

## COMPOSITION AND QUANTITY OF COMBUSTION PRODUCTS DETERMINING IN THE COAL SELF-IGNITION PROCESS

<sup>1</sup>Minieiev S.P., <sup>1</sup>Demchenko S.V., <sup>1</sup>Oparin S.V., <sup>2</sup>Makarenko R.V.

<sup>1</sup>Institute of Geotechnical Mechanics named by N. Poljakov of National Academy of Sciences of Ukraine, <sup>2</sup>MM named «Heroes of Space»

**Abstract.** The study is dedicated to the mining processes research at high temperature, in particular, to determining the composition and quantity of possible combustion products, as well as determining of the thermodynamic properties for the mixture under different combustion conditions, which could be obtained by means of some simplifications applied and under the conditions in which combustion occurs.

In mines, temperature parameters forecast within fire area for the fire development assessing in order to quickly extinguish fire is of considerable interest. These parameters are important for the actual assessment of the environment in the extinguishing area, as they are control ones to determine the rock cooling and, indirectly indicate fire has been extinguished.

The paper presents theoretical thermodynamic studies of the equilibrium composition for gas phase components depending on process temperature and oxidant flow rate  $\alpha$ , using software, designed to model chemical and phase equilibria at wide temperatures, taking into consideration coal of «Heroiv Kosmosu» coal mine. In calculating the parameters of the combustion process the composition and number of possible combustion products were determined as well as their thermodynamic properties under different combustion conditions for further development of new and improvement of existing methods for predicting spontaneous combustion of coal in mines were identified.

The dependences of carbon monoxide content, which is of particular interest from the point of view of coal spontaneous combustion forecasting as well as total volume of the gas phase dependence on the oxidant consumption factor  $\alpha$  are obtained. It was found that the increase in carbon monoxide content (increase in carbon monoxide concentration over 0.001% within the total volume of gas produced) begins in the temperature range from 700 K to 800 K regardless of the oxidant flow rate  $\alpha$ , indicating the self-ignition core of the coal sample.

**Keywords:** self-ignition of coal, fire area, thermodynamic studies, temperature forecast, combustion products.

**Introduction.** A large number of endogenous fires occur every year, which are top-ranked disasters in terms of damage caused in the coal industry of Ukraine. Therefore, for their prevention and extinguishing, the determining of the stages of self-ignition development for coal is of primary importance. The earlier an endogenous fire is detected, the less effort and resources have to be spent for its extinguishing.

The volume fraction of carbon monoxide as well as the temperature of air, side rocks and water is measured while self-ignition of coal in the mine workings of the fire station is under control. In addition, volume fractions of carbon dioxide, methane, oxygen, and hydrogen are monitored. The development of self-ignition process is assessed by the change of abovementioned indicators, mainly being guided by engineering experience and logical inferences. Main features of the early stages for self-ignition of coal are as follows: an increase of the coal temperature, air and water (above natural values for the certain seam); a steady increase of the volume fractions of carbon monoxide, hydrogen, saturated and unsaturated hydrocarbons as well as a decrease of the volume for the oxygen fraction, increase of the volume for the carbon dioxide fraction, smell of coal sublimation products appearance and an increase of the mine air humidity. The main feature of an endogenous fire is a concentration of carbon monoxide that exceeds 0,001 % in three air samples taken at the same control points every 6 hours [1, 2].

During fire extinguishing performance in mines as well as assessment of the process development, much attention has been paid to the temperature parameters fore-

casting within the fire area as well as determining the location of the fire within the coal seam. A number of studies have been conducted in this field of science [3-10]. However, problems arise during the studying of combustion processes as follows: determining of the composition and number of possible combustion products as well as identification of thermodynamic parameters for the mixture properties under different combustion conditions. These parameters are important for assessment of the state of the environment, as they indirectly determine the fact whether fire extinguished or not. Therefore the issues related to the described problems are relevant enough.

**Methods.** The purpose of the study is determining the composition and number of possible combustion products as well as identifying their thermodynamic properties under different combustion conditions in a closed system (closed space) in order to establish the fact of self-ignition of coal, as well as further development of new and improvement of current forecasting methods of coal self-ignition. Thus, thermodynamic studies of the equilibrium composition of gas phase components were carried out depending on the process temperature and the oxidant flow rate  $\alpha$ . The oxidant flow rate is the ratio of the air volume that is actually consumed to its theoretical volume, which corresponds to the stoichiometric one. When the fuel is completely burned out  $\alpha > 1$ , while during its gasification  $\alpha < 1$ . Study was conducted using the software, taking into consideration an example of the chemical and phase equilibria modeling for wide temperature ranges and is based on the fundamental laws of thermodynamics, the laws of mass and energy conservation. [11]. The software allows to create a mathematical model for closed thermodynamic systems that contains gaseous and condensed substances, electroneutral and ionized components that are in a state of equilibrium. The initial data for the calculations are the physicochemical characteristics of the coal from the «Heroiv Kosmosu» coal mine, according to the materials provided by the geological service of the mine, which is listed in the table 1.

Table 1 – Physicochemical characteristics of coal from the «Heroiv Kosmosu» coal mine

	$A^d$	$W^r$	$S^d$	$C^d$	$H^d$	$O^d$	$N^d$	$SiO_2$	$Al_2O_3$	$Fe_2O_3$	$CaO$	$MgO$	$K_2O$
Initial composition, %	15.9	7.40	1.45	71.73	4.44	5.25	1.23	31.82	22.50	34.1	6.08	3.16	2.34
Operating composition, %	14.8	6.89	1.35	66.79	4.13	4.89	1.15	4.71	3.33	5.05	0.90	0.47	0.35

**Results and discussion.** Fuel combustion process was calculated for 1 kg of coal. Results of thermodynamic calculations at  $\alpha=0$ ;  $\alpha=0.25$ ;  $\alpha=0.5$ ;  $\alpha=0.75$  and  $\alpha=1$  for the temperature range from 300 to 2000 K under pressure  $p=0.1$  MPa are given in tables 2-6 and figures 1-5.

Analysis of the results shows that self-ignition is accompanied by the gasification process. The process of carbon self-ignition proceeds according to the following primary chemical reactions:  $C + O_2 = CO_2$ ,  $2C + O_2 = 2CO$ . Carbon dioxide  $CO_2$  and carbon monoxide  $CO$  are simultaneously obtained. Quantitative ratio for  $CO$  and  $CO_2$  depends on some conditions. At a temperature of 1600 K (figures 1-5) ratio of  $CO:CO_2 = 1$ , and while the temperature rises up, its value increases.

Table 2 – Results of thermodynamic calculations of fuel combustion for different process temperatures and the oxidant flow rate  $\alpha=0.0$ 

Temperature, K	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000
Components	The gas phase, m <sup>3</sup> /kg fuel (coal + oxidant)																	
<i>H<sub>2</sub></i>	0.000	0.001	0.005	0.028	0.089	0.203	0.343	0.452	0.506	0.525	0.530	0.535	0.537	0.540	0.543	0.543	0.543	0.543
<i>H<sub>2</sub>O</i>	0.094	0.129	0.134	0.126	0.116	0.099	0.068	0.030	0.009	0.003	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>H<sub>2</sub>S</i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.004	0.007	0.006	0.006	0.003	0.000	0.000	0.000	0.000
<i>N<sub>2</sub></i>	0.006	0.004	0.002	0.002	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>NH<sub>3</sub></i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>CO<sub>2</sub></i>	0.000	0.003	0.007	0.011	0.015	0.020	0.021	0.010	0.003	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>CH<sub>4</sub></i>	0.207	0.208	0.203	0.195	0.169	0.121	0.067	0.031	0.014	0.006	0.003	0.002	0.001	0.001	0.000	0.000	0.000	0.000
<i>C<sub>2</sub>H<sub>6</sub></i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>N<sub>2</sub>C</i>	0.003	0.005	0.007	0.007	0.008	0.008	0.008	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009
<i>CO</i>	0.000	0.000	0.000	0.000	0.001	0.010	0.045	0.105	0.140	0.150	0.153	0.157	0.158	0.164	0.193	0.194	0.196	0.197
Total volume, m <sup>3</sup>	0.341	0.511	0.656	0.811	1.027	1.353	1.821	2.335	2.749	3.068	3.349	3.637	3.907	4.232	4.696	4.987	5.290	5.581
<i>CO</i> content in total volume, %	0.000	0.000	0.000	0.000	0.097	0.739	2.471	4.497	5.093	4.889	4.569	4.317	4.044	3.875	4.110	3.890	3.705	3.530

Table 3 – Results of thermodynamic calculations of fuel combustion for different process temperatures and the oxidant flow rate  $\alpha= 0.25$ 

Temperature, K	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000
Components	The gas phase, m <sup>3</sup> /kg fuel (coal + oxidant)																	
<i>H<sub>2</sub></i>	0.000	0.000	0.003	0.014	0.045	0.092	0.134	0.157	0.173	0.185	0.192	0.195	0.197	0.198	0.198	0.200	0.201	0.201
<i>H<sub>2</sub>O</i>	0.174	0.164	0.144	0.126	0.104	0.078	0.061	0.044	0.028	0.016	0.009	0.005	0.002	0.001	0.001	0.001	0.000	0.000
<i>H<sub>2</sub>S</i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.002	0.003	0.003	0.003	0.001	0.000	0.000
<i>N<sub>2</sub></i>	0.264	0.163	0.104	0.071	0.052	0.043	0.061	0.096	0.131	0.158	0.173	0.181	0.185	0.186	0.188	0.191	0.195	0.196
<i>NH<sub>3</sub></i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>CO<sub>2</sub></i>	0.032	0.046	0.058	0.067	0.077	0.080	0.068	0.049	0.029	0.014	0.006	0.003	0.001	0.001	0.000	0.000	0.000	0.000
<i>CH<sub>4</sub></i>	0.007	0.019	0.028	0.031	0.027	0.016	0.004	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>N<sub>2</sub>C</i>	0.124	0.224	0.284	0.317	0.336	0.345	0.326	0.292	0.256	0.230	0.214	0.207	0.203	0.201	0.200	0.196	0.193	0.192
<i>CO</i>	0.000	0.000	0.000	0.000	0.003	0.023	0.065	0.122	0.178	0.219	0.243	0.254	0.259	0.261	0.263	0.267	0.270	0.271
Total volume, m <sup>3</sup>	0.661	0.904	1.137	1.378	1.650	1.984	2.371	2.784	3.209	3.619	3.994	4.340	4.671	4.994	5.319	5.668	6.017	6.339
<i>CO</i> content in total volume, %	0.000	0.000	0.000	0.000	0.182	1.159	2.741	4.382	5.547	6.051	6.084	5.853	5.545	5.226	4.945	4.711	4.487	4.275

Table 4 – Results of thermodynamic calculations of fuel combustion for different process temperatures and the oxidant flow rate  $\alpha= 0.5$ 

Temperature, K	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000
Components	The gas phase, m <sup>3</sup> /kg fuel (coal + oxidant)																	
<i>H<sub>2</sub></i>	0.000	0.000	0.001	0.004	0.013	0.027	0.042	0.057	0.070	0.079	0.086	0.091	0.095	0.097	0.099	0.101	0.102	0.102
<i>H<sub>2</sub>O</i>	0.109	0.116	0.116	0.113	0.105	0.092	0.076	0.061	0.049	0.039	0.032	0.026	0.022	0.019	0.018	0.016	0.016	0.015
<i>H<sub>2</sub>S</i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001	0.002	0.002	0.001	0.001	0.001
<i>N<sub>2</sub></i>	0.327	0.296	0.296	0.297	0.302	0.311	0.327	0.351	0.380	0.408	0.430	0.446	0.457	0.464	0.469	0.472	0.475	0.476
<i>NH<sub>3</sub></i>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>CO<sub>2</sub></i>	0.084	0.085	0.086	0.088	0.091	0.095	0.095	0.086	0.070	0.053	0.038	0.027	0.020	0.016	0.013	0.011	0.009	0.008
<i>CH<sub>4</sub></i>	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>N<sub>2</sub>C</i>	0.153	0.185	0.185	0.183	0.179	0.170	0.154	0.130	0.101	0.073	0.051	0.035	0.024	0.016	0.011	0.008	0.006	0.004
<i>CO</i>	0.000	0.000	0.000	0.000	0.001	0.007	0.023	0.056	0.101	0.146	0.183	0.209	0.227	0.239	0.247	0.253	0.256	0.259
Total volume, m <sup>3</sup>	0.741	1.001	1.254	1.509	1.773	2.054	2.364	2.714	3.102	3.514	3.914	4.300	4.670	5.027	5.373	5.712	6.047	6.353
<i>CO</i> content in total volume, %	0.000	0.000	0.000	0.000	0.056	0.341	0.973	2.063	3.256	4.155	4.676	4.860	4.861	4.754	4.597	4.429	4.234	4.077

 Table 5 – Results of thermodynamic calculations of fuel combustion for different process temperatures and the oxidant flow rate  $\alpha= 0.75$ 

Temperature, K	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000
Components	The gas phase, m <sup>3</sup> /kg fuel (coal + oxidant)																	
<i>H<sub>2</sub></i>	-	0.000	0.000	0.002	0.005	0.011	0.019	0.027	0.033	0.037	0.038	0.037	0.036	0.035	0.033	0.032	0.031	0.030
<i>H<sub>2</sub>O</i>	-	0.084	0.084	0.082	0.079	0.073	0.065	0.057	0.051	0.047	0.046	0.046	0.047	0.048	0.050	0.051	0.052	0.053
<i>H<sub>2</sub>S</i>	-	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001	0.001	0.001	0.000	0.000
<i>N<sub>2</sub></i>	-	0.435	0.436	0.436	0.438	0.443	0.452	0.466	0.483	0.498	0.508	0.513	0.516	0.517	0.518	0.518	0.519	0.519
<i>NH<sub>3</sub></i>	-	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>CO</i>	-	0.000	0.000	0.000	0.001	0.004	0.014	0.034	0.062	0.088	0.107	0.119	0.126	0.130	0.133	0.135	0.137	0.139
<i>CO<sub>2</sub></i>	-	0.107	0.108	0.109	0.110	0.112	0.111	0.105	0.094	0.083	0.074	0.068	0.063	0.060	0.058	0.056	0.054	0.053
<i>CH<sub>4</sub></i>	-	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>COS</i>	-	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
<i>N<sub>2</sub>C</i>	-	0.084	0.083	0.083	0.081	0.076	0.067	0.053	0.036	0.021	0.011	0.006	0.003	0.002	0.001	0.001	0.000	0.000
Total volume, m <sup>3</sup>	-	1.040	1.302	1.565	1.831	2.107	2.399	2.717	3.057	3.401	3.733	4.049	4.353	4.652	4.949	5.246	5.540	5.836
<i>CO</i> content in total volume, %	-	0.000	0.000	0.000	0.055	0.19	0.58	1.25	2.03	2.59	2.87	2.94	2.89	2.79	2.69	2.57	2.47	2.38



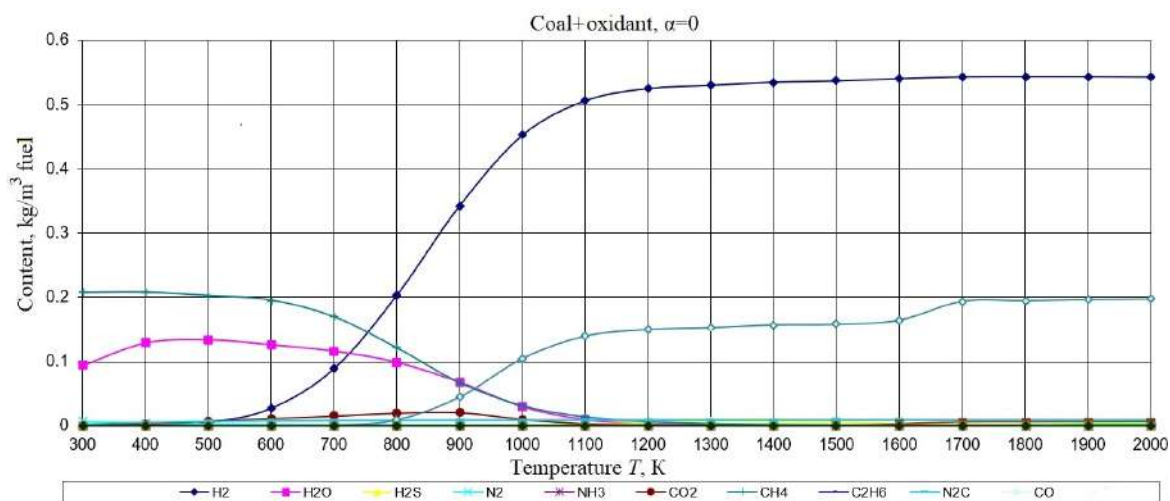


Figure 1 – Results of thermodynamic calculations for gas phase components for  $\alpha=0$  for coal from the «Heroiv Kosmosu» coal mine

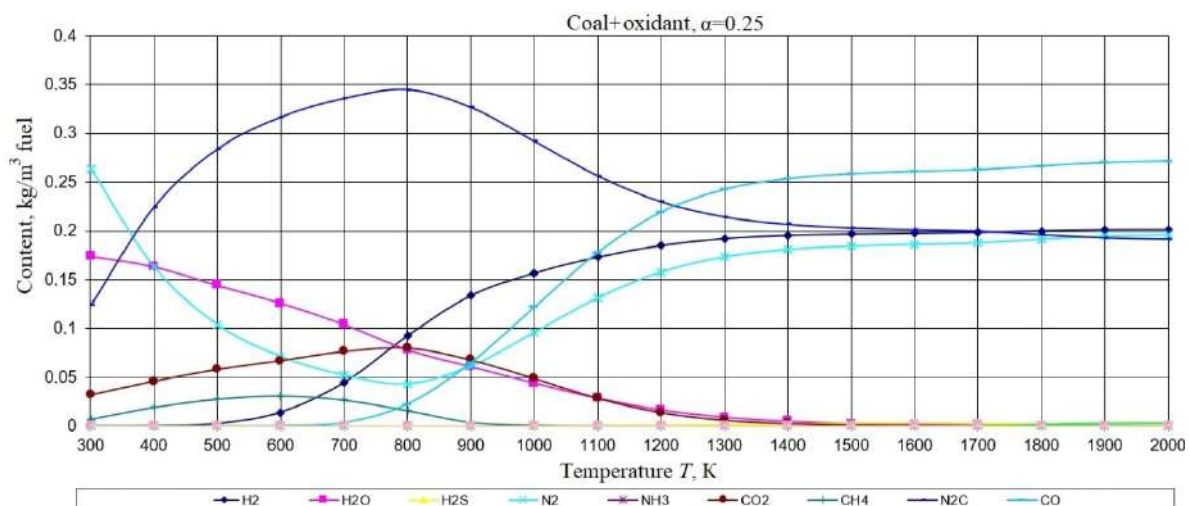


Figure 2 – Results of thermodynamic calculations for gas phase components for  $\alpha=0.25$  for coal from the «Heroiv Kosmosu» coal mine

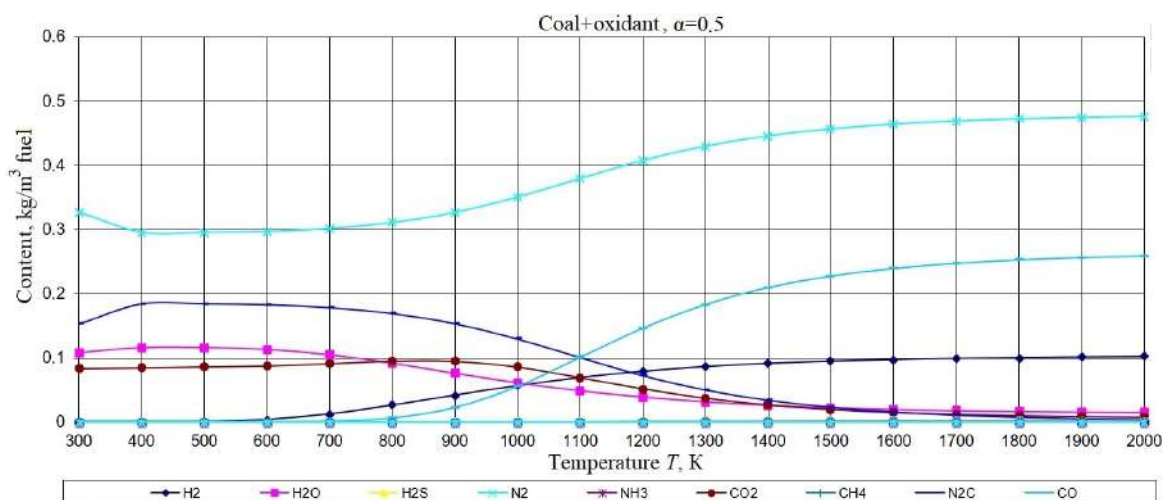


Figure 3 – Results of thermodynamic calculations for gas phase components for  $\alpha=0.5$  for coal from the «Heroiv Kosmosu» coal mine

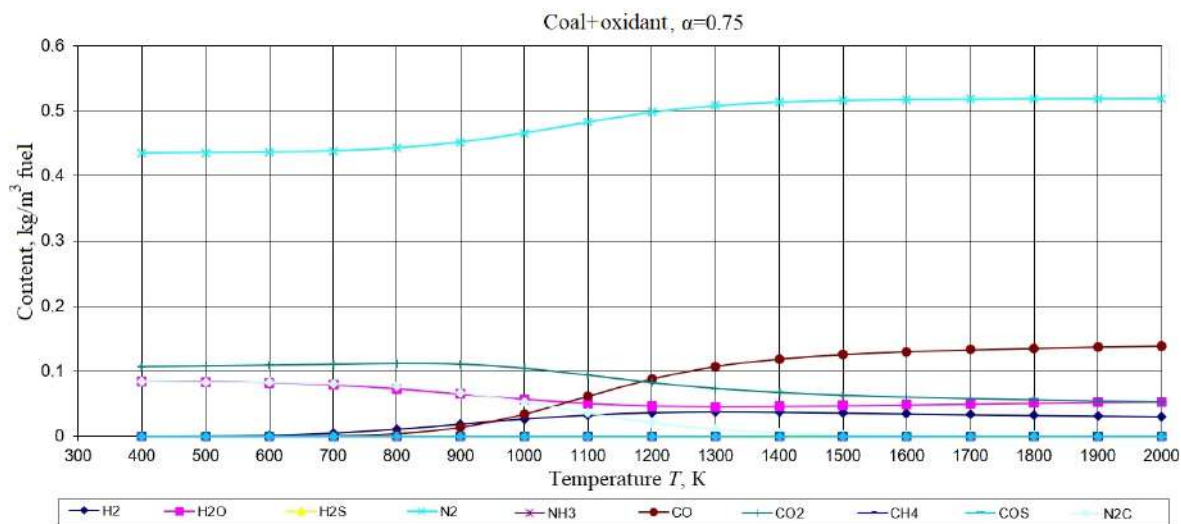


Figure 4 – Results of thermodynamic calculations for gas phase components for  $\alpha=0.75$  for coal from the «Heroiv Kosmosu» coal mine

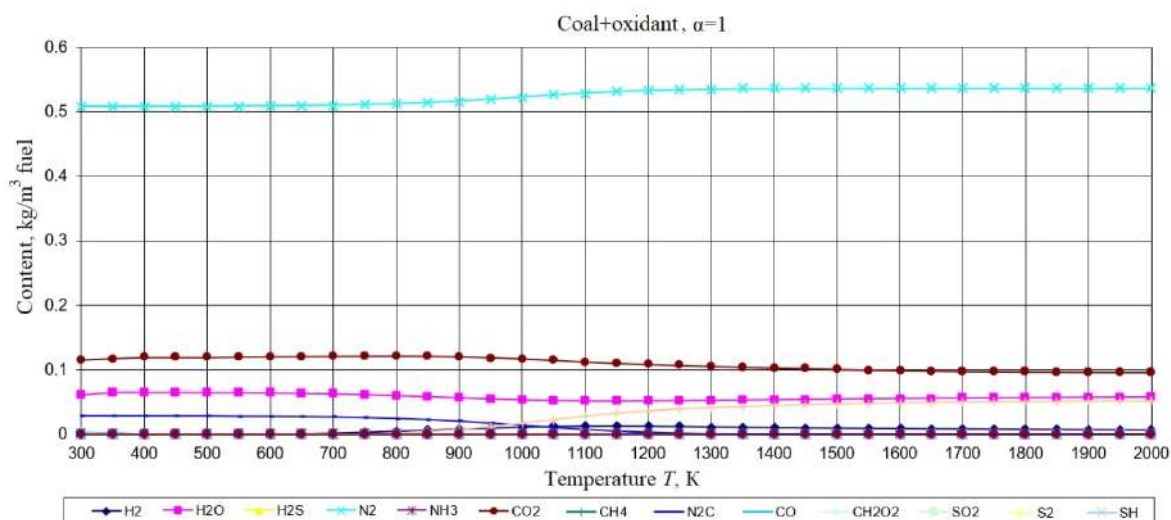


Figure 5 – Results of thermodynamic calculations for gas phase components for  $\alpha=1$  for coal from the «Heroiv Kosmosu» coal mine

By evaluating the dynamics of changes based on theoretical studies of actually measured gas parameters, it is possible to determine the real state of the fire. This assumption requires further research, industry review and discussion.

*CO* content in the total volume of the gas phase is of particular interest for the prediction of coal self-ignition. *CO* content in the total volume of the gas obtained, depending on the oxidant consumption coefficient, for coal from the «Heroiv Kosmosu» coal mine, is shown in the figure 6.

Therefore, it could be stated that the growth of the *CO* content in the total volume of gas occurs in the temperature range from 600 K to 700 K, regardless of the oxidant flow rate. An increase of the carbon monoxide concentration over 0.001% indicates the core location for a coal self-ignition. In fact, self-ignition of the coal samples considered takes place within the mentioned temperature range. It is possible to roughly

estimate the temperature within the coal combustion area based on the carbon monoxide release.

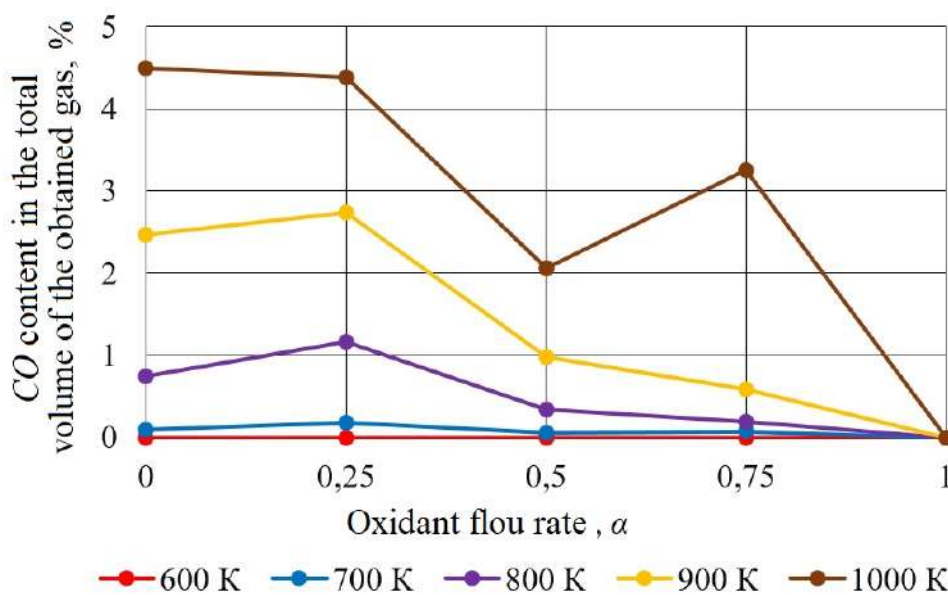


Figure 6 – CO content in the total volume of the obtained gas depending on the oxidant flow rate on the example of coal from the «Heroiv Kosmosu» coal mine

**Conclusions.** As a result of the performed thermodynamic studies, the composition and number of possible combustion products were determined and their thermodynamic parameters during self-ignition and different combustion conditions were found. The results of the study could be applied to assess the fact whether fire extinguished or not, temperature value within the fire area, location of the core for a coal self-ignition within the coal seam, to improve existing and develop new forecasting methods for the coal self-ignition and, in general, to increase the level of endogenous fire safety for coal mines.

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#### About authors

**Minieiev Serhii Pavlovych**, Doctor of Technical Sciences (D.Sc.), Professor, Head of the Department of Pressure Dynamics Control in Rocks, Institute of Geotechnical Mechanics named by N. Poyakov of National Academy of Sciences of Ukraine (IGTM NAS of Ukraine), Dnipro, Ukraine, [sergmineev@gmail.com](mailto:sergmineev@gmail.com)

**Demchenko Serhii Viacheslavovych**, Master of Science, Minor Researcher in Department of Pressure Dynamics Control in Rocks, Institute of Geotechnical Mechanics named by N. Poyakov of National Academy of Sciences of Ukraine (IGTM NAS of Ukraine), Dnipro, Ukraine, [demchikigt@gmail.com](mailto:demchikigt@gmail.com)

**Oparin Serhii Oleksandrovych**, Candidate of Technical Sciences (Ph.D), Senior Researcher, Senior Researcher of the Department of Vibropneumatic Transport Systems and Complexes, Institute of Geotechnical Mechanics named by N. Poyakov of National Academy of Sciences of Ukraine (IGTM NAS of Ukraine), Dnipro, Ukraine, [oparinsa1977@gmail.com](mailto:oparinsa1977@gmail.com)

**Makarenko Roman Volodymyrovych**, Deputy Chief Engineer «Mine Management «Heroes of Space», Pavlograd, Ukraine

### ВИЗНАЧЕННЯ СКЛАДУ ТА КІЛЬКОСТІ ПРОДУКТІВ ГОРІННЯ ПРИ САМОЗАЙМАННІ ВУГІЛЛЯ

*Мінєєв С.П., Демченко С.В., Опарін С.О., Макаренко Р.В.*

**Анотація.** Стаття спрямована на вивчення процесів горіння при високій температурі в шахтних умовах, зокрема на визначення складу та кількості можливих продуктів горіння, а також з'ясування термодинамічних властивостей суміші за різних умов горіння, яка може бути отримана за дотриманням встановлених спрощень, та за умов, у яких відбувається горіння.

У шахтах велике значення приділяється прогнозу температурних показників в осередку пожежі для оцінки процесу розвитку пожежі з метою найшвидшого їх гасіння. Ці показники є важливими для фактичної оцінки стану середовища в осередку його гасіння, оскільки є контрольними для визначення охолодження порід масиву і, зрештою, опосередковано вказують на факт згаслої пожежі.

У статті наводяться теоретичні термодинамічні дослідження рівноважного складу компонентів газової фази в залежності від температури процесу і коефіцієнта витрати окиснювача  $\alpha$ , за допомогою програми «Астра-4», призначеної для моделювання хімічних і фазових урівноважень в широких діапазонах температур, на прикладі вугілля шахти «Героїв Космосу». При розрахунку параметрів процесу горіння визначені склад та кількість можливих продуктів горіння і встановлені їх термодинамічні характеристики (параметри) при різних умовах горіння для подальшої розробки нових і вдосконалення існуючих способів прогнозу самозаймання вугілля в шахтах.

Отримані залежності вмісту оксиду вуглецю, який представляє особливий інтерес з точки зору прогнозу самозаймання вугілля, в загальній кількості газової фази від коефіцієнту витрати окиснювача  $\alpha$ . Встановлено, що зростання вмісту оксиду вуглецю (збільшення концентрації понад 0,001% в загальному об'ємі отриманого газу) починає відбуватися в діапазоні температур від 700 К до 800 К незалежно від коефіцієнта витрати окиснювача  $\alpha$ , що вказує на прояв осередку самозаймання розглянутого зразка вугілля.

**Ключові слова:** самозаймання вугілля, осередок пожежі, термодинамічні дослідження, прогноз температури, продукти горіння.

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