Mathematical model and methods for solving heat-transfer problem during underground coal gasification

Pavlo Saik¹✉, Mykhailo Berdnyk¹✉
¹ Dnipro University of Technology, Dnipro, Ukraine
*Corresponding author: e-mail saik.mnu@gmail.com

Abstract

Purpose. A mathematical model development for heat transfer during underground coal gasification based on the transcendental equation solution by the Newton-Raphson method.

Methods. The heat-transfer model development is based on the research into a temperature field with a variable size of the gasification zone when passing through the phase transformation boundary, which changes abruptly. The research on the coal seam temperature and the displacement length of the phase transition boundary is based on the integration of the differential heat-transfer equation with the fulfillment of one-phase Stefan problem conditions. The proportionality factor, characterizing the ratio of the displacement length of the “generator gas – coal” phase transition boundary to the time of coal seam gasification, is determined by substituting the Boltzmann equation and using the Newton-Raphson method based on solving the obtained transcendental equation.

Findings. The main problems related to laboratory research on the coal gasification process have been identified. A mathematical model of heat transfer during underground coal gasification for a closed georeactor system has been developed, taking into account the effective change in its active zones.

Originality. A mathematical model of heat transfer during underground coal gasification at the phase transition boundary has been developed, under which the one-phase Stefan problem conditions are fulfilled. Dependences of the change in the underground gas generator temperature, taking into account the change in the active zones of chemical reactions along the length of the combustion face and the gasification column, have been revealed. In addition, the dependences of the change in the phase transition boundary of a “generator gas – coal” heterogeneous system have been determined, which characterize the displacement length of the phase transition boundary on time and reveal the relationship between the thermal conductivity coefficient, specific heat capacity, as well as bulk density of coal and its calorific value.

Practical implications. A method has been developed to determine the displacement length of the phase transition boundary of a “generator gas – coal” heterogeneous system and its relationship between the time and temperature of gasification process. This makes it possible to predict in the future the change in the active zones of the underground gas generator along the length of the gasification column.

Keywords: underground gasification, coal, heat transfer, thermal conductivity, Stefan problem

1. Introduction

The rapid development of scientific-technological progress is accompanied by an increasing demand for fuel and energy resources. Ukraine has an extremely high potential for hard and brown coal reserves, which, if properly and efficiently involved in industrial turnover, can compete with natural gas. However, today’s realities are such that since 2014, coal production has decreased almost twice (as of 2018). This is primarily due to the political and military situation in the east of Ukraine [1]. Another reason for such a decrease in production is the complication of conducting mining operations due to the negative rock pressure manifestations in the stope faces and advance workings, as well as the use of outdated equipment, etc. At the same time, Russia’s war against Ukraine further encourages the development and implementation of its own technologies for mining and processing of solid fuels. One of the promising technologies in the mining and energy sector is the introduction of borehole underground gasification technology. Thus, the transformation of mining mines into mining-energy mines is a new stage in the development of the fuel and energy sector of our country. Over the past few years, interest in underground coal gasification as a potential energy source has increased significantly [2]. There are enough reasons to revive such interest. Among these reasons are the growing demand for energy, the decrease in the availability of the best traditional energy sources and the amount of potential energy resources in our country. Obviously, underground coal gasification can be a process capable of producing large volumes of clean fuel. This fuel is particularly suitable for use in combined power generation cycle, which is based on material, financial, human and organizational resources [3]-[5]. Of
course, evaluation of such technology must be substantiated by taking into account discounting and financial activity of the enterprise and its process management [6]-[8].

Moreover, it should be noted that an important component of this cycle is to ensure an acceptable ecological state of the territories within which the solid fuel deposits are concentrated [9]-[12] while maintaining the safety of workers [13].

2. Analysis of recent research and publications

Underground coal gasification (UCG) technology is an unconventional method of mining the fields that opens up new opportunities in the development of solid energy fuel reserves. In other words, UCG technology is a controlled process of coal gasification at the place of its occurrence to obtain a crude mixture containing CO, CO2, H2, CH4, O2, higher hydrocarbons, resins and impurities in its composition [14], [15]. The essence of UCG technology is in drilling the directional boreholes through the coal seam from the earth’s surface with their subsequent connection, formation of a reaction channel, inflammation of the coal seam, its gasification, production of generator gas and its removal to the earth’s surface [16]-[18]. Over the last decade, a number of research works have been performed on the problems of the gasification process efficiency. Intensive research and practical work has been conducted on the territory of Europe, which has a long history of field trials and laboratory research [19]. The research performed has allowed to form the main three parameters by which it is necessary to control:

1) the process parameters, such as flow rate of blast mixtures, their temperature and pressure, synthesis gas content and calorific value [20];
2) geomechanical parameters, such as pressures in cavities and coal seams, cavity development, subsidence and deformation of coal seam roof rocks [21], [22];
3) environmental parameters, such as groundwater chemical composition and air quality [23], [24].

3. Feasibility of conducting research on this issue

The specifics of UCG technology makes it impossible to monitor chemical, thermal, hydrological and geomechanical processes occurring both in the coal seam plane and in the rocks around the formed georeactor system (underground gas generator). The temperature field distribution parameters can be assessed using thermal imaging devices and temperature sensors, the course of chemical reactions, qualitative and quantitative analysis of the initial gas mixture. The pollution level is assessed by sampling water from aquifers. In addition, it is necessary to further study the wastewater generated during the processing of gasification products [25]. With regard to geomechanical processes, it is extremely difficult to assess the stress-strain state of a rock mass without having data on the velocity of combustion face advance in space and time. That is, directly in the conditions of a working system. Therefore, the stress-strain state is studied by numerical simulation methods [26]-[28]. Accordingly, the urgent task of ensuring the predictive performance of the georeactor system (underground gas generator) is the development of a mathematical algorithm that allows obtaining data on the heat-transfer model. The developed mathematical models make it possible to qualitatively and quantitatively assess the parameters of temperature fields [29]-[32]. Thus, an analytical calculation method based on Fourier’s law of thermal conductivity is proposed in the work [33]. This method makes it possible to study the thermal effect of the combustion and gasification process on the rocks containing the underground gas generator in order to use groundwater as an intermediate mobile heat carrier. In the work [34], a mathematical model of filtration and heat transfer in the roof rocks of an underground gas generator has been developed and tested, which makes it possible to assess the convection and conduction components of the heat flow. At the same time, the underground gasification process takes place in the underground space and is characterized by a variety of factors depending on the thermophysical and geometrical dimensions of both the reaction channel and the underground gas generator [35], [36].

Despite the prospects of the analyzed technologies for the introduction of underground coal gasification, there are few examples of its practical implementation [37]-[39]. This is primarily due to the lack of data, as well as the absence of generally accepted and practically confirmed theories regarding the heat and mass transfer processes in the rock mass containing the underground gas generator. It is impossible to select the main technological operating modes of underground gas generators only by conducting experimental studies. It is necessary to form a theory of the underground coal gasification process based on mathematical models that take into account a set of basic heat and mass transfer processes occurring during underground gasification.

4. Research methods

4.1. Physical formulation of the problem

Coal gasification is based on either incomplete fuel combustion (with a lack of oxygen), or complete fuel combustion with subsequent reaction of carbon with carbon dioxide and water vapor to obtain combustible generator gases (CO, H2, CH4). The last reactions are endothermic in nature. The general mechanism of the process of underground coal gasification is shown in Figure 1.

![Figure 1. Mechanism for conducting the coal gasification process](image)

By taking into account the mechanism for conducting the underground coal gasification process, which is presented in Figure 1, it is possible to substantiate the mathematical model parameters of heat transfer occurring in the underground gas generator.

4.2. Mathematical model of heat transfer during underground coal gasification

In mathematical modeling of the underground gasification process, it is assumed in our case that there are no inhomogeneities in the coal seam, and heat and mass transfer conditions along the upper and lower surface of the seam do not change. Modeling of the heat-transfer process during underground coal gasification is accompanied by a change in the aggregate state of the medium as a result of coal com-
The rock-coal mass formation is performed in two stages. At the first stage, the coal seam modeling is conducted, and at the second stage, the modeling of the coal-overlaying formation is performed. As an equivalent material, pieces of coal with a size of 200×150×100 mm are used, which, in terms of their qualitative composition, correspond to the studied area; coal dust; water and M400 cement. There is a space left in the seam to model injection and gas production boreholes with a diameter of d = 0.05 m and a reaction channel. The reaction channel is formed from coal pieces with a fraction of 2.5-6.8 cm, modelling hydraulic fracturing between the blast-hole and gas production borehole.

The lithological varieties of the mass are identified in accordance with the in-situ conditions of the studied mine field areas. Based on scaling factors and peculiarities of forming complex systems, simplification are introduced into the modeling process by combining rock seams with similar metamorphic properties. For the conditions of the model, the thickness of such layers does not exceed 0.2 m. To ensure the system autothermicity, the underground gas generator is thermally insulated. This makes it possible to maintain the gasification process without supplying heat from the outside due to exothermic reactions. A refractory brick serves as a heat-insulating material, which is laid out in one row along the bench contour to the height of the lithological variety layers.

The temperature field distribution parameters are studied at individual points of the modelled area, in places of setting the stationary temperature sensors of the TEP-109 type (Fig. 3).

Figure 2. General view of the interphase boundary S(t): “generator gas – coal”

The phase transition boundary x = S(t) at any time separates coal from combustion products, moving at a certain velocity v = dS/dt towards the coal seam. From the problem formulation S(0) = 0.

4.3. Laboratory facilities for conducting research

The need for laboratory research is to determine the temperature fields in the underground gas generator, depending on the combustion face position along the length of the gasification column [43]. This makes it possible to obtain data on the temperature in the coal seam, which is the basis for conducting the computational experiment.

Experimental studies are conducted using a laboratory setup in the laboratory of thermochemical transformation technologies of the Dnipro University of Technology [44]. In general terms, the setup consists of four main elements: a test bench, blast and gas exhaust systems, as well as control and measuring equipment. The central part of the setup is a test bench – a metal box welded from 5 mm thick sheet steel. The bench is made sectional, which makes it possible to model an underground gas generator by two methods of mining the coal seam: a borehole – a gas generator and pillar mining. On the front part of the bench, there are holes for supplying blast and removing generator gas.

According to the presented schematic diagram (Fig. 3), the sensors are set on the plane of the coal seam contact with the immediate roof.

5. Results and discussion

Mathematically, determining the coal seam temperature field T(x, t) and the displacement length of the phase transition boundary S(t) consists in integrating the differential equation of thermal conductivity [45, 46] in the area

\[ D = \{ (x,t) \mid x \in \{S(t), \infty\}, \ t \in (0, \infty) \} \],

which, given the accepted assumptions, takes the following form:

\[ \frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2}, \]  

(1)

with the initial condition:

\[ T(x,0) = T_0. \]  

(2)
and boundary conditions:

\[ T(0, t) = T_p \] \hspace{1cm} (3)

\[ T(\infty, t) = T_0 \] \hspace{1cm} (4)

at the phase transition boundary, the conditions (Stefan problem conditions) are fulfilled:

\[ T\left(S(t), t\right) = T_c \] \hspace{1cm} (5)

\[ \lambda \frac{\partial T\left(S(t), t\right)}{\partial S} = -\gamma \cdot Q \frac{dS}{dt} \] \hspace{1cm} (6)

where:

\( a = \lambda \gamma \) – temperature conductivity coefficient;

\( \lambda \) – thermal conductivity coefficient;

\( c \) – specific heat capacity;

\( \gamma \) – coal bulk density;

\( Q \) – specific calorific value.

Using the Boltzmann transformation \( \theta = \frac{x}{\sqrt{t}} \), Equation 1 is reduced to the ordinary differential equation for the function \( T(\theta) \):

\[ \frac{d^2 T(x, t)}{d\theta^2} + 1 \cdot \theta \frac{dT}{d\theta} = 0. \] (7)

Having substituted \( \theta = \frac{dT}{d\theta} \), Equation 7 takes the form:

\[ \frac{1}{\theta} \frac{d\theta}{d\theta} = -\frac{1}{2a} \theta. \] (8)

The solution of the ordinary differential Equation 8 is as follows:

\[ \theta(\theta) = B \exp\left(-\frac{\theta^2}{4a}\right). \] (9)

where:

\( B \) – unknown constant.

By integrating Equation 9, the general solution of Equation 7 can be found:

\[ T(\theta) = A + B \int_0^\theta \exp\left(-\frac{\xi^2}{4a}\right) d\xi = A + B \Phi\left(\frac{\theta}{2\sqrt{a}}\right). \] (10)

where:

\( A \) – unknown constant;

\[ \Phi(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp\left(-\xi^2\right) d\xi \] – Laplace function.

The Laplace function is also called the error function and is denoted as \( \text{erf}(z) \). In particular, the Laplace function satisfies the conditions:

\[ \Phi(0) = 0. \] (11)

Returning to the variables \( x, t \), the found Solution 10 can be written in the form:

\[ T(x, t) = A + B \cdot \Phi\left(\frac{x}{2\sqrt{a} \sqrt{t}}\right). \] (12)

where:

\( a = \sqrt{a} \).

From the boundary condition 5, we obtain:

\[ A + B \cdot \Phi\left(\frac{S(t)}{2\sqrt{a} \sqrt{t}}\right) = T_c. \] (13)

For Condition 13 to be satisfied, it is necessary that the function \( \Phi \) argument in Equation 13 be constant, that is, proportional to \( \sqrt{t} \). Let:

\[ S(t) = \beta \cdot \sqrt{t}, \] (14)

where:

\( \beta \) – the proportionality factor between the displacement length of the phase transition boundary and time.

Then, Equation 13 takes the form:

\[ A + B \cdot \Phi\left(\frac{\beta}{2\sqrt{a}}\right) = T_c. \] (15)

From the boundary Condition 3 we obtain:

\[ A = T_p. \] (16)

Thus, from Equation 15 we have:

\[ B = \frac{T_c - T_p}{\Phi\left(\frac{\beta}{2\sqrt{a}}\right)}. \] (17)

Given 16-17, \( T(x, t) \) takes the form:

\[ T\left(x, t\right) = T_p + \frac{T_c - T_p}{\Phi\left(\frac{\beta}{2\sqrt{a}}\right)} \cdot \Phi\left(\frac{x}{2\sqrt{a} \sqrt{t}}\right). \] (18)

Having substituted Condition 6 in 18, the transcendental equation is obtained for determining \( \beta \):

\[ F(\beta) = \sqrt{\pi} \cdot Q \cdot \alpha_1 \cdot \beta + \frac{\exp\left(-\frac{\beta^2}{2\sqrt{a}}\right)}{\Phi\left(\frac{\beta}{2\sqrt{a}}\right)} = 0. \] (19)

Hence, from Equation 19, which has a quadratic convergence, successive approximations by the Newton-Raphson method are calculated by the formula:

\[ \beta_{n+1} = \beta_n - \frac{F(\beta_n)}{dF(\beta_n)/d\beta} \] (20)

where:

\[ \frac{dF(\beta)}{d\beta} = F'(\beta) = \frac{\sqrt{\pi} \cdot Q \cdot \alpha_1}{2\lambda (T_c - T_p)} + \exp\left(-\frac{\beta}{2\sqrt{a}}\right) \left[ \frac{\beta}{2(a_1)^2} - \frac{1}{a_1} \frac{1}{\sqrt{\pi}} \right] \]

\[ + \left[ \Phi\left(\frac{\beta}{2\sqrt{a}}\right)^2 \right] \frac{2}{\sqrt{\pi}} \]

When performing a computational experiment by solving the transcendental Equation 19, depending on the temperature regime of the formed closed georeactor system (\( T_c, T_p \)), thermal conductivity coefficient (\( \lambda \)), specific heat capacity (\( c \)), bulk density of coal (\( \gamma \)) and its specific calorific value,
(Q), the coefficient (β) is determined, which characterizes the proportionality between the displacement length of the “generator gas – coal” phase transition boundary and time. Having determined this coefficient, it is possible to determine the rate of change in the aggregate state of the studied system along the combustion face length, which is characterized by a balance between the oxidizing and reducing zones.

The proportionality factor is determined on the basis of solving transcendental Equation 19. The basis of the initial data on the bulk density of coal (γ) and the specific calorific value (Q) is the mining-geological conditions of bedding the coal seam y^2 of the Stepova mine, SE Lvivvuhilja. Coal grade is G. The nature of the temperature distribution around the underground gas generator is studied for grade G coal of the seam c0 at the Soleniwska site, Donets coal basin (site #1). In the course of laboratory research, the parameters of the temperature field distribution in the plane of the coal seam roof have been determined, both in the combustion face and in the gassed-out space.

In the coal gasification process, the formation of active zones and thermal intensification of the process is provided by supplying blast mixture to the combustion face “mirror”. An air blast mixture is used for the studied conditions. The oxygen content is 21%. The average pressure of the supplied mixture is 0.24 MPa. This makes it possible to form chemical reaction zones along the combustion face length, characterized by a change in temperature in the plane of the coal seam contact with the immediate roof (Fig. 4).

![Figure 4. Parameters of temperature distribution in the plane of the coal seam contact with the immediate roof when supplying air blast mixture: 1 - 6 - rows of setting the temperature sensors along the length of the gasification column (0.2 m step); 7 - blast-hole placement; 8 - production borehole placement](image)

The temperature maximum is observed at a distance of 0.25 m from the blast-hole and distributed to 0.1 m from both sides. This indicates the formation of the transition zone of the underground gas generator. At the same time, when the combustion face moves towards the gasification column, the temperature field distribution is described by the power-law relation (Fig. 5): \( t = k_1 t^k \) (\( k_1 \) – empirical coefficients characterizing the temperature distribution in the coal seam roof influenced by the zone of chemical reactions along the length of the combustion face). From the data analysis in Figure 5, it can be argued that the thermal zone of the underground gas generator is uniformly formed along the length of the gasification column. In the course of subsequent research, the parameters of temperature change during the combustion face advance have been determined. The research is conducted with the position of the combustion face under the second (\( T_4^d - T_5^d \)), third (\( T_4^d - T_5^d \)) and fourth (\( T_4^d - T_5^d \)) rows of set thermocouples (Fig. 3).

![Figure 5. Dependences of temperature change in the coal seam when supplying air blast mixture along the length of the gasification column: A – E – rows of setting the temperature sensors](image)

Data from two adjacent thermocouples are taken to analyze the temperature field distribution data. This makes it possible to obtain patterns of temperature change along the length of the gasification column (Fig. 6). And this, accordingly, confirms that the combustion face moves in a specified direction.

![Figure 6. Cyclicity of temperature change in the coal seam when supplying air blast mixture along the length of the gasification column: T1 – T6 – thermocouple number](image)

After 30 minutes of research, the temperature in the first row of thermocouples (\( T_1^d - T_6^d \)) increases to 110-150°C. This indicates that the combustion face moves towards the second row of thermocouples \( T_1^d - T_6^d \). The temperature maximum in the second row of thermocouples is observed after 2.4 hours of gasification and is 585-660°C. Hence, it can be argued that the velocity of the combustion face advance is 0.083 m/hour. A similar situation regarding the change in the combustion face velocity is observed in the course of research on the temperature maximum for the third (\( T_1^d - T_6^d \)) and fourth (\( T_1^d - T_6^d \)) row of thermocouples.

Based on the obtained data analysis, it has been determined that the effective change in the active zones (oxidizing and reducing) of the gas generator in the combustion face plane occurs at the level of thermocouples \( T_1^g - T_6^g \), \( T_1^g - T_6^g \), \( T_1^g - T_6^g \). This indicates that the oxidizing zone is ahead of the reducing zone by more than 50%. This leads to the thermal energy transfer from thermochemical reactions into the reducing zone of the gas generator and creates conditions for imbalance in the gasification process.

The obtained results on the temperature parameters in the coal seam serve as the initial data for solving the transcendental Equation 19, which makes it possible to determine the coefficient (β) characterizing the proportionality between the “generator gas – coal” and gasification time. When conducting a computational experiment, the data given in Table 1 are taken as initial ones.
The gasification time ranges from 50 to 200 s with a step of 50 s. The coal gasification temperature is set as an average value, that is \((T^2 + T^3 + T^4)/3\), \((T^2 + T^3 + T^4)/3\), \(\ldots\), \((T^2 + T^3 + T^4)/3\). Chemical reactions in the coal gasification zone are accompanied by a significant heat release, since they are exothermic. The methane gas released from the coal seam enters the reaction channel and is combusted. The oxygen present in the blast mixture also reacts with oxygen. The carbon monoxide produced is partially combusted. As a result of exothermic reactions, the gas temperature in the medium of the underground gas generator reaches 1100°C [47], [48].

Using the data from Table 1, the authors have conducted a computational experiment and obtained data on the change in the displacement length of the phase transition boundary from the proportionality factor \((\beta)\) (Fig. 7).

![Figure 7. Displacement lengths of the phase transition boundary \(S(t)\) depending on the proportionality factor \((\beta)\): \(A50 \rightarrow D50, A50 \rightarrow D50, A50 \rightarrow D50\) gasification time: 50, 100, 150 and 200 s, respectively, at the studied point of the underground gas generator](https://example.com/image)

Data analysis in Figure 7 characterizes the change in the displacement length of the phase transition boundary, the parameters of which are not constant and characterize the active zones of chemical reactions. To obtain the dependences of the change of proportionality factor \((\beta)\) on the length of the phase transition boundary and the time of gasification, the values of temperatures at study points \(T^2\), \(T^3\), \(T^4\) from the inlet borehole were excluded from this sample. Since these temperatures are in the range of 664-590°C.

6. Conclusions

An unequal temperature distribution along the length of the combustion face and the gasification column is a sign of a significant impact of oxidation and reduction reactions occurring in the underground gas generator. The obtained
dependences of the temperature change along the length of the combustion face make it possible to determine the size of the gas generator active zones: oxidizing zone, in which the coal combustion process occurs, and reducing zone, in which reduction reactions occur with the production of combustible generator gases.

Substituting the Boltzmann equation and using the Newton-Raphson, as well as solving the transcendental equation, a proportionality factor \(\beta\) has been determined, which characterizes the ratio of the displacement length of phase transition boundary of the “generator gas – coal” heterogeneous system to the time of coal gasification process. This makes it possible to develop a mathematical model of heat transfer during underground coal gasification, taking into account the effective change in the active zones of chemical reactions of an underground gas generator in the form of a one-phase Stefan problem. The parameters of the displacement length of the phase transition boundary characterize the intensity of the coal gasification process. This intensity contributes to the process acceleration from the side of the blast-hole with the occurrence of exothermic processes of thermochemical reactions for the formation of gases and thermal energy, providing the kinetics of endothermic reactions in the reducing zone.

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References


Математична модель та метод розв'язання задачі теплообміну при підземній газифікації вугілля

П. Саїк, М. Бердник

Мета. Розробка математичної моделі теплообміну при підземній газифікації вугілля на основі розв'язання трансцендентного рівняння методом Ньютона-Рафсона.

Методика. Основою розробки моделі теплообміну є дослідження температурного поля при змінному розмірі області газифікації на переході через межу фазових перетворень, яка змінюється стрибкоподібно. Дослідження температурного поля вугільного пласта \( T(x, t) \) та довжини переміщення межі фазового переходу \( S(t) \) проводились на інтегруванні диференціального рівняння теплопровідності з використанням умов однофазної задачі Стефана. Коефіцієнт пропорційності \( (\beta) \), що характеризує відношення довжини переміщення межі фазового переходу “генераторний газ – вугілля” до часу газифікації вугільного пласта знаходився за допомогою підстановки Больцмана та методом Ньотона-Рафсона на основі розв'язання отриманого трансцендентного рівняння.

Результати. Виділено основні проблеми, пов'язані з проведенням лабораторних досліджень процесу газифікації вугілля. Розроблена математична модель теплообміну при підземній газифікації вугілля для замкнутої геореакторної системи із врахуванням ефективної зміни активних її зон.

Наукова новизна. Отримана математична модель теплообміну при підземній газифікації вугілля на межі фазового переходу, при якій виконуються умови однофазної задачі Стефана. Встановлено залежності зміни температури підземного газогенератора з врахуванням зміни активних зон хімічних реакцій за довжиною вогневого вибою та стовпа газифікації. Встановлені залежності зміни межі фазового переходу гетерогенної системи “генераторний газ – вугілля”, що характеризують довжину переміщення межі фазового переходу від часу та показують взаємозв’язок між коефіцієнтом теплопровідності, питомою теплоємністю та об’ємною вагою вугілля й його теплотою згоряння.

Практична значимість. Розроблена методика, що дозволяє визначити довжину переміщення межі фазового переходу гетерогенної системи “генераторний газ – вугілля” та її взаємозв’язок між часом і температурою газифікації. Це дозволяє в подальшому прогнозувати зміну активних зон підземного газогенератора за довжиною стовпа газифікації.

Ключові слова: підземна газифікація, вугілля, теплообмін, теплопровідність, задача Стефана