(\mathrm{I}) = 135$ nm, which is close to anthracite (Table 1) [13, 14]. From Table 1, the thickness of the surface layer of coals is within the range of $R(\mathrm{I}) \approx 0.2$–$0.15$ microns.

In Table 2, (right column), the number of carbon monolayers (~400–500) obtained by dividing the coal nanolayer

Table 1

Thickness of the surface layer of coals

Coal, grade	M – molar mass (g/mol)	ρ – density (g/cm^3)	volume υ, cm^3/mol	R(I), nm	$T(h)$, K	R(II), nm
Brown coal B	1,575	1.25	1,260.0	214.2	1,473	2,142
Open-burning coal D	1,578	1.35	1,168.9	198.7	1,588	1,987
Gas coal G	1,448	1.24	1,167.7	198.5	1,590	1,985
Fat coal ZH	1,400	1.25	1,120.0	190.4	1,657	1,904
Coking coal K	1,351	1.27	1,063,8	180.8	1,745	1,808
Forge coal OC	1,340	1.29	1,038.8	197.4	1,598	1,974
Noncoking coal T	1,332	1.31	1,016.8	172.8	1,826	1,728
Antracite A	1,310	1.47	891.2	151.5	2,083	1,515

Table 2

Thickness of the surface layer of coal formations of the Karaganda basin [9]

Layer	Coal grade	M – molar mass (g/mol)	P – density (g/cm^3)	R(I), nm
Ashlarik	KZH	1,376	1.42	164.7 (458)
	OC	1,340	1.56	146.0 (406)
Karaganda	K	1,351	1.27	180.8 (502)
	GZH	1,424	1.34	180.7 (501)
	KZH	1,376	1.48	158.1 (439)
Dolinsk	K	1,351	1.23	186.7 (519)
	ZH	1,400	1.44	165.3 (459)
	GZH	1,424	1.50	161.4 (448)
	KZH	1,376	1.27	184.2 (512)
Tentek	K	1,351	1.42	161.7 (449)
	ZH	1,400	1.44	165.3 (459)
	KZH	1,376	1.39	168.3 (467)

R(I) by the average distance between coal macromolecules, (~0.36 nm), determined by X-ray scattering, is given in parentheses. The thickness of the surface layer R(I) of the coal substance is above the technological limit of 100 nm according to G. Glater [15]. In the surface layer R(I), dimensional effects occur that are determined by the entire collective of atoms in the system (collective processes). Such "quasi-classical" size effects are observed only in nanoparticles and nanostructures, (size effects of the II kind). They characterize changes in physicochemical properties of nanomaterials: (crystalline, supramolecular structure of coal, electronic structure, electrical conductivity, change of conditions of stress state of coal and conditions of methane diffusion in coal, etc.).

The layer R(II) extends, as already noted, from size $R(\mathrm{I}) \approx 9R$ to $R\infty$, it is a bulk phase.

The equilibrium structures of the upper coal nanolayer differ from the corresponding atomic plane in the volume. Two main types of atomic surface remodeling are distinguished.

In fullerenes, the number of monolayers subjected to surface distortion is, on the order of 30 or more [16]. And in coal matter the distortion is even greater, ~400–500 atomic layers (Table 2), which are in completely different conditions compared to the rest of the volume.

It follows from [9, 17] that for nano- and mesostructures the dimensional effects are described by the next equations

$$A(h) = A_0 \cdot \begin{cases} \left(1 - \dfrac{R(I)}{h}\right), & h \gg R(I) \\ \left(1 - \dfrac{R(I)}{R(I)+h}\right), & 0 \le h \le R(I) \end{cases}, \tag{3}$$

here $A(h)$ is physical property of the surface layer with thickness h; A_0 – physical property of a massive sample (excluding the surface layer).

Adhesion energy of coal seams. Adhesion is caused by intermolecular interaction in the surface layer, and is characterized by the specific work required to separate surfaces.

Atomic rearrangement processes occur in the surface layer R(I) in the coal substance: remodeling or relaxation. To separate the layer R(I) from the other volume of carbon matter R(II), the adhesion energy W_a must be expended, which is determined by Dupre's equation

$$W_a = \sigma_1 + \sigma_2 - \sigma_{12} \approx \sigma_1 + \sigma_2, \tag{4}$$

where σ_{12} is surface energy at the interface, (due to phase transition of II kind it is not significant).

To calculate σ_1, it is necessary to take into account the dimensional dependence of the melting temperature according to the formulas (3), where $A(h) = T(h)$ and $A_o = T_m$; $T(h)$ – melting temperature in the layer R(I) and T_m – melting temperature of a massive sample of coal substance, K [18].

The value of surface energy σ1, according to [13] is equal to

$$\sigma_1 = 0.7 \cdot 10^{-3} \cdot T(h). \tag{5}$$

Table 1 shows that the relationship between the melting temperature of the surface layer of coals ($T(h)$, K) and the thickness of the nanolayer is determined by a regularity: the thinner the coal layer, the lower its melting temperature is. This regularity is important for understanding the activation energy of methane-bearing coal solution in the zone of GDPH characterized by the fact that the amount of methane ejected from the zone is often much larger than the volume of the cavity from which the coal and methane were released.

Using formulas (3–5) we calculate the work of adhesion (Table 3), which is necessary to calculate the internal stresses, at section R(I) and R(II).

The internal stresses ε_{is} between phases σ_1 and σ_2 can be calculated by the formula (Table 3).

$$\varepsilon_{is} = \sqrt{\left[W_a / R(I)\right] \cdot E}. \tag{6}$$

All values, formulas (6), are given in Tables 1 and 2, and Young's modulus in ranges from $E = 3.4 \cdot 10^9$ Pa (brown coal) to Pa (brown coal) to $E = 4.3 \cdot 10^9$ Pa (antracite). Adhesion force for coal of different grades is equal to

$$F_1 = \sigma_1 \cdot R(\mathrm{I}). \tag{7}$$

In this case, the internal stress ε_{is} is approximately equal to 1/6 of the longitudinal elasticity σ u of coals of different grades.

Table 3 shows that in the surface nanolayer of size R(I), the following relation is satisfied: F_1 = const, from which it follows that the force F_1 corresponds to intermolecular interactions in the near-surface layer of coal, for all grades – from brown to anthracite. This pattern is due to the fact that the intermolecular interaction in coals of different grades is related to the structure of the core of the macromolecule, which is a benzene ring. The number and composition of side groups, to a large extent, account for all the diversity of coals, but has no influence on intermolecular interactions.

Table 3 shows that the internal stress εis and longitudinal elasticity σu increase from brown coal to anthracite. This is due to the fact that the thickness of the surface layer in brown coal is 1.5 times greater than that in anthracite. This effect for coals is similar to the presence of a solid inclusion, a model of which is presented in [19], where the role of the inclusion is played by the surface nanolayer R(I).

Table 3

Adhesion energy and parameters of different coal grades in Karaganda basin

Coal, grade	Adhesion energy			Adhesion parameters		
	σ_1, mJ/m^2	σ_2 mJ/m^2	W_a, mJ/m^2	F_1, nN	ε_{is}, MPa	σ_u, MPa
Brown coal B	389	1,178	1,567	83	158	26.3
Open-burning coal D	419	1,270	1,689	83	173	28.8
Gas coal G	420	1,272	1,692	83	176	29.3
Fat coal ZH	438	1,326	1,764	83	187	31.2
Coking coal K	461	1,396	1,857	83	200	33.3
Forge coal OC	422	1,278	1,700	83	183	30.5
Noncoking coal T	482	1,461	1,943	83	212	35.3
Antracite A	550	1,667	2,217	83	250	41.7

Gas energy in coal seam. Table 4 shows physical and chemical properties of coals of Karaganda basin from which it follows that in the series from brown coal to anthracite decreases: molar mass M; surface layer thickness R(I); heat capacity Cs; humidity W; volatile matter yield V^{daf}; and increases: density ρ; adhesion energy W_a; internal stress ε_{is}; longitudinal elasticity σ_u; heat of combustion Q^G; gas content c_o.

The established regularities correlate with the thickness of the nanolayer and surface energy of coals, they define a physical and mathematical model linking coal nanostructures with its technological characteristics that determine gas-dynamic phenomena in mines.

According to the energy theory of emissions, the energy conditions under which their occurrence is possible are written in the form of an energy balance

$$W_u + W_g > A_u + A_g, \qquad (8)$$

where W_u is energy of elastic deformation of coal seam, MJ; W_g – energy of free gas contained in the coal seam, MJ; A_u – work of coal destruction, MJ; A_g – work of displacement of coal destroyed at coal emission, MJ. The calculated values of these parameters are given in Table 5.

Energy $W_u = \sigma_u/2E$, for different grades of coal $W_u = (\sigma_u/2E + 2.72 \cdot 10^{-3}H)$ MJ, where H is coal seam depth.

Work $A_u = \sigma_u/(597r_n)^{1.75}$, where r_n is a particle size of coal particles destroyed during emission, cm; W_g – free gas energy, which can be calculated by formula

$$W_g = \frac{RT}{X-1} \cdot \frac{V}{22.4 \cdot 10^{-3}} \left(1 - \left(\frac{P_2}{p_1}\right) \cdot \frac{X-1}{X}\right), \qquad (9)$$

where R is the universal gas constant equal to 0.848 kg m/mol, deg; X – adiabatic index, for methane $X = 1.32$; P_1 and P_2 – initial and final gas pressure, MPa; V – gas volume, m^3/t; T – absolute temperature of coal, gas system, K.

Displacement work $A_g = mgL$, where m is mass of emitted coal or rock, kg; g – acceleration of gravity, cm/s^2; L – distance by which the center of gravity of the emitted coal moves in case of sudden emission, m.

When calculating the energy of coal seam gas involved in the emission, it is necessary to take the gas, which is contained in the outburst-prone coal seams in the free state and the actual pressure of free gas.

From equation (7) and Table 5, it is clear that coal and gas explosion capability is inherent in all coal seams. It is considered [20] that coal and gas emissions occur in coal seams of G, ZH, K, OC, T and A grades, i. e. excluding B and D grades. However, the latter is characterized by self-ignition.

Thus, the data in Tables 4 and 5, should be used in assessing the coal seams' ability to release coal and gas.

Table 4

Technological properties of coal of different grades

Coal grade	C_s, J/kg K	W, %	V^{daf}, %	Q^G, kcal/kg	c_o, m^3/t
Brown coal B	1,440	20–40	41 and more	6,900–7,500	5–8
Open-burning coal D	1,380	10	>39	7,500–8,000	6–9
Gas coal G	1,333	7	36	7,900–8,600	9–10
Fat coal ZH	1,280	5	30	8,300–8,700	10–12
Coking coal K	1,080	3,5	20	8,400–8,700	15–18
Forge coal OC	1,327	2	15	8,450–8,780	20–24
Noncoking coal T	1,161	1	12	7,300–8,750	25–30
Antracite A	815	1	≤8	8,100–8,750	40–45

Table 5

Energy balance for coal and gas emissions ($H = 250$ m)

Coal grade	W_u, MJ	W_g, MJ	A_u, MJ	A_g, MJ
Brown coal B	0.79	0.11	0.73	0.08
Open-burning coal D	0.85	0.12	0.75	0.09
Gas coal G	0.85	0.12	0.75	0.10
Fat coal ZH	0.89	0.14	0.81	0.11
Coking coal K	0.94	0.16	0.83	0.13
Forge coal OC	0.86	0.12	0.81	0.10
Noncoking coal T	0.98	0.18	0.95	0.15
Antracite A	1.12	0.21	0.99	0.17

The result of the conducted research is the conclusion that the stress-strain state of the coal seam, associated with the disturbance of the coal structure at the meso-level, plays a determining role in coal and gas emission.

Activation energy of methane-bearing coal solution. One of the main forms of methane content in coal under SSS in the coals of Karaganda basin, at the depth of the seam above 800 m, is solid methane-bearing coal solution. Thus, 70–80 % of the methane is in the intermolecular space of coal substance; 8–16 % – on coal surfaces of natural pores and defects of coal continuity, including interblock gaps and macroscopic defects in adsorbed form; 2–12 % – inside macropores, microcracks and other defects of coal continuity; 1–2 % – defects of aromatic layers of crystallites – chemically sorbed methane and 1–3 % – inside quatratite-like structures-solid solution of introduction.

Areas of coal seams containing highly dispersed coal (nanoparticles) are areas of unstable methane state, where there is a transition of methane from the bound state to the free state at unloading of the seam and temperature increase in this zone, this leads to a sharp increase in the activation energy of methane-bearing coal decay. In [13] this energy is defined by the expression

$$A = \frac{E_m - G^0/c}{kT} \quad , \qquad (10)$$

where G^0 is Gibbs energy of a carbon substance; c – methane concentration; T – temperature; $E_m = 200$ kJ/mol – average methane binding energy in coal substance; k – Boltzmann constant.

The activation energy of methane-bearing coal decomposition depends on temperature, and it is determined by the thickness (size) of carbon nanoparticles.

At temperature $T' = T_p$ the decomposition of methane-bearing coal begins, forming centers of high stress and temperature in the coal seam, leading to GDPH.

For coals of the whole range of metamorphism the activation energy was determined by derivatography, which turned out to be equal to $E_a = 0.65$ kJ/mol. Temperatures of the onset of outgassing are as follows: in fusenite (390 °C), vitrinite (335 °C), and exinite (250 °C). Then $kT \approx 825 \times \times 10^{-23}$ JK^{-1}. Using these numerical estimates, we obtain that $\frac{G^0}{c} = 200 - 536 \cdot 10^{-23}$. This value is negligibly small. Then from E_m, in the ratio

$$\frac{G^0}{c} = E_m, \qquad (11)$$

which indicates that the activation energy of the process of decomposition of carbon methane is smaller the smaller the Gibbs energy of the carbon matter is.

In works [8, 13], the formula determining methane ability of coal seam was obtained (c)

$$c=\frac{kT}{C_1}\cdot\frac{A}{G^0}\cdot c_0^2, \quad (12)$$

where c_0 is initial concentration of methane in the coal seam (methane content); A – work (energy) of external forces (field); C_1 – constant.

Formula (12) defines a quadratic dependence of methane availability on the methane content of the formation, and the more G^0 of solid coal-gas solution is, provided that $G^0=\sum_1^n c_i\cdot G_i^0$, where c_i – concentration of the i^{th} sort of molecules (nitrogen, carbonaceous gas, and others) of the gas; G_i^0 – its Gibbs energy, the greater is the activation energy of the coal-gas solution.

The gas emitted during decomposition, as well as gas adsorbed in the pore space of coal, diffuses through the system of cracks and open pores into the bottomhole space. It has been established that the temperature of the beginning of volatile substances appearance at heating of different types of humus coal seams naturally increases in the row: brown coals → stone coals → anthracite. The results of gas extraction are greatly influenced by the speed of their heating with its increase, the temperature of the start and the maximum of gas extraction, increased.

The kinetics of the reaction is described by the formula

$$-\frac{dc}{d\tau}=kc^n, \quad (13)$$

where k is rate constant; n – order velocity; τ – time.

The constant k is related to temperature and is expressed by the Arrhenius law

$$k=k_0\cdot e^{\frac{E}{RT}}, \quad (14)$$

where E is activation energy; k_0 – pre-exponential factor; T – experimental temperature.

Reaction rate under isothermal conditions is

$$-\frac{dc}{d\tau}=k_0\cdot e^{\frac{E}{RT}}\cdot c^n. \quad (15)$$

To describe all the processes of decomposition of methane-bearing coal solution by one equation of the 1st order (monomolecular transformation) is impossible, because in real conditions the decomposition of the organic mass of coal seam occurs in the interaction of substances and gases of different nature constituting this solid solution.

Griffith's theory of ***fracturing crack in coal seam.*** Equations (1, 2) determine the thickness of the surface layer of coal matter, and equation (3) determines the surface energy of the coal nanolayer.

Theoretically, in a layer composed of one-dimensional spherical particles, the average pore size will be equal to the size of the empty space formed by a single-layer staggered arrangement of three spheres. The radius of the pore, in this case, is equal to

$$r=0.154\cdot L. \quad (16)$$

When particles have the form of spheres of the same diameter L, the specific surface area S_{sp}, is defined by the expression

$$S_{sp}=\frac{6}{\rho}\cdot L. \quad (17)$$

Using formulas (1, 2, 5, 16), we calculate the surface layer crack length and pore radius for different coal grades: brown coal (B) → open-burning coal (D) → gas coal (G) → fat coal (ZH) → coking coal (K) → noncoking coal (OC) → forge coal (T) → antracite (A) (Table 6).

Table 6 shows that the surface energy σ_1 and specific surface area S_{sp} increase with the degree of metamorphism associated with the change in carbon content C in coal from brown coal (C 76 %) to anthracite (C 91 %). Conversely, the fracture length and pore radius decrease from brown coal to anthracite. Crack length in coals $L \approx 0.2$–0.15 micron, is the field of mesoscopic physics or mesoscopics (MC). It is typical for MC that the properties of these bodies are determined by the behavior of a single microscopic particle [20].

Table 6

Thickness L and properties of coals

Coal grade	L, nm	σ_1, J/m^2	r, nm	S_{sp}, m^2/g
B	214.2	1.178	33.0	795
D	198.7	1.270	30.6	857
G	198.5	1.272	30.6	858
ZH	190.4	1.326	29.6	894
K	180.8	1.396	27.8	942
OC	176.2	1.278	27.1	966
T	172.8	1.461	26.6	985
A	151.5	1.667	23.3	1,124

Mineral inclusions in coals are mainly gypsum, calcite, siderite, pyrite and others. The specific surface area, fracture length and pore radius correspond to the nanostructures of these minerals.

According to the IUPAC definition [21], porous bodies are divided into microporous (pore diameter of at least 2 nm), mesoporous (between 2 and 50 nm) and macroporous (greater than 50 nm) bodies. In our case (Table 1) we have a mesoporous coal substance.

The microcrack length (Table 6) is formed due to the formation of dislocations. After coal seam remodeling and relaxation, edge and helical dislocations can occur (Kittel Ch., 1978).

Griffiths A. [22–24] considered the energy change of a body with a crack under loading and obtained an energy criterion of fracture, according to which a crack acquires the ability to propagate spontaneously only when the rate of release of elastic energy during growth becomes equal to or exceeds the energy of the newly formed surface

$$\Delta W=\frac{\sigma_{av}^2\pi L^2}{2E}+2\delta L, \quad (18)$$

where ΔW is total energy change for the case of plane stress state; where δ – specific surface ending; E – Young's module; σ_{av} – applied voltage; L – crack size; ν – Poison's ratio.

The value of critical stresses at which the crack is capable of unstable growth can be found from the following conditions

$$\frac{\partial W}{\partial L}=0;\quad \frac{\sigma_{av}^2\pi L}{E}=2(\delta_1+\delta_2). \quad (19)$$

From formula (19) calculate the crack length L for brown coal B, using the data in Table 6, and $\delta=\delta_1+\delta_2$ and $\sigma_{av}=\varepsilon_{is}$, Young's modulus in [25–27] is equal, on average, to, $E = 4.9\cdot10^9$ Pa for brown coal.

So, $L = 2\cdot1.571\cdot4.9\cdot10^9/3.14\ (158)^2\cdot10^{12} = 15.4\times10^9/0.078\cdot10^{18} = 197.4$ nm, instead of $L = 214.2$ nm from Table 6, which is an error of $\delta \approx 8$ %, which is acceptable for Griffiths' theory. The same data can also be obtained for other coal grades.

Coal can be destroyed by applying stress

$$\sigma_{av}=\sqrt{2W_aE/\pi L}. \quad (20)$$

Griffiths' theory, proposed by him in the 20s of the last centuries, was not properly recognized due to the inconsistency of theoretical data with experimental results. Hence, it follows that corrections must be made to the Griffiths theory related to the microcrack length L (1, 2). A number of models of microcrack formation, noted in the works by Zener-Stroh-

Petch, Cottrell, Ballaf-Gilman, Orvan-Stroh, Koble, Nabarro-Herring, develop the model of Griffiths, but do not determine the length of the microcrack, in particular coals.

Conclusions. The regularities that determine the contribution of the surface layer of coals to the main processes describing gas-dynamic phenomena of the coal seam have been established.

A model for the decomposition of a solid solution of methane-bearing coal is described, and it is shown that the activation energy of the methane-bearing coal decomposition process is smaller the lower the Gibbs energy of the carbon substance is.

A regular decrease in the melting temperature of the nanolayer from the thickness of coal of different grades has been established, which is an important factor for understanding the process of activation of the decomposition of methane-bearing coal solution in the zone of GDPH; it is shown that the ability to release coal and gas is inherent in all coal seams and the stress-strain state of coal seams is responsible for this, taking into account the surface coal nanolayer, in which critical stresses are formed that contribute to the unstable growth of microcracks; the crack length is estimated taking into account the thickness of the coal nanolayer, which is comparable to the Griffiths theory.

Thus, to the already known parameters of coal assessment, from the point of view of explosion hazard, the parameters are determined by the results of our research, such as: molar mass, thickness of coal surface layer, adhesion energy, activation energy of coal methane decomposition, internal stress, longitudinal elasticity, heat of combustion, volatiles yield, gas content, i.e. parameters, which are characteristics of coals taking into account the surface nanolayer, the thickness of which is different for different coal grades, which is a physical and mathematical model of connection.

To identify areas dangerous for the manifestation of GDPH in coal seams, it is necessary to make regular measurements of physical quantities that react to the fact that the conditions for sudden release of coal and gas are approaching, as well as to create three-dimensional models of coal seams, to predict the geological factors that are concentrators of zones of change in SSS, textural and structural factors of the coal seam, gas content.

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Оцінка впливу поверхневого шару вугілля на газодинамічні явища у вугільному пласті

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Мета. Розробити фізичну-математичну модель, що зв'язує наноструктурний поверхневий шар вугільної речовини з геодинамічними явищами вугільного пласта, через енергію агдезії різних шарів і марок вугілля, температуру плавлення наношару, визначення ролі напружено-деформованого стану пласта у формуванні тонкодисперсного вугілля й метану при їх викидах у гірничу виробку.

Методика. Математичні та експериментальні дослідження закономірностей зміни поверхневого наношару вугільної речовини в залежності від марки вугілля для різних світ Карагандинського басейну; оцінка впливу поверхневого шару вугілля на енергію агдезії, що визначає напружено-деформований стан вугільного пласта. Фізичні методи вивчення температури розпаду вуглеметану, зміни його концентрації, швидкості реакції з виділення метану з вугілля.

Результати. Показано закономірне зниження товщини поверхневого наношару вугільної речовини різних марок вугілля і світ у метоморфічному ряду вугілля. Встановлено, що це зниження супроводжується зростанням поверхневої енергії та енергії адгезії. Показано зв'язок газодинамічних явищ (ГДЯ) з напружено-деформованим станом вугільного пласта, що формує тонкодисперсні структури вугілля, форми знаходження метану, енергію активації твердого вуглеметанового розчину, швидкість реакції термічного розкладання, критичні напруження формування й розвитку тріщин у вугільній речовині.

Наукова новизна. Уперше розроблена фізична модель розрахунку товщини поверхневого наношару та його поверхневої енергії для вугілля різних марок Карагандинського басейну; встановлено зв'язок товщини наношару з температурою плавлення, енергією агдезії, що зв'язують напружено-деформований стан вугільного пласта в зоні ГДЯ й концентрацію метану. Встановлено, що величина внутрішніх напружень у поверхневому шарі вугілля різних марок є постійною величиною. Також встановлено зв'язок енергії активації розпаду твердого вуглеметанового розчину з енергією Гіббса й концентрацією метану, що пояснює його значну кількість при ГДЯ.

Практична значимість. Фізико-математична модель описує вплив поверхневого шару на процеси, які відбуваються в зоні ГДЯ, і закономірності їх зміни в залежності від товщини поверхневого наношару, що визначає такі параметри як: напружено-деформований стан, дисперсність вугілля, а також виділення великої кількості метану при викиді вугілля й газу в гірничу виробку.

Ключові слова: *газодинамічне явище, марка вугілля, агдезія, енергія Гіббса, метан, тріщини, температура*

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