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Kutovyi D.S.
National Technical University "Kharkiv Polytechnic Institute"

Kazakov V.V.
National Technical University "Kharkiv Polytechnic Institute"

OPTIMIZATION OF THE GASIFICATION PROCESS OF LOW-METAMORPHOSED COAL: REGRESSION ANALYSIS

In recent decades, global changes in the world's natural environment have become a significant restraining factor in the development of society, which requires the development of scientific approaches to reducing the negative technogenic impact on the environment. The need to establish a balance between meeting the modern needs of humanity and protecting the interests of future generations requires the harmony between social, economic, and ecological components of the transformation of society. In European countries, particularly in Ukraine, environmental risks are mainly caused by the industrial sector. The production activity of coal industry enterprises leads to a significant territorial deterioration of the environment. Therefore, increasing environmental safety in the direction of energy development of Ukraine is relevant, has practical significance, and involves research on the creation of ecological methods of thermochemical processing of substandard carbon-containing raw materials.

The article provides a comprehensive analysis of the gasification process of a solid product obtained by the thermolysis of low-metamorphosed coal. The article's main goal is to optimize the gasification process parameters depending on the intended use of the obtained gas, using regression analysis. To solve this problem and explore different approaches to its solution, the latest research and publications in this field were analyzed.

The article presents the obtained regression equations for determining the degree of influence of various technological conditions on the final parameters of the gasification process. Each regression equation is presented as a graph that provides a visual representation of the data and makes it easier for readers to understand the relationships between variables.

The unsolved parts of the general problem, which are investigated in the article, are shown. The challenges and limitations of current approaches are reviewed and future directions for research in this area are outlined.

The authors' detailed analysis and approach to solving the problem make this article a valuable scientific resource for scientists and energy specialists and can serve as a basis for further research on the parameters of the gasification process depending on the intended use of the obtained gas.

Key words: *gasification, thermolysis, low-metamorphosed coal, optimization, process conditions, regression equations, energy industry.*

Formulation of the problem. The problem of optimizing the gasification process of solid products from the thermolysis of low-metamorphosed coal is a crucial challenge in the energy industry. The production of gas, which can be used for various purposes such as energy production, methanol production, or other chemical processes, requires precise control of process conditions. These conditions, such as air and steam consumption, the temperature in the reaction zone, and the residence time of the material, have a significant impact on the yield and composition of the resulting gas. The article aims to present regression equations that capture the relationship between process conditions and the final parameters of the gasification process, as well as to provide insights into how these parameters can be optimized for different uses of the resulting gas through graphs that demonstrate the degree of the process conditions' influence. This research provides a valuable contribution to the scientific and practical tasks of improving the efficiency and sustainability of energy production through the gasification process of solid products from the thermolysis of low-metamorphosed coal.

An analysis of the latest research and publications. Research, modernization, and improvement of the processes of gasification of carbon-containing raw materials to increase their energy efficiency is an urgent task for the development of Ukrainian industry. The importance of this problem is emphasized in many other publications [1–2, 4–6]. However, there are still certain difficulties in the development of modern technologies, namely their large volume, and cost. The current direction of research in this field is aimed at reducing their volume and costs. The use of mathematical modeling allows you to implement this approach, choose and make a choice of rational process parameters.

Formulation of the goals of the article. The article aims to present the regression equations for the gasification process of the solid product of thermolysis of low-metamorphosed coal and to analyze the effect of process parameters (air consumption, steam consumption, temperature, residence time) on the yields of various gases (methane, carbon dioxide, hydrogen, carbon monoxide, nitrogen, oxygen) as well as the final parameters of the process (dry gas yield, humidity, net calorific value, density, the conversion rate of carbon, the conversion rate of steam). The article also aims to provide insights on how to optimize these parameters to achieve the best gas for different purposes (methanol production, energy industry).

Outline of the main research material. Table 1 provides technological parameters and results of 20 laboratory experiments on the gasification of the solid product of thermolysis of low-metamorphosed coal carried out by the authors, where x1 is air consumption, l/100g of the solid product, x2 is steam consumption, g/100g of the solid product, x3 is the temperature in the reaction zone, ° C, x4 – residence time of the material in the reaction zone, min.

Data analysis in the Minitab® software yielded the following regression equations describing the available data.

Composition of dry gas:

- Methane

$$CH_4 = 6{,}35 - 0{,}017x1 - 0{,}01x2 - 0{,}005x4 + 0{,}000015x1^2$$

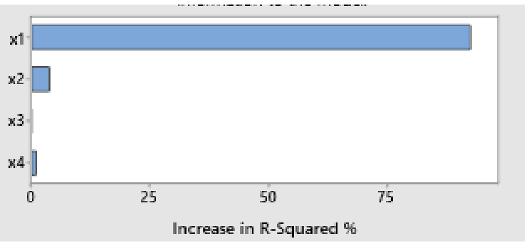

Fig. 1. Influence of initial parameters on methane yield

Table 1

	Technological factors of the process				Composition of dry gas, % vol						Dry gas properties				Conversion rate, %	
№	x1	x2	x3	x4	CH_4	CO_2	H_2	CO	N_2	O_2	Yield, m^3/kg semi-coke	Humidity, g/m^3	Net calorific value, MJ/m^3	Density, g/m^3	Carbon	Steam
1	500	80	1000	60	0,5	11,7	12,3	18,0	51,7	1,1	4,21	138	3,6	1198	95,8	25,0
2	300	80	1000	60	1,4	10,3	12,8	21,4	50,9	0,4	4,71	134	4,9	1043	96,4	21,8
3	500	60	1000	60	0,7	13,9	15,8	16,0	54,6	1,6	4,09	67	3,8	1236	91,2	44,5
4	300	60	1000	60	1,7	11,1	16,4	20,4	56,5	0,8	4,44	70	4,8	1130	99,3	40,1
5	500	80	800	60	0,5	11,5	16,4	17,9	56,4	1,1	4,73	98	4,1	1140	101,1	42,9
6	300	80	800	60	1,4	11,5	16,1	20,5	51,8	0,7	4,65	132	5,2	1086	92,0	29,8
7	500	60	800	60	0,7	16,2	17,2	14,4	50,2	1,4	4,18	65	4,1	1107	88,9	48,3
8	300	60	800	60	1,6	11,5	15,2	18,5	47,9	0,4	4,93	65	4,8	1093	96,7	51,6
9	500	80	1000	40	0,5	13,1	13,7	16,5	56,8	1,5	4,19	156	3,7	1151	93,4	23,3
10	300	80	1000	40	1,6	10,9	12,6	19,7	55,0	0,1	3,92	157	4,8	1186	100,3	17,9
11	500	60	1000	40	0,8	14,8	14,1	12,5	52,8	0,9	4,24	80	3,3	1265	89,5	33,4
12	300	60	1000	40	1,9	11,9	13,4	15,6	49,7	0,9	4,38	96	4,3	1066	80,3	34,3
13	500	80	800	40	0,6	16,7	13,8	14,6	52,8	1,6	4,47	130	3,5	1292	95,6	27,4
14	300	80	800	40	1,6	14,0	15,0	15,3	54,4	0,1	4,68	121	3,9	1279	91,5	29,3
15	500	60	800	40	0,8	16,6	14,9	10,6	50,9	1,1	4,31	76	3,2	1076	83,3	39,0
16	300	60	800	40	1,9	14,3	13,9	14,1	49,4	0,5	4,02	83	4,0	1061	90,9	42,3
17	400	70	900	50	1,0	14,2	14,2	14,7	52,7	1,0	4,26	126	3,9	1206	77,5	21,4
18	400	70	900	50	1,2	14,0	12,2	16,6	52,4	1,1	3,76	138	4,1	1267	88,4	17,2
19	400	70	900	50	0,9	14,2	12,1	14,4	60,2	1,1	4,45	134	3,8	1168	86,3	20,4
20	400	70	900	50	0,9	14,4	12,8	13,9	52,3	1,3	3,91	123	3,7	1235	82,5	19,5

Analyzing the equation and Fig. 1 we can see that air consumption (x1) has a negative linear effect and a positive quadratic effect on the methane yield. An increase in air consumption will reduce the methane yield, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) also has a negative linear effect on methane yield. An increase in steam consumption will reduce the methane yield.

The temperature in the reaction zone (x3) does not affect the methane yield.

The residence time of the material in the reaction zone (x4) has a negative linear effect on methane yield. An increase in residence time will reduce the methane yield.

- Carbon dioxide

$$CO_2 = -8{,}49 + 0{,}1806x1 - 0{,}0688x2 – 0{,}00712x3 – 0{,}0787x4 – 0{,}000209x1^2$$

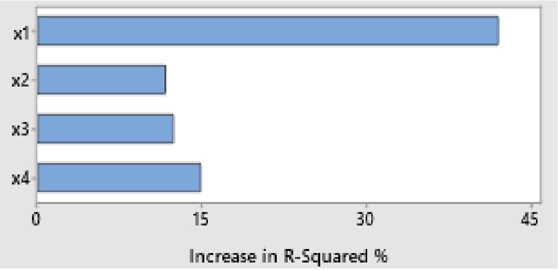

Fig. 2. Influence of initial parameters on the yield of carbon dioxide

Looking at the equation and Fig. 2 it is clear that air consumption (x1) has a positive linear effect and a negative quadratic effect on the carbon dioxide yield. An increase in air consumption will increase the carbon dioxide yield, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) has a negative linear effect on carbon dioxide yield. An increase in steam consumption will reduce the carbon dioxide yield.

The temperature in the reaction zone (x3) has a negative linear effect on carbon dioxide yield. An increase in temperature will reduce the carbon dioxide yield.

The residence time of the material in the reaction zone (x4) has a negative linear effect on carbon dioxide yield. An increase in residence time will reduce the carbon dioxide yield.

- Hydrogen

$$H_2 = 43{,}62 – 0{,}1278x1 -0{,}05063x2 – 0{,}004062x3 +0{,}03562x4 +0{,}000161x1^2$$

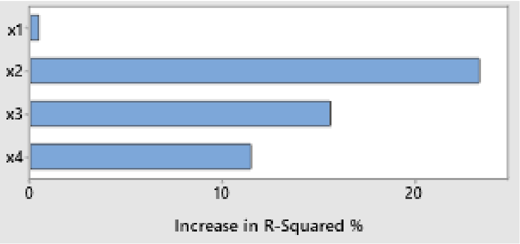

Fig. 3. Influence of initial parameters on hydrogen yield

Judging from the equation model for hydrogen and Fig.1 we can see that air consumption (x1) has a negative linear effect and a positive quadratic effect on the hydrogen yield. An increase in air consumption will reduce the hydrogen yield, but the effect becomes weaker as air consumption increases. Change in air consumption almost does not impact hydrogen yield.

Steam consumption (x2) has a negative linear effect on hydrogen yield. An increase in steam consumption will reduce the hydrogen yield.

The temperature in the reaction zone (x3) has a negative linear effect on hydrogen yield. An increase in temperature will reduce the hydrogen yield.

The residence time of the material in the reaction zone (x4) has a positive linear effect on hydrogen yield. An increase in residence time will increase the hydrogen yield.

- Carbon monoxide

$$CO = 20{,}76 – 0{,}1564x1 + 0{,}1238x2 + 0{,}01363x3 + 0{,}1562x4 + 0{,}000174x1^2$$

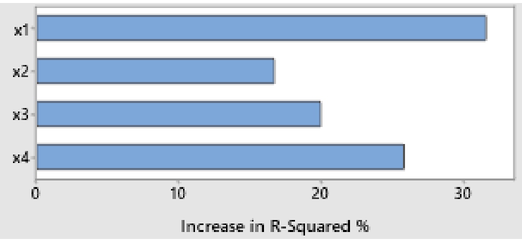

Fig. 4. Influence of initial parameters on the output of carbon monoxide

By looking at the equation and Fig. 4 we can say that air consumption (x1) has a negative linear effect and a positive quadratic effect on the carbon monoxide yield. An increase in air consumption will reduce the carbon monoxide yield, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) has a positive linear effect on carbon monoxide yield. An increase in steam consumption will increase the carbon monoxide yield.

The temperature in the reaction zone (x3) has a positive linear effect on carbon monoxide yield.

An increase in temperature will increase the carbon monoxide yield.

The residence time of the material in the reaction zone (x4) has a positive linear effect on carbon monoxide yield. An increase in residence time will increase the carbon monoxide yield.

The influence of parameters fluctuates from 17% (steam consumption) to 32% (air consumption).

- Nitrogen

$N_2 = 40{,}35 + 0{,}0981x1 - 0{,}1125x4 - 0{,}000117x1^2$

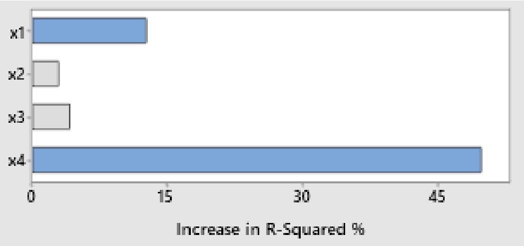

Fig. 5. Influence of initial parameters on nitrogen yield

From the equation and Fig. 5, we can see that Air consumption (x1) has a positive linear effect and a negative quadratic effect on the nitrogen yield. An increase in air consumption will increase the nitrogen yield, but the effect becomes weaker as air consumption increases.

The residence time of the material in the reaction zone (x4) has a negative linear effect on nitrogen yield. An increase in residence time will reduce the nitrogen yield.

The residence time has the most impact on the nitrogen yield and steam consumption with temperature does not impact it at all.

- Oxygen

$O_2 = -3{,}70 + 0{,}0208x1 - 0{,}00750x2 + 0{,}000125x3 + 0{,}00625x4 - 0{,}000021x1^2$

Looking at this equation we can say that air consumption (x1) has a positive linear effect and a negative quadratic effect on the oxygen yield. An increase in air consumption will increase the oxygen yield, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) has a negative linear effect on oxygen yield. An increase in steam consumption will reduce the oxygen yield.

The temperature in the reaction zone (x3) has a positive linear effect on oxygen yield. An increase in temperature will increase the oxygen yield.

The residence time of the material in the reaction zone (x4) has a positive linear effect on oxygen yield. An increase in residence time will increase the oxygen yield.

Dry gas properties:

- Yield, m^3/kg semi-coke

$\text{Yield} = 6{,}06 - 0{,}02534x1 + 0{,}0525x2 + 0{,}00295x3 + 0{,}00719x4 + 0{,}000032x1^2 - 0{,}000057x2x3$

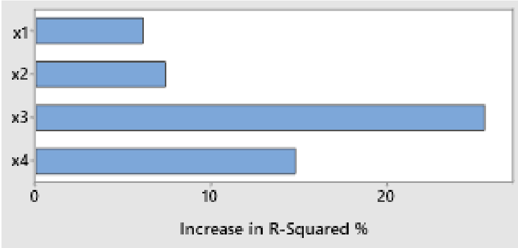

Fig. 6. Influence of initial parameters on the yield of dry gas, m^3/kg semi-coke

Fig. 6 shows that the dry gas yield is most affected by the temperature in the reaction zone (25%) and the Residence time of the material in the reaction zone (15%).

The corresponding equation shows that air consumption (x1) has a negative linear effect and a positive quadratic effect on the dry gas yield. An increase in air consumption will reduce the dry gas yield, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) has a positive linear effect on dry gas yield. An increase in steam consumption will increase the dry gas yield.

The temperature in the reaction zone (x3) has a positive linear effect on dry gas yield. An increase in temperature will increase the dry gas yield.

The residence time of the material in the reaction zone (x4) has a positive linear effect on dry gas yield. An increase in residence time will increase the dry gas yield.

The interaction between steam consumption (x2) and temperature in the reaction zone (x3) has a negative linear effect on dry gas yield. The effect of temperature on dry gas yield is weaker as steam consumption increases.

- Humidity, g/m^3

$\text{Humidity} = -340 + 2{,}519x1 - 1{,}11x2 – 0{,}196x3 – 0{,}681x4 – 0{,}003169x1^2 + 0{,}00419x2x3$

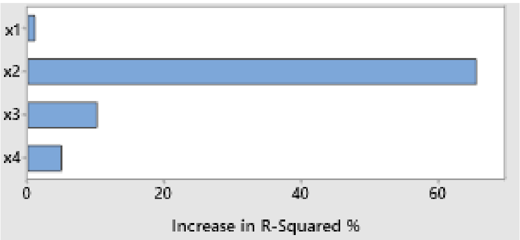

Fig. 7. Influence of initial parameters on gas humidity, g/m^3

Fig. 7 shows that the gas humidity is most influenced by the Steam consumption (65%), the temperature in the reaction zone slightly affects (7%), and the other parameters practically do not affect the gas humidity (<5%).

From the equation, we can conclude that Air consumption (x1) has a positive linear effect and a negative quadratic effect on the humidity in the resulting gas. An increase in air consumption will increase the humidity in the resulting gas, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) has a negative linear effect on the humidity in the resulting gas. An increase in steam consumption will decrease the humidity in the resulting gas.

The temperature in the reaction zone (x3) has a negative linear effect on the humidity in the resulting gas. An increase in temperature will decrease the humidity in the resulting gas.

The residence time of the material in the reaction zone (x4) has a negative linear effect on the humidity in the resulting gas. An increase in residence time will decrease the humidity in the resulting gas.

The interaction between steam consumption (x2) and temperature in the reaction zone (x3) has a positive linear effect on the humidity in the resulting gas. The effect of temperature on the humidity in the resulting gas is stronger as steam consumption increases.

- Net calorific value, MJ/m^3

$NHV = 8{,}987 – 0{,}03487x1 + 0{,}00625x2 + 0{,}001x3 + 0{,}0225x4 + 0{,}000039x1^2$

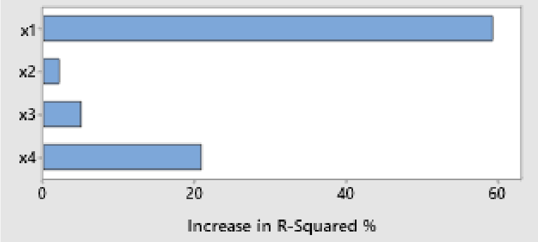

Fig. 8. Influence of initial parameters on the net calorific value, kcal/m^3

Fig. 8 shows that the lower calorific value is most affected by air consumption (60%), the residence time of the raw material in the reaction zone affects it less (21%) and the other parameters practically do not affect it (<5%).

From the equation, we can see that air consumption (x1) has a negative linear effect and a positive quadratic effect on the net calorific value of the resulting gas. An increase in air consumption will decrease the net calorific value of the resulting gas, but the effect becomes weaker as air consumption increases.

Steam consumption (x2) has a positive linear effect on the net calorific value of the resulting gas. An increase in steam consumption will increase the net calorific value of the resulting gas.

The temperature in the reaction zone (x3) has a positive linear effect on the net calorific value of the resulting gas. An increase in temperature will increase the net calorific value of the resulting gas.

The residence time of the material in the reaction zone (x4) has a positive linear effect on the net calorific value of the resulting gas. An increase in residence time will increase the net calorific value of the resulting gas.

- Density, g/m^3

$Density = 637{,}9 + 2{,}923x1 - 0{,}0025x3 + 0{,}125x2 - 0{,}937x4 - 0{,}003500x1^2$

We can see that the density of the resulting gas is positively influenced by air consumption (x1), and negatively influenced by temperature (x3) and steam consumption (x2) in the reaction zone. The density also decreases with increased residence time (x4) in the reaction zone. The effect of air consumption (x1) on the density of the resulting gas is more significant as it is multiplied by a higher coefficient (2.923) compared to temperature (x3) and steam consumption (x2).

Conversion rate, %:

- Carbon

$CarbConvRate = 162{,}67 - 0{,}4995x1 - 0{,}001500x3 + 0{,}15000x2 + 0{,}36500x4 + 0{,}000597x1^2$

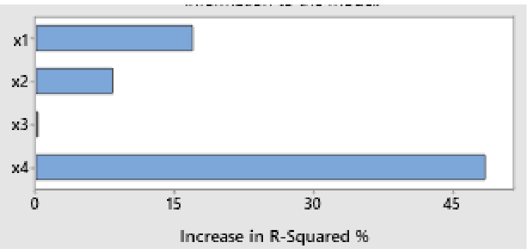

Fig. 9. Influence of initial parameters on the degree of carbon conversion, %

Fig. 9 shows that the lower calorific value is most affected by the residence time of the raw material in the reaction zone (48%), air consumption (17%) and steam consumption (8%) affect it less, the temperature in the reaction zone practically does not affect it (< 1%).

From the equation, we can conclude an increase in air consumption (x1) leads to a decrease in the conversion rate of carbon. This can be seen by the negative coefficient of -0,4995 associated with x1.

An increase in steam consumption (x2) leads to an increase in the conversion rate of the carbon, as seen by the positive coefficient of 0.15000 associated with x2.

The temperature in the reaction zone (x3) has a negative effect on the conversion rate of the carbon. A higher temperature leads to a decrease in the conversion rate, as indicated by the negative coefficient of -0.001500 associated with x3.

The residence time of the material in the reaction zone (x4) has a positive effect on the conversion rate of the carbon, which can be seen by the positive coefficient of 0.36500 associated with x4.

The influence of the square of air consumption (x1^2) on the conversion rate of carbon is not straightforward. The coefficient of 0.000597 associated with x1^2 suggests that the effect of x1 on the conversion rate is not linear, and further analysis may be needed to determine the specific relationship.

- Steam

SteamConvRate = 335,3-1,221x1 – 0,7625x2 – 0,04150x3 + 0,3512x4 + 0,001538 $x1^2$

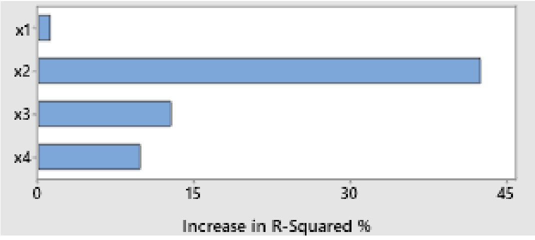

Fig. 10. Influence of initial parameters on the degree of steam conversion, %

Fig. 10 shows that the lower calorific value is most affected by steam consumption (42%), the temperature in the reaction zone and the residence time of the raw material in the reaction zone affect it less, and the air consumption practically does not affect it (<1%).

The equation shows that increasing air consumption (x1) results in a decrease in the conversion rate of steam while increasing steam consumption (x2) leads to a further decrease in the conversion rate.

The higher temperature in the reaction zone (x3) has a negative effect on the conversion rate, while the longer residence time of the material in the reaction zone (x4) leads to an increase in the conversion rate.

The influence of the square of air consumption (x1^2) on the conversion rate is positive.

Conclusions. An analysis of the obtained regression equations shows that with an increase in airflow, the methane content will decrease, the amount of carbon dioxide will increase, and the content of nitrogen and unreacted oxygen will increase.

An increase in steam consumption entails a decrease in the methane content in the final gas since methane is formed during gasification by thermochemical transformations of raw materials without the participation of a blast.

The amount of carbon dioxide and hydrogen also decreases, which is explained by a decrease in the conversion of water vapor due to its excess, in contrast to carbon monoxide, the content of which increases. The decrease in water vapor conversion also explains the increase in the humidity of the resulting gas.

Increasing the temperature in the reaction zone promotes the reactions:

$C + H_2O \rightarrow CO + H_2$

$C + 2\ H_2O \rightarrow CO_2 + H_2$

$C + CO_2 \rightarrow 2CO$,

the result is a decrease in the percentage of carbon dioxide and hydrogen, with an increase in the proportion of carbon monoxide.

Increasing the residence time of the raw material in the reaction zone increases the proportion of hydrogen and carbon monoxide in the generator gas, and reduces the proportion of carbon dioxide. And since it is the reactions of obtaining CO and H2 that are characterized by the highest volumetric yield per unit mass of raw materials, the percentage of ballast nitrogen in the gas obtained after gasification decreases, the lower calorific value and the degree of conversion of carbon and hydrogen increase.

The regression equations obtained as a result of calculations show a complex dependence of the parameters of the produced gas and the conditions for carrying out the gasification process. This leads to the impossibility of choosing the ideal reaction parameters for all cases of using the generator gas. For example, to achieve the best gas for the energy industry, the parameters must be optimized to maximize the net calorific value and minimize the humidity of the resulting gas, while maintaining a high conversion rate of carbon and steam. Some steps that can be taken to achieve these goals are:

Increase the temperature in the reaction zone, as this has a positive impact on the net calorific value and a negative impact on the humidity of the resulting gas.

Decrease air consumption, as this has a positive impact on the net calorific value and a negative impact on the humidity of the resulting gas.

Increase steam consumption, as this has a positive impact on the net calorific value and a negative impact on the humidity of the resulting gas.

Adjust the residence time of the material in the reaction zone to optimize the net calorific value while maintaining a low humidity and a high conversion rate of carbon and steam.

To achieve the best gas for methanol production, the parameters must be optimized to maximize the hydrogen and carbon monoxide yields and minimize the carbon dioxide and nitrogen yields, while maintaining a high conversion rate of carbon and steam. Some steps that can be taken to achieve these goals are:

Increase the temperature in the reaction zone, as this has a positive impact on the carbon monoxide yield and a negative impact on the carbon dioxide yield.

Decrease air consumption, as this has a negative impact on the methane and hydrogen yields, and a positive impact on the carbon monoxide yield.

Increase steam consumption, as this has a positive impact on the hydrogen yield and a negative impact on the carbon dioxide yield.

Adjust the residence time of the material in the reaction zone to optimize the yield of the desired gases while maintaining a high conversion rate of carbon and steam.

The method for determining the optimal technological parameters of the process of gasification of a solid thermolysis product based on the theory of multicriteria vector optimization is described by the authors in [3, 97-100].

As a result of the work carried out in the course of this article, regression equations for the gasification process were derived that are as close as possible to the process, without crossing the "overfitting" line, which occurs when the equation is overcomplicated in an effort to fit all the data for a perfect match. The resulting equations are easily analyzed, which simplifies the work with them. The article also presents graphs for each regression equation on the degree of influence on the final parameters of the process conditions, which makes it possible to understand the change in which specific technological factors will give the greatest result.

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Кутовий Д.С., Казаков В.В. ОПТИМІЗАЦІЯ ПРОЦЕСУ ГАЗИФІКАЦІЇ МАЛОМЕТАМОРФІЗОВАНОГО ВУГІЛЛЯ: РЕГРЕСІЙНИЙ АНАЛІЗ

У останні десятиліття глобальні зміни навколишнього природного середовища світу стали суттєвим стримуючим фактором розвитку суспільства, що потребує розроблення наукових підходів до зменшення негативного техногенного впливу на екологію. Необхідність встановлення балансу між задоволенням сучасних потреб людства і захистом інтересів майбутніх поколінь передбачає гармонізацію соціальних, економічних та екологічних складових трансформації суспільства. У країнах Європи, зокрема в Україні, екологічні ризики переважно спричинені промисловим сектором. Виробнича діяльність підприємств вугільної галузі призводить до значного територіального погіршення стану довкілля. Отже, підвищення екологічної безпеки у напряму енергетичного розвитку України є актуальною, має практичне значення та передбачає проведення досліджень щодо створення екологічних способів термохімічного перероблення некондиційної вуглецевмісної сировини.

У статті проведено комплексний аналіз процесу газифікації твердого продукту, отриманого термолізом малометаморфізованого вугілля. Основною метою статті є оптимізація параметрів процесу газифікації в залежності від цільового використання отриманого газу шляхом використання регресійного аналізу. Для вирішення цієї проблеми та дослідження різних підходів до її вирішення проаналізовано останні дослідження та публікації в цій галузі.

У статті наведено рівняння регресії, які були виведені для визначення ступеня впливу різних умов процесу на кінцеві параметри процесу газифікації. Графічно охарактеризовано кожне рівняння регресії, надаючи візуальне представлення даних і полегшуючи читачам розуміння зв'язків між змінними.

Показано невирішені частини загальної проблеми, які досліджуються в статті. Розглянуто проблеми та обмеження поточних підходів і окреслюють майбутні напрямки досліджень у цій галузі.

Детальний аналіз та підхід авторів до вирішення проблеми роблять цю статтю цінним науковим ресурсом для науковців та фахівців енергетики та може слугувати підґрунтям для подальших досліджень щодо параметрів процесу газифікації в залежності від цільового використання отриманого газу.

Ключові слова: *газифікація, термоліз, малометаморфізоване вугілля, оптимізація, умови процесу, рівняння регресії, енергетика.*