Mathematical Modeling of Gas Generation in Underground Gas Generator

Y. N. Zakharov(✉)

ICT of SB RAS, Kemerovo State University,
6, Krasnaya Street, Kemerovo, Kemerovo Region 650043, Russia
zaxarovyn@rambler.ru, zyn@kemsu.ru

Abstract. Underground coal gasification is an in-situ underground physical and chemical process which converts coal into combustible gases using injections of free or bound oxygen. The paper presents two dimensional nonstationary mathematical model of underground gas generator performance based on flux method. It takes into account physical, chemical and gas dynamic processes. Gas medium consists of the following gases: CH_4, H_2, CO, O_2, H_2O, N_2. The research shows the numerical calculations of gas composition change inside the gas generator describing table values of brown and bituminous coal combustion products. *abstract* environment.

Keywords: Underground coal gasification · Compressible flow · Difference methods · Lateral fire well · Combustion face

1 Introduction

Advanced coal processing is one of the most complex and time consuming tasks of coal industry. This task solution can improve economic performances of fuel and energy industry and deal with the issues of ecological safety. Underground coal gasification (UCG) can be one of these problem solutions. Underground coal gasification is an in-situ underground physical and chemical process which converts coal into combustible gases using injections of free or bound oxygen. Establishing UCG production is possible for those places where deep mining and surface mining are not commercially viable. Underground coal gasification enables to dig for coal in the context of flat-lying high ash coal seams. One of the UCG advantages is that there are no severe surface damages caused. Moreover gas is considered to be environmentally friendly fuel: processed UCG gas has no hydrogen sulfide and does not release sulfur dioxide during combustion. The gas produced with oxygen injection has no nitrogen oxides [1]. UCG production has significant health and safety advantages: no people required to work underground, no work accidents associated with deep mining.

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Underground coal gasification technology was developed by the Soviet engineers in the 30's. Some experimental facilities were built in the USSR in the 50's. Yuzhno-Abinskaya station "Podzemgas" in Kuzbass (1955–1996) is one of them. Underground coal gasification seemed to be of great interest for foreign countries in the 70's and 80's. Major coal mining countries paid for UCG technology licenses. Though early UCG experiments naturally took place 80 years ago, there have been no industrial facilities until quite recently because of the complexity of UCG process technology, depending on many factors (mine engineering, hydrodynamic, hydro geologic, etc).

Nowadays scientists identify possible hydrocarbon energy potential of the Earth as 100% that includes oil (4.2%), gas (2.5%) and coal (93.3%) [2]. Steady increase of coal importance for the future economy is registered not only in Russia but in the whole world as well and makes unconventional coal mining technology (UCG) be the issue of great interest.

A great interest for UCG commercialization has been observed abroad during recent years. China and Australia are demonstrative example of it. The article [3] lists Chinese coal companies that are currently engaged in UCG implementation, e.g.: Xinwen Coal Industry Group; Feicheng Coal Industry Group; Xiyang Chemistry Company, etc. Now Australia has taken top position in the field of UCG. There are group of the companies in Australia that succeed in UCG exploitation. Here is the list of the most known and largest companies in the world: "Linc Energy" (global UCG leader) and "Australian Syngas Association Inc" (represents the group of Australian UCG companies). Currently UCG technology has small amount of theoretical backgrounds. Though UCG technology is widely used today, though development of relevant mathematical model and its validation is still considered to be a crucial task despite the researches [4–8].

Most researches contain simplified models that are basis for engineering formulae for received gas content calculation. The literature reviewing UCG issues also contains researches devoted to the more extensive description of physical and chemical transformations in the reaction site. In the same time there are no data on the complete composition of the received gas, and there is no comparison with the results of in situ tests. Thus, the task of validation of the reviewed UCG model has not been solved. Published in 2004 E. V. Kreinin's research contains much information comparing mathematical simulation based on engineering methods and in situ measurements taken at the operating flow method UCG companies.

Most researches contain simplified models that are basis for engineering formulae for received gas content calculation. The literature reviewing UCG issues also contains researches devoted to the more extensive description of physical and chemical transformations in the reaction site [9]. In the same time there are no data on the complete composition of the [8] received gas, and there is no comparison with the results of in situ tests. Thus, the task of validation of the reviewed UCG model has not been solved. Published in 2004 E. V. Kreinin's research contains much information comparing mathematical simulation based

on engineering methods and in situ measurements taken at the operating flow method UCG companies.

Consequently, computational modeling of gas generation based on flux method and UCG mathematical model validation (described in [10]) are the key goals of the paper. Gas composition determined at the exit of the gas production well (with the help of numerical calculations) is compared to the results of in-situ measurements of gas composition changes.

2 UCG Model

The paragraph is devoted to the UCG model based on flux method [8] (1).

To install gas generator, coal seam with at least 5 m thickness and 30–800 m formation depth is needed.

Two wells are drilled on either side of an underground coal seam, a lateral well (so called "lateral fire well") is drilled to connect the two vertical wells. It is used to ignite and fuel the underground combustion process, so the coal face ("combustion face") burns. One well is used to inject air or steam-oxygen (injection well) into the coal seam. The second well (gas collecting well) is used to collect the gas that is formed from the gasification reactions and to pipe it to the surface. As the coal face burns, the immediate area is depleted from the bottom up. Burning front shifts in the same direction. The remaining cavity usually contains the left over ash and fallen parts of the roof. The lateral fire well section barely changes due to coal burning, and the burning face surface remains available for injected blast, and as shown in [8] the gasifier operation is being stabilized. The injected blast flows round combustion face surface, gasifies coal and causes combustion gas generation. Both burning process and gasification process is considered to be single process. Part of the heat formed from the combustion process is transmitted to the immediate coal area. Heating process contains two stages. Firstly, coal moisture evaporates (drying of coal), the process decomposes coal and generates combustible volatiles (mostly CH_4, H_2) and carbon residue that contains carbon and ash. Coal temperature increases. Afterwards, coking residue carbon heterogeneously reacts with free and bound oxygen and water vapor to transform into CO and incombustible gases. The temperature can be 1500K–1700K. Remaining part of the heat is used to heat up gases in the lateral fire well. Gases generated during the decomposition reaction and further oxidation of coke carbon can be divided into two portions. Some gas portion is filtered and gets into unmined coal due to pressure gradient. The remaining gas portion gets into lateral fire well to heat up gas mixture and cause homogeneous oxidizing reactions due to convection and diffusion. The research [10] shows mathematical model of UCG that takes into consideration the physical processes of coal gasification mentioned above, gas flow in lateral fire well and mine face form change.

Two dimensional mathematical model of UCG [10] that describes UCG processes taking place both in unmined coal and lateral fire well is under consideration. As far as gas quality basically depends on the processes taking place on the

combustion face surface and in the lateral fire well, so when computational modeling is concerned, the quotation describing UCG only in gasifier channel Ω_2 and at combustion face (Γ_1) is under consideration in this paper (Fig. 1). Solution of a complete model including gas seepage, ash fall and fire face move demands another article layout. Here we are not concerned by mass values of gas seepage, here it is necessary to determine the content of the receiving gas and compare it with the gas content received by UCG from different coal basins. According to the mathematical model [6] the gas in lateral fire well is compressible and viscous and consists of seven components: CH_4, H_2, CO, O_2, H_2O, N_2

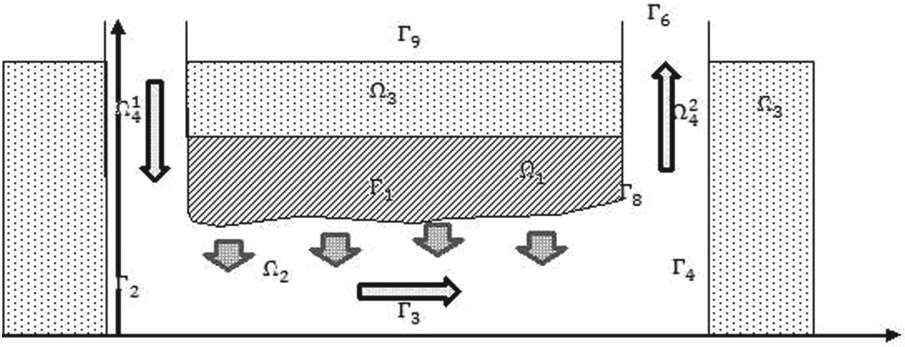

Fig. 1. Underground coal gasification (UCG)

Here are the main symbols used:

Ω_1 - coal seam, Ω_2 - lateral fire well, $\Omega_4^1 \cup \Omega_4^2$ - injection well and gas collection well, Ω_3 - soil, Γ_1 - combustion face, Γ_2, Γ_7 - side boundaries of the gas collecting well, Γ_4, Γ_8 - side boundaries of the gas collection well, Γ_3 - bottom interface of the lateral fire well, Γ_5, Γ_6 - entry and outlet section of the wells, Γ_9 - ground surface, $\rho(x, y, z)$ and $p(x, y, z)$ - density and pressure of the gas mixture, $u(x, y, z)$, $v(x, y, z)$ - projection of the gas velocity vector on the axis x and y relatively; $T(x, y, z)$ - temperature of the gas mixture, μ, μ_k - viscosity of the gas mixture and gas k-element, M, M_k - molar mass of the k-element mixture, λ, λ_k and c_p, c_{p_k} - thermal conduction and specific thermal capacity of the gas mixture and gas k-element, D_k - effective diffusion factor of the k- gas, c_k - proportion of k-element of the gas mixture, R - universal gas constant; q_k and P_k - enthalpy of formation, C_k^{out} and T_{out} - fractional gas composition and exterior temperature, α - heat-transfer coefficient, k_j, E_j, q_j - pre-exponential factor, activation energy and thermal effect of homogeneous reactions, W_k - mass change rate of gas phase k-component, R_j - mass rates of heterogeneous reactions, M_y - molar mass of dry coal, v_i, v_{3k} - stoichiometric coefficients, s - pore surface per unit volume of porous medium, ω_i - volume ratio of porous medium i-phase, where $i = 1$ - dry coal, $i = 2$ - moisture, $i = 3$ - gas phase, $i = 4$ - charred coal, $i = 5$ - ash, $f(x)$ - combustion face form, n - normal vector to the boundary.

Gaseous phase is considered to be a combination of non-viscous perfect gases, while its component diffusion is independent. The flow in the fields is laminar.

In $\Omega_2 \cup \Omega_4^1 \cup \Omega_4^2$ (Fig. 1) viscous compressible heat-conducting gas flow is defined by the Navier-Stokes equation system that describes nonstationary flow of viscous heterogeneous compressible fluid:

$$\begin{aligned} \rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) &= -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right), \\ \rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) &= -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial y}\right), \end{aligned} \tag{1}$$

Here are the initial: $v_0(x, y, 0) = u_0(x, y, 0)$, and boundary conditions: $v\big|_{\Gamma_1} = v_1(x, y, t)$, $v\big|_{\Gamma_5} = v_5(x, y, t)$, $v\big|_{\Gamma_6} = v_6(x, y, t)$, $u\big|_{\Gamma_1} = u_1(x, y, t)$, $u\big|_{\Gamma_5} = u_5(x, y, t)$, $u\big|_{\Gamma_6} = u_6(x, y, t)$.
$\frac{\partial v}{\partial n}\big|_{\Gamma_2,\Gamma_3,\Gamma_4,\Gamma_7,\Gamma_8} = \frac{\partial u}{\partial n}\big|_{\Gamma_1,\Gamma_2,\Gamma_3,\Gamma_4,\Gamma_5,\Gamma_6,\Gamma_7,\Gamma_8} = 0.$

The gas mixture viscosity is determined in accordance with k-gas proportion.
$\mu = \sum_{k=1}^{7} \mu_k c_k$
and v_0, u_0, v_1, v_5, v_6 - specified functions.

The Eq. (1) are closed by the state equation

$$p = \frac{\rho R T}{M}, \tag{2}$$

and molar mass of the gas phase is calculated in the following way
$\frac{1}{M} = \sum_{k=1}^{7} \frac{c_k}{M_k}$

The following heat-transfer equation governs heat transfer, absorption and emission in the gasifier:

$$\rho c_p\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right) = \frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right) + \sum_{k=3}^{6} q_k P_k \tag{3}$$

taking into consideration the initial: $T_0 = T_0(x, y, 0)$ and boundary conditions: $T\big|_{\Gamma_1} = T_1(x, y, t)$, $T\big|_{\Gamma_5} = T_5(x, y, t)$, $\frac{\partial T}{\partial n}\big|_{\Gamma_2,\Gamma_3,\Gamma_4,\Gamma_7,\Gamma_8} = 0$, $\frac{\partial T}{\partial n}\big|_{\Gamma_6} = \alpha\,(T - T_{out})$,
where α - heat-transfer coefficient, T_0, T_1, T_5 - specified functions of initial temperature and temperatures on the boundaries Γ_1 and Γ_5.

Mass rates of the reactions P_k, $k = 3, \ldots, 6$ are calculated by using the following formulas

$$\begin{aligned} P_3 &= k_3 \rho c_1 e^{-\frac{E_3}{RT}}, P_4 = k_4 \rho c_2 e^{-\frac{E_4}{RT}}, \\ P_5 &= k_5 \rho c_3 e^{-\frac{E_5}{RT}}, P_6 = k_6 \rho c_4 e^{-\frac{E_6}{RT}}, \end{aligned}$$

where k_j, E_j, q_j - thermokinetic constants, λ and c_p coefficients are calculated for the gas mixture taking into consideration proportion of each component

$$\lambda = \sum_{k=1}^{7} \lambda_k c_k, \qquad c_p = \sum_{k=1}^{7} c_k c_{pk}.$$

Equation of continuity is relevant for the gas in gasifier channel

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0 \tag{4}$$

with initial data $\rho_0 = \rho_0(x, y, 0)$ where ρ_0 is a specified function, $(x, y) \in \Omega_2 \cup \Omega_4^1 \cup \Omega_4^2$.

As long as gas phase contains seven components, and each component has its own physical specifications, diffusion and transfer process is considered to be determined by individual convection-and-diffusion equation for each component:

$$\begin{gathered} \rho\left(\frac{\partial c_k}{\partial t} + u\frac{\partial c_k}{\partial x} + v\frac{\partial c_k}{\partial y}\right) = \frac{\partial}{\partial x}\left(\rho D_k \frac{\partial c_k}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho D_k \frac{\partial c_k}{\partial y}\right) + W_k, k = 1, ..., 6 \\ \sum_{k=1}^{7} c_k = 1. \end{gathered} \tag{5}$$

with initial conditions

$$\begin{gathered} c_1(x, y, 0) = c_1^0, c_2(x, y, 0) = c_2^0, c_3(x, y, 0) = c_3^0, c_4(x, y, 0) = c_4^0, \\ c_5(x, y, 0) = c_5^0, c_6(x, y, 0) = c_6^0, c_7(x, y, 0) = c_7^0, \end{gathered}$$

and boundary conditions

$$\begin{gathered} c_k\big|_{\Gamma_1} = c_{k1}(x, y, 0), c_k\big|_{\Gamma_5} = c_{k5}(x, y, 0), k = 1..6 \\ \frac{\partial c_k}{\partial y}\big|_{\Gamma_6} = \beta(c_k - c_k^{out}), k = 1..6 \\ \frac{\partial c_k}{\partial n}\big|_{\Gamma_2, \Gamma_3, \Gamma_4, \Gamma_7, \Gamma_8} = 0, k = 1..6, \end{gathered}$$

where c_{k1}, c_{k5}, $k = 1..6$ - specified functions of the proportions of the gas mixture k-element on the boundaries Γ_1 and Γ_5.
In this case, the formulas for W_k demand $P_1 = P_2 = s = 0$, $\varphi_3 = 1$ as Ω_2 is gas flow region.
For example, for methane $CH_4 : W_1 = \frac{\nu_{31}}{\nu_1}\frac{M_1}{M_y}P_1 - \varphi_3 P_3$,
For hydrogen $H_2 : W_2 = \frac{\nu_{32}}{\nu_1}\frac{M_2}{M_y}P_1 + \varphi_3(\frac{M_2}{M_3}P_6 - P_4) + s\frac{M_2}{M_c}R_4 = \varphi_3(\frac{M_2}{M_3}P_6 - P_4)$.

The following heterogeneous chemical reactions of carbon oxidizing and carbon monoxide reduction can take place during UCG process

$$\begin{gathered} (1)\, C + O_2 = CO_2 + q_{s1}, \qquad (2)\, C + \tfrac{1}{2}O_2 = CO + q_{s2}, \\ (3)\, C + CO_2 = 2CO + q_{s3}, \qquad (4)\, C + H2O = CO + H_2 + q_{s4}, \end{gathered}$$

taking into consideration corresponding absolute value of mass rates:

$$\begin{gathered} R_1 = \frac{M_c}{M_4} k_{s1} \rho_3 c_4 e^{-\frac{E_{s1}}{RT}}, \quad R_2 = \frac{M_c}{M_4} k_{s2} \rho_3 c_4 e^{-\frac{E_{s2}}{RT}} \\ R_3 = \frac{M_c}{M_4} k_{s1} \rho_3 c_5 e^{-\frac{E_{s3}}{RT}}, \quad R_4 = \frac{M_c}{M_4} k_{s2} \rho_3 c_6 e^{-\frac{E_{s3}}{RT}} \end{gathered} \tag{6}$$

Absolute values of mass rates of pyrolysis reaction - P_1 and moisture evaporation - P_2 are determined by the Arrhenius law and simplified Hertz-Knudsen law

$$P_i = k_i \rho_i \phi_i e^{-\frac{E_i}{RT}}, i = 1, 2, .$$

Mass rates of the W_k gas phase k-component changes are determined in the following way

$$\begin{aligned}
&CH_4 : W_1 = \tfrac{v_{31}}{v_1}\tfrac{M_1}{M_y} P_1 - \phi_3 P_3,\\
&H_2 : W_2 = \tfrac{v_{32}}{v_1}\tfrac{M_2}{M_y} P_1 + \phi_3 \left(\tfrac{M_2}{M_3} P_6 - P_4\right) + s\tfrac{M_2}{M_c} R_4,\\
&CO : W_3 = \tfrac{v_{33}}{v_1}\tfrac{M_3}{M_y} P_1 - \phi_3 (P_5 + P_6) + s\tfrac{M_3}{M_c} (R_2 + 2R_3 + R_4),\\
&O_2 : W_4 = -\phi_3 \left(2\tfrac{M_4}{M_1} P_3 + \tfrac{1}{2}\tfrac{M_4}{M_2} P_4 + \tfrac{1}{2}\tfrac{M_4}{M_3} P_5\right) - s\tfrac{M_4}{M_c} \left(R_1 + \tfrac{1}{2} R_2\right),\\
&CO_2 : W_5 = \tfrac{v_{35}}{v_1}\tfrac{M_5}{M_y} P_1 + \phi_3 \left(\tfrac{M_5}{M_1} P_3 + \tfrac{M_5}{M_3} P_5 + \tfrac{M_5}{M_3} P_6\right) + s\tfrac{M_5}{M_c} (R_1 - R_3),\\
&H_2O : W_6 = \tfrac{v_{36}}{v_1}\tfrac{M_6}{M_y} P_1 + P_2 + \phi_3 \left(2\tfrac{M_6}{M_1} P_3 + \tfrac{M_6}{M_3} P_4 - \tfrac{M_6}{M_3} P_6\right) - s\tfrac{M_6}{M_c} R_4,\\
&N_2 : W_7 = 0.
\end{aligned}$$

Combustion face form $f(x,t)$ is identified as the solution of nonlinear equation [8]

$$\rho_4 \frac{\partial f}{\partial t} - \sqrt{1 + \left(\frac{\partial f}{\partial x}\right)^2 \cdot \sum_{j=1}^{4} R_j} = 0 \tag{7}$$

with initial data $f\big|_{t=0} = f^0(x)$, where $f^0(x)$ - specified initial form of the combustion face, and the function R_j is calculated by the formula (6).

Consequently, the equation system (1)–(6) with corresponding initial and boundary conditions describes the processes in lateral fire well and combustion face. Numerical algorithm of the UCG problem is determined in accordance with the presented mathematical model. Firstly, the Cauchy problem is solved for the continuity equation (4) by using known values of velocities and specified initial data. Secondly, temperature propagation equations are solved (3). Thirdly, Navier-Stokes motion equations are solved after calculating the pressure value determined by state equation (2). As soon as all necessary flow state changes are determined at a new time step, changes of gas composition are calculated (5) and new state of mine face form is identified (7).

3 Results of the Numerical Experiments

This section is devoted to the results of the numerical experiments of nondimensionalized UCG mathematical model (1)–(6) (black coal and brown coal).

Numerical experiments are carried out in full accordance with common methods: calculations take into consideration progressively fine meshes and solutions' comparison, robustness test of numerical methods, solutions of the problems depending on various initial data, etc.

Unequally spaced mesh (as far as space variables are concerned) Ω_h with steps $h_{x_{ij}}$, $h_{y_{ij}}$ and constant time-step $\tau > 0$ is considered to be in the domains

$\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4^1 \cup \Omega_4^2$. N and M define number of points on the axis OX and OY respectively.

The Eqs. (1), (3)–(5) are approximated on Ω_h in a standard way [11] by using difference schemes. To solve continuity Eq. (4) the Lax-Wendroff-type scheme [11] with implicit viscosity is used. The system (1) and the Eq. (3), (5) are solved with the help of difference scheme of stabilizing correction with directional differences [12]. Viscosity coefficient μ as well as other coefficients use fractional gas composition of the previous time moment to solve all the equations. The equation of mine face form change is solved by the first approximation order scheme in the context of time and space.

Coefficient values μ_k, λ_k, c_{pk} for k-gas are mentioned in [13–15], and thermokinetic constants q_{3-6}, k_{3-6}, E_{3-6}, M_{3-6}, M_y, M_c are mentioned in [16–18]. Brown coal ash content is considered to be 30% that is similar to coal ash content in Moscow lignite basin [19]. Field observation results (mentioned in [20]) are considered to be input data for gas composition that is caused by coal thermal decomposition.

Comparison on a percentage base of rated gas composition to gas compositions described in different researches is presented further. Table 1 shows percentage composition of the gas calculated for uniform gasification process of bituminous coal and the in-situ measurements of gas composition, which are relevant for different coal-bearing basins [8,21]. Table 1 shows the intervals that limit test values of gas composition. The researches [8,21] show in-situ measurements (in the context of air blast) taken in Kuzbass Yuzhno-Abinskaya coalmine "Podzemgas". The column No3 shows real measurements taken by E .V. Kreinin, who is considered to be one of the principal UCG researchers and to spend much time on its analysis and development. He presents UCG engineering model in his paper [8]. His natural experiments are based on that model.

Table 1. The percentage of gas in the gasification of coal.

	1. Rated gas composition according to the model (1)–(7) %	2. Real gas composition (Yuzhno-Abinskaya station) [21] %	3. Gas composition according to Kreinin [8] %
CH_4	1.9	1.6–3.	2.6
H_2	10.6	10–15	12.5
CO	17.2	10–20	11.9
O_2	0.2	0.2	0.2
CO_2	10.9	8.0–14.5	13.2
N_2	59.1	53–63	59.5
Nonregistered impurity	0.1	0.1–0.5 0.01–0.02	0.1

Table 2 shows the comparison results of numerical calculations to in-situ measurements of brown coal. The research [20] presents a range of gas composition values taken in Moscow lignite basin and at Shatskay station. The table columns 2–3 show that different types of gas can be generated (in the context of brown coal) because of various coal characteristics in different basins. Calculation results based on laboratory data concerning coal decomposition show true burning processes registered in brown coal of different deposits.

Table 2. The percentage of gas in the gasification of drilling coal.

	1. Rated gas composition according to the model (1)–(7) %	2. Real gas composition (Podmoskovnaya and Shatskaya) [21] %	3. Gas composition according to Kreinin [8] %
CH_4	1.97	1.0–1.5	2.0
H_2	14.8	15–17	22.5
CO	9.7	5–7	4
O_2	0.2	0.3–0.5	0.4
CO_2	18.9	17–18	21.5
N_2	53.2	56–59	49.0
Nonregistered impurity	1.23	–	0.2

The presented calculations show that the underground gasifier model described is able to perform real UCG processes, which take place in both bituminous and brown coal mines and enables to get valid quantitative agreement with in-situ measurements.

The presented calculations show that the underground gasifier model described taking account of physical and chemical transformations and gasdynamics of thermally conductive compressible gas is able to perform real UCG processes flow method, which take place in both bituminous and brown coal mines and enables to get valid quantitative agreement with field measurements. Thus, the validation of the mathematical model carried out will allow the conducted experiments to determine the input parameters for the optimal operation of the gas generator.

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