

Article

The Prediction of Possibilities of CO Poisoning and Explosion during Syngas Leakage in the UCG Process

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Abstract: Underground coal gasification (UCG) is an industrial process that converts coal into product gas (syngas). This technology makes it possible to obtain energy without mining coal and post-processing. The UCG process is considered a safe technology with various advantages over conventional mining techniques. However, a small amount of potentially dangerous syngas may escape from the UCG cavity, and it is necessary to pay attention to the safety of the process in this respect. This article analyses the impact of a syngas leak from UCG on a possible CO poisoning and explosion hazard in the vulnerable zones. Measured data from experiments and proposed mathematical models were used for the analysis of the UCG process and simulation studies. It is mainly a mathematical model mixing of gases, which evaluated the danger of explosion and CO poisoning in sensitive zones. This model predicts the composition of the syngas mixture with air because this mixture can be dangerous at a certain concentration. Simulation studies focused mainly on CO poisoning in vulnerable areas based on the measured data from laboratory experiments. Simulation studies have shown that the critical value of CO poisoning can achieve with a certain composition of syngas and its escape into vulnerable areas. The results of the studies here indicate a possible hazard. However, by monitoring and control of UCG process, this risk can be minimized. Based on the obtained results, the control of the supply of fresh air to the endangered area during the monitoring of the syngas composition was proposed to prevent the occurrence of possible poisoning.

Keywords: underground coal gasification; mathematical model; explosion; CO poisoning; mixing of gases; control process; material balance



Citation: Laciak, M.; Durdán, M.; Kačur, J.; Flegner, P.; Benková, M. The Prediction of Possibilities of CO Poisoning and Explosion during Syngas Leakage in the UCG Process. *Processes* **2021**, *9*, 1912. <https://doi.org/10.3390/pr9111912>

Received: 25 August 2021

Accepted: 25 October 2021

Published: 26 October 2021

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1. Introduction

Coal is converted into syngas during the underground coal gasification process in the coal seam (i.e., in situ). The gas is produced and extracted by a well drilled into the gasified coal seam. The injection well is used to inject oxidants (i.e., air, oxygen, vapor, or their mixture). Production wells are used to transport the product gas to the earth's surface (see recovered gases in Figure 1) [1,2]. High-pressure gasification is carried out at a temperature of 700–900 °C, but under certain conditions, a temperature of up to 1500 °C can be achieved [2,3]. Finally, coal is decomposed and mainly produces carbon dioxide (CO₂), hydrogen (H₂), carbon monoxide (CO), small amounts of methane (CH₄), and hydrogen sulfide (H₂S) in the UCG process [3,4]. The UCG technology is not new; its history dates back more than 100 years, demonstrated in publications [5–7].

The choice of the UCG method depends on, e.g., the hydrogeological conditions of the coal seam and environment, the coal seam internal structure (i.e., thickness, continuous layer, intercalations, etc.), the structure and thickness of the overburden, and the type and properties of surrounding rocks and their changes after exploitation. Impermeable layers with low porosity and less deformation are most suitable because they prevent the leakage of dangerous substances (e.g., TOC-total organic carbon, BTEX-benzene, toluene,

ethylbenzene, xylene in tar) from the gasified coal seam to the surrounding rock layers [8,9]. Various technical problems and risks to the environment can occur when the UCG process is realized [10]. Fracturing and cracks are created in the gasified coal seam and surrounding rocks during underground coal cavity formation. The localization of microseismic sources in the rock mass structure can provide the basis for determining the potential areas of rock mass instability and rockburst in the underground mining. In addition to monitoring sensors, there are various methods for determining cracks in the rock mass [11–13]. This localization is also very important in terms of syngas leakage from UCG process. Also, operational conditions influence the evolution of these defects, as stated by Su et al. [14]. This method can create danger by generating liquid and gas gasification products such as CO, CO₂, H₂, and CH₄ [15]. Measurement results showed that over time, the dislodging effect of the coal seams based on the thermal explosion is gradually improved, the temperature rate is raised quickens, and the temperature gradient of the coal deposit is continuously decreased [16]. Usually, investors do not pay enough attention to environmental risks affecting the atmosphere, groundwater, working space, etc. [17]. The whole world is currently facing the challenge of minimizing the negative impacts of the UCG process on the environment while increasing the safety and health of operating personnel. That requirement must correspond to the goal of producing gas with the highest possible calorific value. Due to these requirements, many algorithms and methods are being developed by researchers around the world for the UCG process examination. These are, for example, methods for reducing the production of carbon dioxide (i.e., CO₂) or depositing its excess in an underground cavity describe McInnis et al. [18]. Hower et al. [19] described ways of observing accompanying phenomena (e.g., temperature changes), which can lead to fires in coal mines and subsequently to explosions. Tokarz et al. [20] studied methods for mitigating the risk of contaminants migration outside a georeactor zone in emergencies by using reactive materials in the underground coal gasification. Prodan et al. [21] showed that mathematical and geostatistical methods for reducing hazards and explosion risks of the UCG process by determining the methane content are of great importance, mainly in the preliminary stage. Great attention is focused on the development of methods that deal with the conditions of thermal explosion in the UCG process. Molayemat et al. [22] showed in their study that the methane content can be calculated by a multivariate adaptive regression splines (i.e., MARS) model based on data as seam depth, thickness, and ash content. The fault tree methodology for determining main factors that may lead to the explosion using calculations based on the Le Chatelier formula to evaluate the risk level of explosion for the gas mixture and determine the minimum level of oxygen in the mixture necessary to initiate an explosion describe Krause et al. [23]. Yang et al. [24] describe the model test method of the thermal explosion of oxygen-steam underground coal gasification to investigate the changing characteristics of the temperature field in a georeactor. The process of the relationships between the moving velocity of the flameworking face and the time interval for a thermal explosion was examined in Yang et al. [25]. Obileke et al. [26] describe to develop and validate a mathematical model for predicting methane production in an underground biogas digester. The developed model can predict methane gas production as a separate entity differing from other models.

The lack of control of the parameters controlling the UCG process and the effects of host rock behavior makes cavity formation in space and time difficult to predict. One of the consequences is the transmission problem generated in the overburden (i.e., gas components, chemical species, etc.). The pore diameter and tortuosity have an essential role in transferring gaseous contaminants through surrounding rocks [27,28]. These characteristics affect the risk of explosion or poisoning in the vulnerable area due to gas leakage through the porous layers. These risks are the subject of extensive research to determine their potential occurrence and reduce their impact. The unexpected leak of methane from the excavation has been investigated, where mixing methane with fresh air caused a gas explosion [29,30]. It has been found that this leak may occur from the methane drainage system or pipelines of devices. The minimum content of oxygen in the mixture to initiate

an explosion was also analyzed [31]. The results showed that an explosion might occur in the area where gas may leak from the in-situ reactor.

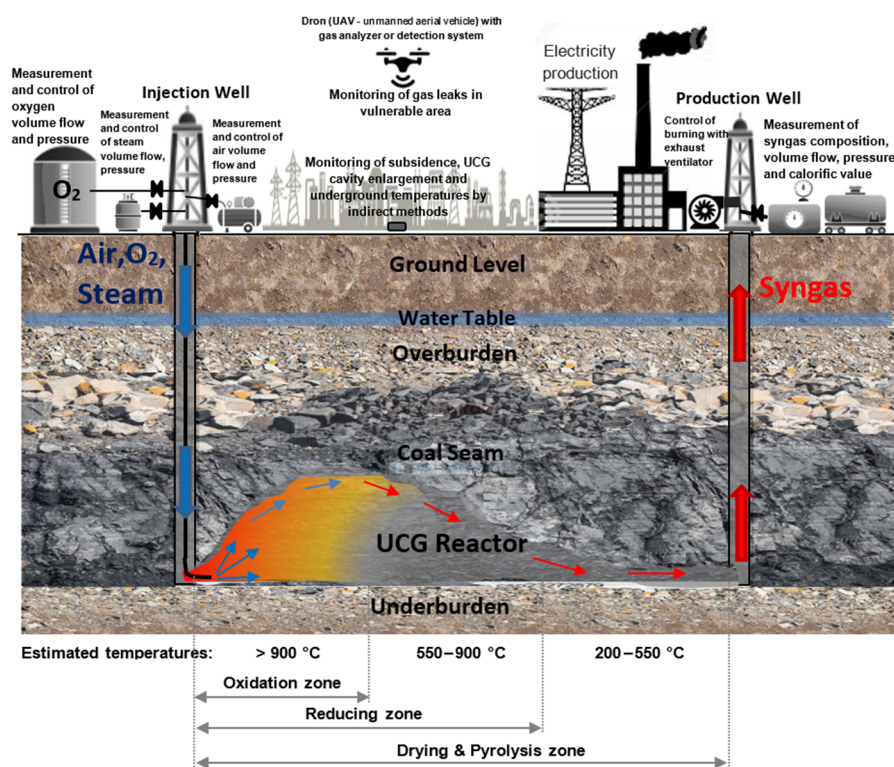


Figure 1. Principle of the UCG process.

Nowadays, numerical models are widely used to simulate processes of extraction and processing raw materials, including the UCG process. A thermal-mechanical numerical model for examining thermal impacts of the UCG process on the surrounding rock (e.g., the degradation of their mechanical properties) [32,33]. There are many physical processes occurring during in situ combustion, including multi-phase flow, heat and mass transfer, chemical reactions in porous media, and geomechanics. A key tool in analyzing and optimizing the technologies involves using numerical models to simulate the processes. Perkins [32] presents a brief review of mathematical modeling of in situ combustion and gasification with an emphasis on developing a generalized framework. Ekrieligoda et al. [33] presents details of a numerical model that was developed to analyze several key features that take place during the process of underground coal gasification. The model was developed based on the UCG trial site at the Wieczorek mine in Poland. Using a thermodynamics model, which minimizes Gibbs energy, is possible on based inputs such as e.g., weight and composition of coal, amount oxidizers, to determine syngas composition [34,35]. The model accounts for 44 species in the product which also includes solid carbon and sulfur. The result of the gasification model is presented in terms of the equilibrium composition of product gases with the inclusion of minor.

Based on the above, it is evident that the implementation of the UCG is associated with various problems such as the formation of cracks in the coal seam and its surroundings, which can cause gas leakage into vulnerable areas and cause CO poisoning or explosion. CO poisoning can occur in the UCG process since the output of this process is syngas with a relatively high CO content. Carbon monoxide (CO) is a colorless, odorless, nonirritant gas that accounts for numerous cases of CO poisoning every year from a variety of sources of incomplete combustion of hydrocarbons. Once CO is inhaled it binds with hemoglobin to form carboxyhemoglobin (COHb) with an affinity 200 times greater than oxygen, leading to decreased oxygen-carrying capacity and decreased release of oxygen to tissues leading

to tissue hypoxia [36,37]. Due to the complexity of this process, it is still possible to develop new approaches to reduce the risk in implementing this process. One of the possibilities is the use of mathematical and simulation models based on physical laws.

This article focused on the UCG process on the environment and process safety by proposing a mathematical model to predict the harmful effects of gases leaking from a gasified coal seam into vulnerable areas. The task of the proposed model is to predict the time in which a gas poisoning or explosion will occur if the set limit values in the monitored area are exceeded. This information enables the regulation of the air in vulnerable areas or will enable the timely evacuation of endangered personnel. Data from four experiments performed on a laboratory gasifier (i.e., ex-situ reactor) were used to test the proposed model. The individual experiments differed in the proposed physical model, which represented different hydrogeological conditions of the coal seam using the proposed insulating materials. It was used to investigate the leakage of syngas through the coal seam and its surroundings into vulnerable areas respectively outside the ex-situ generator.

The amount of leaking gas was determined by the material balance model. An algorithm for predicting dangerous side effects was built using the gas mixing model. Based on information about the critical time for possible CO poisoning, the control system of fresh air supply to the vulnerable area (underground or on the surface) has been proposed. The proposed control using a mathematical model is an innovative solution to increase the safety of the UCG process.

2. Materials and Methods

2.1. Experiments

For the analysis of simulation studies, we used experiments of the UCG process in laboratory conditions. The experiments were performed in an ex-situ generator (see Figure 2). The ex-situ reactor vessel is semi-cylindrical and consists of a forehead (front and rear) and a vessel body. Its length is 3.14 m, width 1.14 m, and height 0.5 m (see Figure 2b). The isolation of 0.1 m thick is placed on the inner surface of the generator vessel, and it is covered cover steel plate. There are three holes in the inlet of the generator vessel. The first hole serves as an input for the oxidizer. The second is for igniting the coal at the beginning of the experiment, and the third serves to discharge the condensed tar during the experiment. At the vessel's outlet, there is a hole for the syngas outlet, in which a sliding probe for gas extraction is located.

Four experiments were performed in the generator, which differed from each other by the physical model of the coal seam and the amount of gasified coal. The coal seam model was created by coal blocks or broken (split) brown coal from the Cigel mine, Slovakia. Within the research project, we analyzed and researched UCG process at different variants of the coal seam model. Overburden and underburden rocks were modeled by a mixture of gravel and water glass. Isolation materials (i.e., Sibril and Nobasil) were used to prevent heat leaking. These components were embedded in ex-situ generator before the experimental gasification. The physical model for the first experiment was split coal with a total coal weight of 521 kg (see Figure 3a). In the second experiment, coal cubes with a total weight of 532 kg were used (see Figure 3b). In the third and fourth experiments, the physical model of the coal seam was the same (see Figure 3c). However, experiments differed in the weight of the coal. In the third experiment, the weight of coal was 214 kg, and in the fourth experiment, it was 472 kg. Table 1 shows the analysis of input coal (coal from the Cigel mine) and unburned coal. As gasification agent was used air, oxygen, or a mixture of air and oxygen [38].

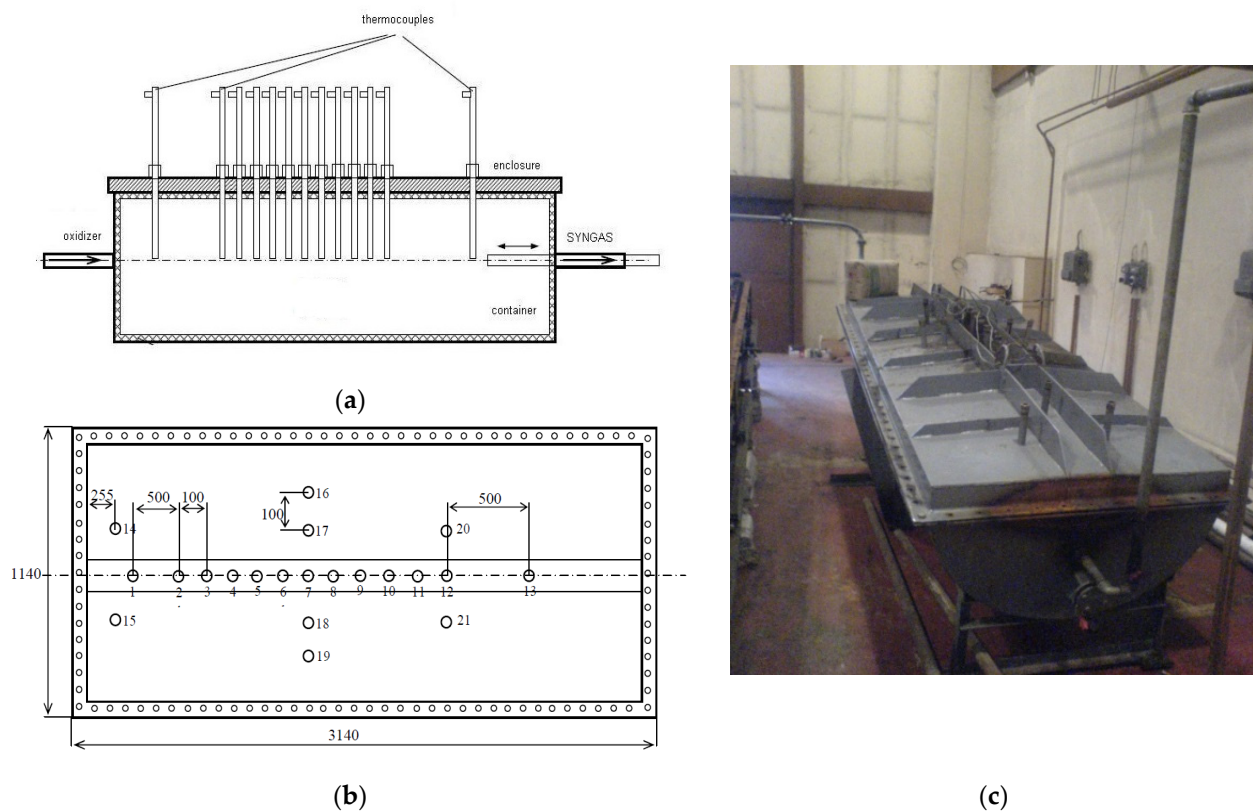


Figure 2. Scheme (a), parameters top view (b), and real view (c) of UCG generator (ex-situ reactor).

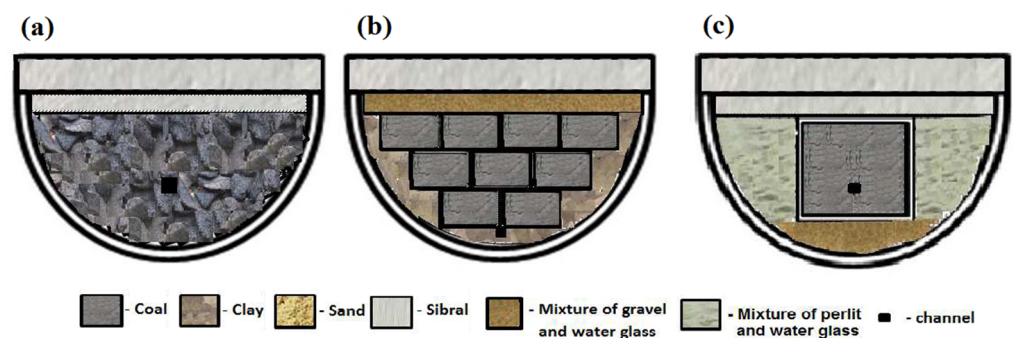


Figure 3. Physical coal seam model for the (a) experiment #1, (b) experiment #2, (c) experiments #3 and #4.

Table 1. The analysis of the input and unburned coal.

	Moisture (%)	Ash (%)	C (%)	H (%)	N (%)	O (%)	S (%)
input coal	20.4	24.1	35.9	3.1	0.6	15	0.9
unburned coal	0	30.4	45.1	3.9	0.7	18.8	1.1

The percentages of the CO, CO₂, H₂, and CH₄ components in the syngas during the experiment are shown in Figure 4. These components were determined from syngas by the analyzer. The time length of each experiment varied. For example, the first and the fourth experiments lasted approximately 70 h, the third experiment lasted about 170 h, and the second experiment lasted the longest, around 200 h. The maximal value of CO was measured in the third experiment (approx. 30%), the maximal value of H₂ was in the

third experiment (approx. 30%), and the maximal value of CH_4 in the fourth experiment (approx. 25%).

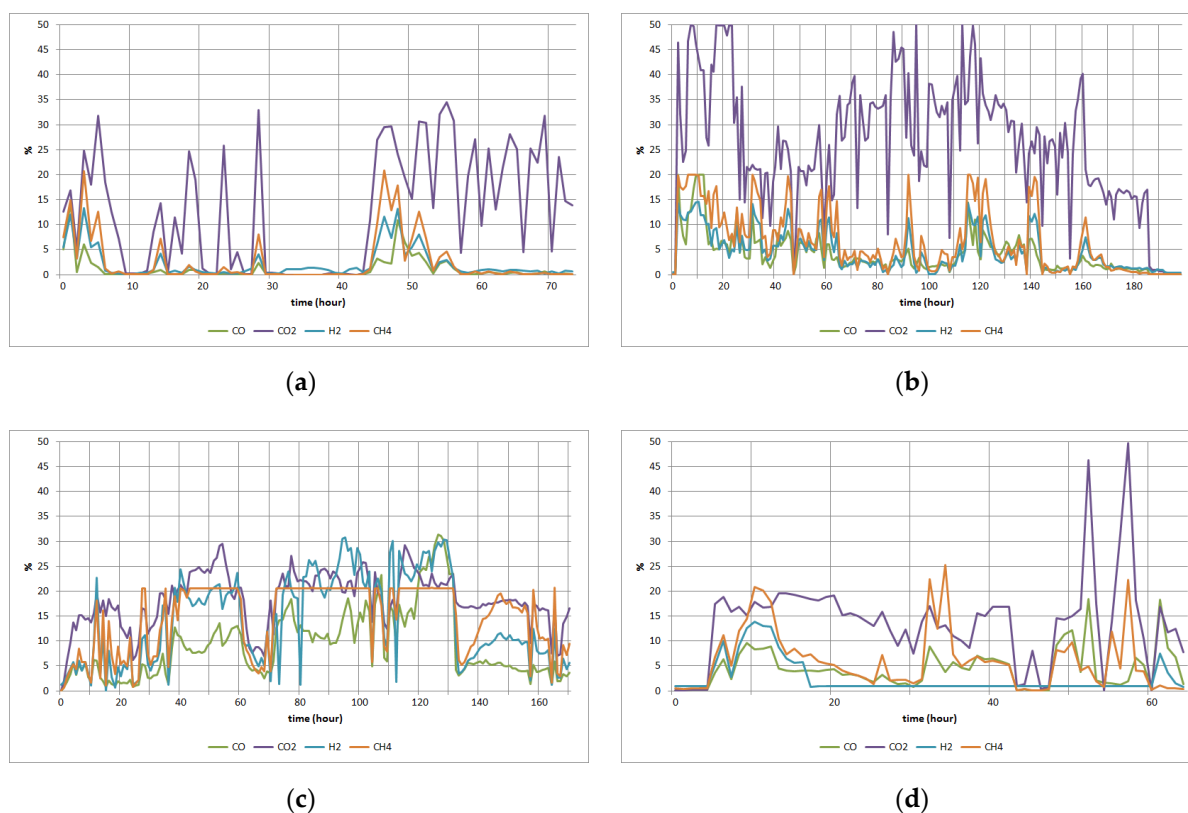


Figure 4. The behavior of %CO, %CO₂, %H₂, %CH₄ in syngas during experiments for the (a) experiment #1, (b) experiment #2, (c) experiment #3, (d) experiment #4.

Figure 5 shows the behaviors of the volume flow of the produced syngas. The volume flow values were in the range of 4–10 m³ per hour during the experiment. At the beginning of the experiments, they were higher due to the higher amount of input oxidizers (ignition of coal and reaching temperatures of about 900–1000 °C, almost zero leaks of syngas out of the ex-situ generator).

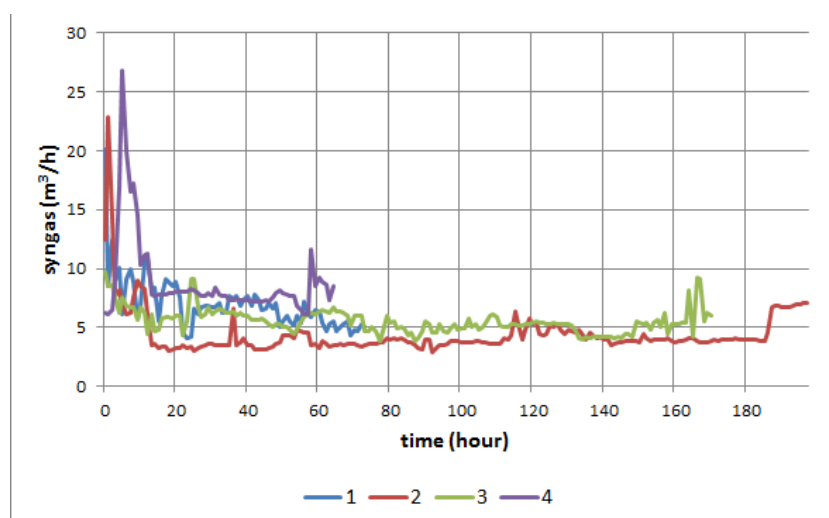


Figure 5. The volume flow of syngas for individual experiments.

2.2. Theoretical Background

Two mathematical models were used to analyze the possibility of CO poisoning and explosion in the UCG process. The first is the material balance model in the UCG process, which provides us with information about the expected syngas leaking from the generator during gasification. The second model is a mathematical model for the mixing of gases. Thus, it is possible to predict the violation of the limits of dangerous components of syngas for CO poisoning or explosion.

2.2.1. The Mathematical Model of Material Balance for UCG Process

The mathematical model of material balance is based on the assumption of conservation of mass in the UCG process. The mathematical model aims to calculate mass flow by accounting for material flow entering (input) and leaving (output) a system (ex-situ reactor). The inputs in the process in term of material flow are coal and oxidants (i.e., a mixture of air and oxygen). The outputs from the process are syngas, ash, condensate, and unburned coal. Thus, the mathematical model of general mass balance in the overall UCG process can be written as follows:

$$G_{coal} + G_{air} + G_{oxygen} = G_{coalunburn} + G_{ash} + G_{syngas} + G_{condensate} \quad (1)$$

where G_{coal} is the mass of input coal (kg), G_{air} is the mass of air (kg), G_{oxygen} is the mass of oxygen (kg), $G_{coalunburn}$ is the mass of unburned coal (kg), G_{ash} is the mass of ash (kg), G_{syngas} is the mass of product gas (kg), and $G_{condensate}$ is the mass of condensate (kg) [38–41].

Applying the material balance model to the UCG process and using data from experiments makes it possible to determine losses respectively syngas leak during coal gasification according to Equation (2).

$$G_{x,losses} = \sum_{i=1}^m G_{x,input_i} - \sum_{j=1}^n G_{x,output_j} \quad (2)$$

where $G_{x,losses}$ is the losses of the x -th chemical element, $G_{x,input_i}$ is the mass of the x -th chemical element (i.e., C, H, N, O, and S) in the individual input materials (kg), and $G_{x,output_j}$ is the mass of the x -th chemical element (i.e., C, H, N, O, and S) in the individual output materials (kg).

2.2.2. The Mathematical Model for Mixing of Gasses

The proposed model (3) predicts gas composition in a closed space. At each time period, the model calculates the composition of the gas (CO, CH₄, H₂, CO₂, N₂, and O₂) in enclosed space based on the volume flow of input and output gas. The detailed mathematical description of the model (3) can be found in [42].

$$\begin{aligned} \frac{dX(1)}{d\tau} &= (Q_{IN} \cdot X_{IN}(1) - Q_{OUT} \cdot X(1)) \cdot \frac{1}{V} \\ \frac{dX(2)}{d\tau} &= (Q_{IN} \cdot X_{IN}(2) - Q_{OUT} \cdot X(2)) \cdot \frac{1}{V} \\ &\vdots \\ \frac{dX(n)}{d\tau} &= (Q_{IN} \cdot X_{IN}(n) - Q_{OUT} \cdot X(n)) \cdot \frac{1}{V} \end{aligned} \quad (3)$$

Initial conditions ($\tau = 0$):

$$\begin{aligned} X(1)_{\tau 0} &= 0, X(2)_{\tau 0} = 0, X(3)_{\tau 0} = 0, X(4)_{\tau 0} = 0, X(5)_{\tau 0} = 79, X(6)_{\tau 0} = 21 \\ Q_{IN} &= 0 \end{aligned}$$

where $X(1)$ is the concentration of the first component of the internal gas element, $X_{IN}(1)$ is the concentration of the first component of inlet gas, $X(n)$ is the concentration of the n -th component of the internal gas element, $X_{IN}(n)$ is the concentration of the n -th component of inlet gas, Q_{IN} is the volume flow of the input gas, Q_{OUT} is the volume flow of the output gas, and V is the volume of element, $X_{IN}(\text{CO}, \text{CH}_4, \text{H}_2, \text{CO}_2, \text{N}_2, \text{O}_2)$.

The using of the proposed model in UCG process can be for CO poisoning prediction and the possibility of the explosion estimation.

3. Results

Simulation analyzes were performed using the above two mathematical models on data obtained from four laboratory experiments. We focused on predicting undesirable effects of the UCG process, such as explosion and CO poisoning in areas with possible access to syngas leaking from this process. Simulation studies for an explosion and CO poisoning were investigated for vulnerability areas, i.e., mining shafts or populated areas near the UCG process. In the first step, we determined losses (syngas leak) during the experiment using the mathematical model of material balance (3). Subsequently, the possible impacts were simulated with respect to the possibility of explosion and CO poisoning in individual experiments for the calculated syngas leak from individual experiments. The last part of this analysis is the proposal of a model for predicting the critical time for CO poisoning in areas where the gas leak may occur.

3.1. Results of the Model of Material Balance

The model of material balance was verified in the experiments in laboratory conditions. Results were published in the paper [38]. Based on the measurements from the experiments, the losses during the experiments were calculated using the material balance model (1)–(3). The losses (syngas leak) from the generator can be through generator leaks (i.e., between generator vessel and cover steel plate, through a hole for syngas outlet, through-holes for thermocouples in the cover of the generator). The results of the material balance model are shown in Table 2. The most significant losses or syngas leak were in experiment 1, namely 15.4%, and the smallest in experiment 2, namely 7.9%. The more significant losses (experiments 1 and 4) can be caused by a type of gasified coal (i.e., the broken coal was gasified at the first experiment) and modeled overburden in ex-situ reactor. The broken coal caused the gasification agent and syngas to leak from the gasified channel through the coal seam, and the overburden cracked under the influence of high temperatures.

Table 2. Material balance for four experiments.

Entering Material (kg)								Leaving Material (kg)		Losses/Syngas Leak
exp.	G_{coal}	G_{air}	G_{oxygen}	$G_{unburncoal}$	G_{ash}	G_{gas}	$G_{condensate}$	G_{losses} (kg)	G_{losses} (%)	
1	521	1504	21	167	75	1403	85	316	15.4	
2	532	903	130	32	119	1238	53	123	7.9	
3	214	1179	129	0	52	1285	11	174	11.4	
4	472	1946	130	66	94	2001	11	376	14.8	

3.2. Simulation Study for an Explosion

The impact of gaseous components in terms of the explosion was examined at a syngas leak, which was calculated by the model of material balance (see Table 2) for each experiment. The gaseous components with the critical values when the explosion can occur are: H_2 —4%, CH_4 —5%, and CO —12.5% [43,44].

The simulations were performed by the model of mixing gasses for the individual experiments. The concentration of the gaseous components obtained from experiments (see Figure 4) was considered as input to the simulations. The volume flow of leaking syngas to the area was calculated by losses and volume flow of syngas from the ex-situ reactor (see Figure 5). The input volume flow of fresh air to the area (i.e., vulnerability space) was set at 25 m³/h. Simulation studies showed that not even one experiment achieved a concentration that could cause an explosion. The highest concentration of dangerous gaseous components was achieved in the third experiment (see Figure 6a). Even when the volume flow of fresh air was minimized to 1 m³/h, the limits of explosive components were not violated above the limit values (see Figure 6b).

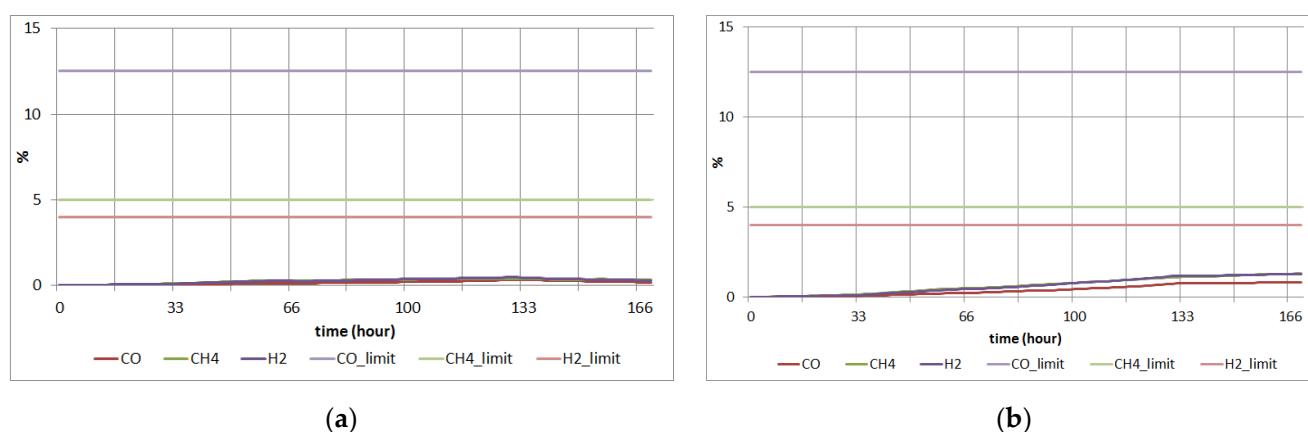


Figure 6. The simulation results of potential explosion at gas leak for the experiment #3 (a) volume flow of fresh 25m³/h (b) volume flow of fresh 1m³/h.

3.3. Simulation Study for CO Poisoning

The impact of CO in terms of the possible poisoning was also examined from the syngas leak obtained by the material balance model. The first critical value is 0.1% of CO which leads to death after 2 h [45,46]. Also, in this case, the computer simulations were performed by the gas mixing simulation model for individual experiments. The volume of the space (vulnerability areas) in which the leaking syngas is mixed with air is 1000 m³ and the volume flow of fresh air to this space is 25 m³/h. The simulation results for individual experiments are shown in Figure 7. In the first and second experiments, the limit for CO poisoning (i.e., 0.1% CO) was not violated. The third experiment was exceeded the critical value of CO in the 50th hour of the experiment (see Figure 7c), and in the fourth experiment, it was in the 12th hour of the experiment (see Figure 7d). It is due to the higher CO content in the produced syngas in these experiments. In the third experiment, the maximum value of CO content in the syngas is at the level of 30% CO (see Figure 4c). In the fourth experiment, the maximum value of CO content in the syngas is 18% (see Figure 4d). Average values of CO content in the syngas are following: 1.16% CO for the first experiment, 3.98% CO for the second experiment, 9.06% CO for the third experiment, and 4.47% CO for the fourth experiment. Average values are similar at the second and fourth experiments, but the syngas leak is more significant for the fourth experiment (see Table 2). The critical value of CO poisoning was exceeded in the fourth experiment for this reason.

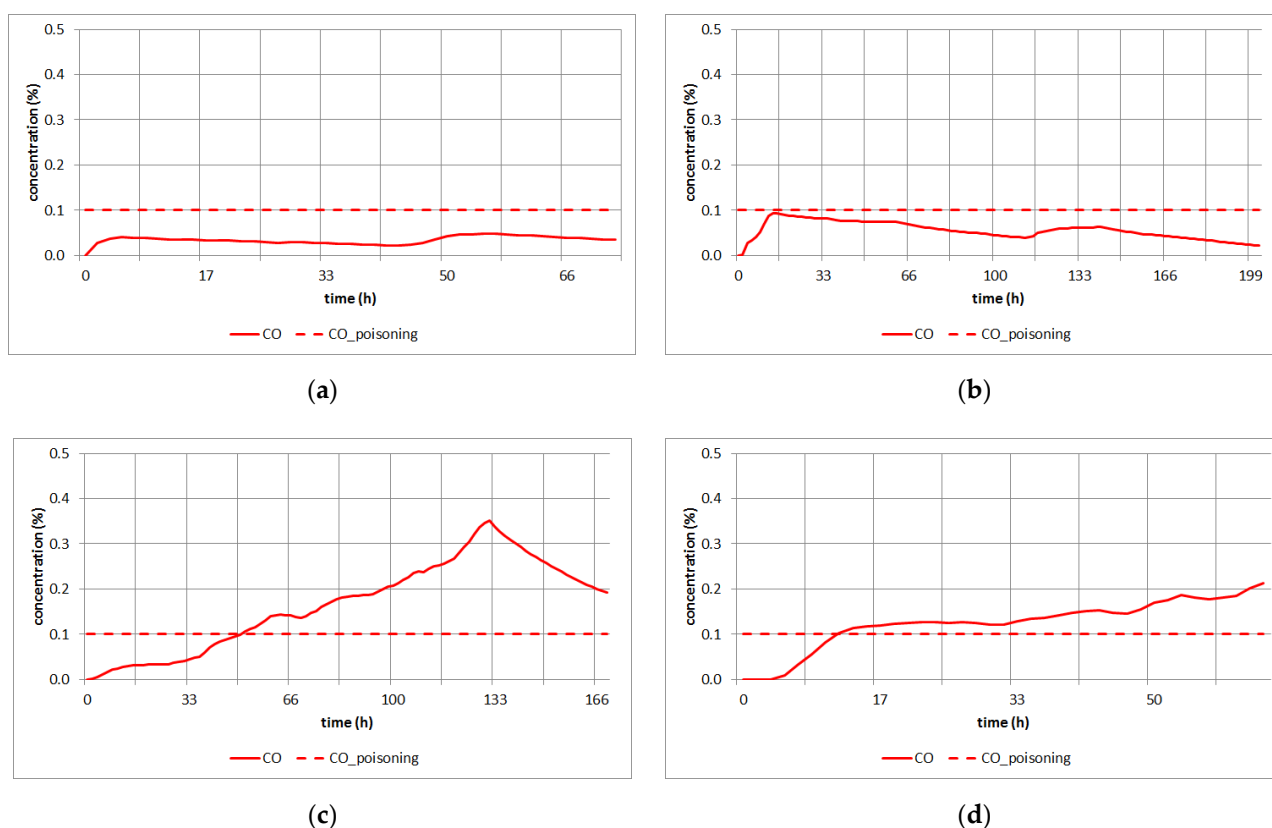


Figure 7. The impact of CO in terms of possible poisoning for the (a) experiment #1, (b) experiment #2, (c) experiment #3, and (d) experiment #4.

3.4. The Proposal of the Model for Prediction Critical Time of CO Poisoning

Safety is first in the UCG process, whether in an experimental generator or real conditions (in-situ reactor). The main product of this technology is syngas, which can be dangerous under certain conditions. For example, it can cause an explosion in the areas where the technology takes place or CO poisoning the personnel who provide it. For this reason, we focused on the proposal of the model and control of the UCG process to prevent the adverse effects of technology such as explosion and CO poisoning.

In terms of the results obtained from previous simulation studies, we focused on predicting the critical time for CO poisoning. This value determines how long it will take to reach the critical value of CO poisoning (0.1%) in a given space, with the expected leak and content of the syngas. Figure 8 shows the critical time ($t_{critical}$) behavior for the four experiments, which was calculated at each hour during the experiment based on the model for mixing gasses and syngas composition. This critical time was calculated from the actual syngas composition for the area (room) with a volume of 1000 m³. As shown in Figure 8a, in the first experiment, the lowest value of the critical time is at the beginning of the experiment and approximately at the 50th hour of the experiment, for 10 h. In the rest of the experiment, we can consider the experiment safe in terms of possible CO poisoning. It is similar in the second experiment also (see Figure 8b). For the third and fourth experiments (see Figure 8c,d) is the critical time in the second part of the experiments equal zero, which means that CO poisoning can occur immediately. It is also evident from the previous results of simulation studies shown in Figure 7, where it exceeded the limit for CO poisoning.

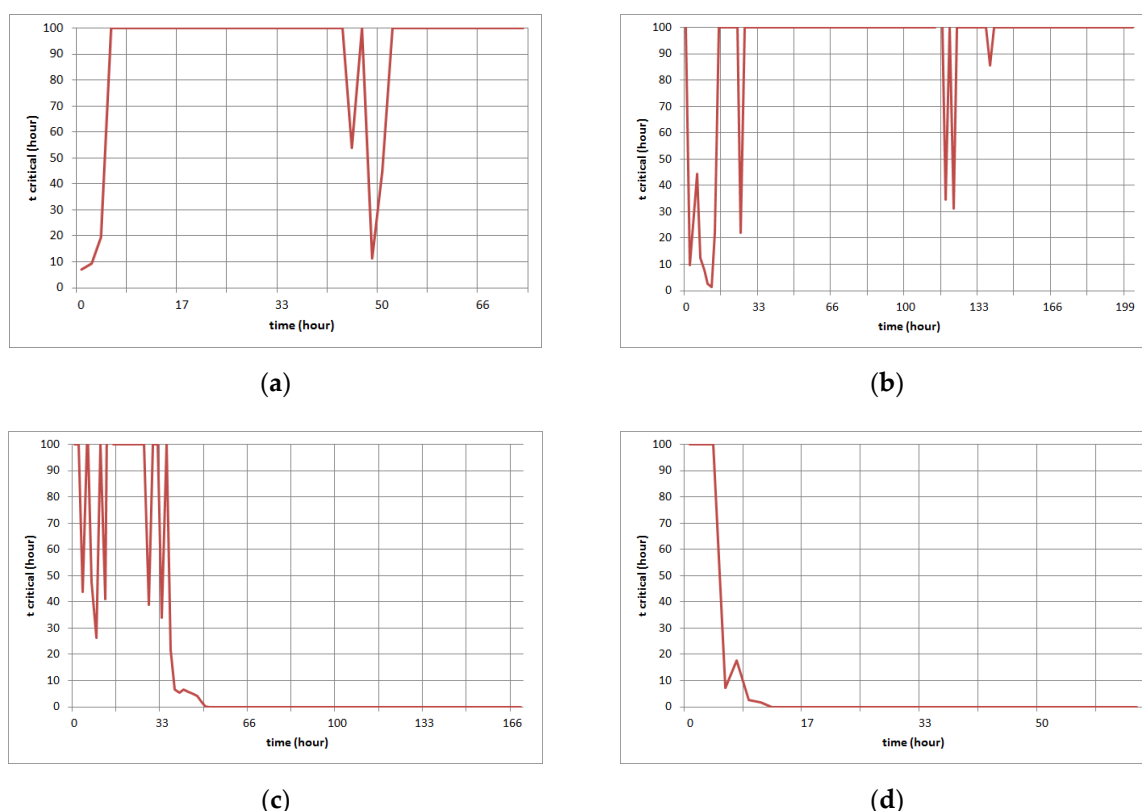


Figure 8. The critical time for the possibility of CO poisoning during experiment for the (a) experiment #1, (b) experiment #2, (c) experiment #3, and (d) experiment #4.

The proposal for the model, respectively the control of the UCG process based on the critical time for CO poisoning we have divided into two parts. In the first part, the so-called static model for determining the value of the critical time of CO poisoning, and in the second part of this proposal, it is a dynamic process control based on the analysis of the composition of the syngas using the supplied fresh air.

3.4.1. The Static Model for Prediction of the Critical Time of CO Poisoning

The basic inputs to the model for prediction of the critical time of CO poisoning include:

- The size (volume) of the space in which is mixed the leaking syngas from the UCG process with air,
- Percentage of leaking syngas,
- The volume flow of fresh air supplied to space.

The inputs to the static model for predicting the critical time of CO were based on the model of mixing gases (3). These inputs have in the mixing model the following form: the size (volume) of the space as the volume element, percentage of leaking syngas as the concentration of the components of inlet gas, the volume flow of fresh air supplied to space as the added amounts of oxygen and nitrogen to inlet gas.

Three mathematical models have been proposed to determine the critical time of CO poisoning based on the above input parameters. The models have the following structure:

$$t_{critical} = a_0 + a_1 V_{flow_{air}} + a_2 \% V_{leak_{syng}} \quad (4)$$

$$t_{critical} = a_0 + a_1 V_{space} + a_2 V_{flow_{air}} + a_3 \% V_{leak_{syng}} \quad (5)$$

$$t_{critical} = a_0 + a_1 V_{space} + a_2 V_{flow_{air}} + a_3 \% V_{leak_{syng}} + a_4 \frac{\% V_{leak_{syng}}}{V_{flow_{air}}} \quad (6)$$

where a_0, a_1, a_2, a_3, a_4 —parameters of the static model, V_{space} is the volume of space, $V_{flow_{air}}$ the volume flow of air supplied to space, and $\%V_{leak_{syng}}$ the leaking of syngas in% into space

The critical time of CO poisoning was calculated for different inputs using the model for mixing gases. Then, the parameters for these models were calculated by the least-squares method. The least-squares method is most often used to estimate the regression parameters of multiple linear regression models. Calculated parameters of the static model (see Table 3) show the influence of individual independent variables included in the model, namely force (size of the coefficient) and terms of type (direct/indirect dependence). These parameters for model no. 3 were calculated from inputs shown in Table 4. The critical time is the time during which the concentration of gas in the monitored space can occur, which causes CO poisoning. The composition of the leaking syngas was used from the fourth experiment, as this experiment was the worst in terms of the simulation results of the critical time for CO poisoning. Regression statistics of all static models are shown in Table 3. The correlation coefficient R is approximately the same for all three models, about 0.9, which confirms the relatively strong correlation between the inputs and the dependent variable. Using the multiple coefficient of determination R Square, we can calculate the share of the variability of the dependent variable $t_{critical}$, which the model expresses, i.e., a combination of selected independent variables used in the regression model. At best, it is equal to R Square = 1. Therefore, we can use the adjusted multiple coefficient of determination Adjusted R Square to consider the number of independent variables in the proposed linear regression model. The results of model no. 3 (6) are shown in Figure 9, where the critical time calculated by the gas mixing model (GMM) and the critical time calculated from the static model 3 (StM).

Table 3. Regression statistics and parameters of static models.

	Model 1 (6)	Model 2 (7)	Model 3 (8)
Multiple R	0.898	0.915	0.918
R Square	0.807	0.836	0.843
Adjusted R Square	0.751	0.755	0.717
Standard Error	6.969	5.706	6.127
a_0	80.910	61.847	59.006
a_1	−0.492	0.006	0.007
a_2	−3.656	−0.310	−0.177
a_3	—	−2.955	−3.165
a_4	—	—	1.890

Table 4. Inputs and output of static model no. 3 (6).

V_{space} (m ³)	$V_{flow_{air}}$ (m ³ /h)	$\%V_{leak_{syng}}$ (%)	$\frac{\%V_{leak_{syng}}}{V_{flow_{air}}}$	$t_{critical}$ (hour)
1000	25	15	0.60	15.24
900	22	10	0.45	30.62
800	20	8	0.40	36.50
700	15	20	1.33	0.47
600	10	15	1.50	16.80
1100	28	15	0.54	15.29
1200	30	15	0.50	15.57
1300	14	17	1.21	14.13
1400	20	14	0.70	22.29
500	5	20	4.00	5.88

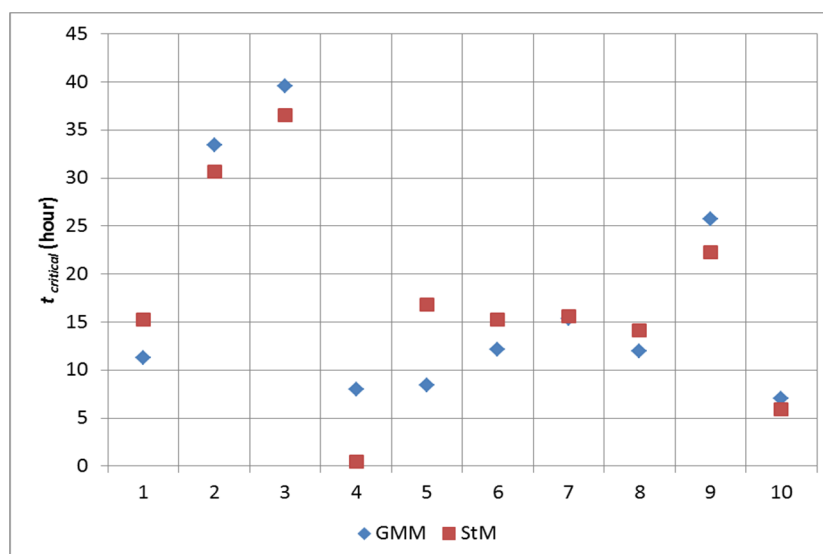


Figure 9. The critical time for CO poisoning calculated by static model no. 3.

The boundaries of the model are determined by the limits of model inputs (e.g., positive values, volume flow of air higher as zero for the third model), technological equipment (e.g., maximal power of the compressor). The model's output ($t_{critical}$) is not limited to the maximum in real conditions, but the maximal value of the model was set at 100 for simulation. It is important to monitor its minimal value. The critical time is the time during which the concentration of gas in the monitored space can occur, which can cause CO poisoning.

3.4.2. Dynamic Control of the Process as Prevention CO Poisoning in Vulnerability Zones

The proposed dynamic process control to prevent possible CO poisoning in the space into which the syngas can escape consists controlling the supply of fresh air to this space. The principle diagram of the control system is shown in Figure 10. The core of the control system is the control algorithm (see Figure 11), whose task is to set the airflow so that the CO limit in the vulnerable space is not exceeded. The control algorithm cooperates with the gas mixing model, the output of which is the critical time of CO poisoning based on which it is increased or reduced flow of fresh air into space.

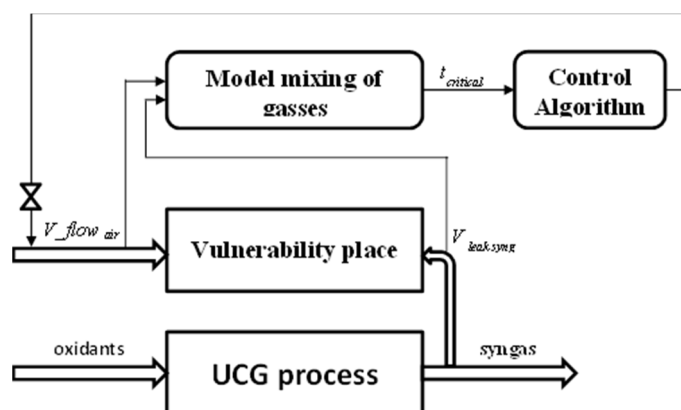


Figure 10. The principle diagram of the control process.

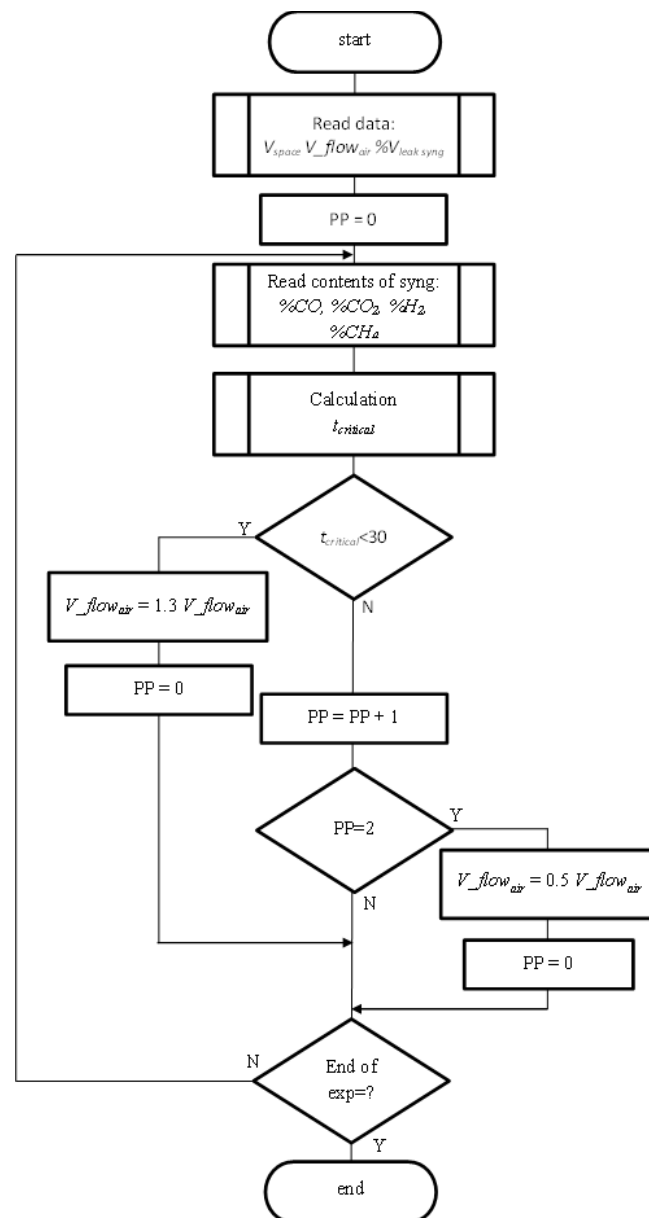


Figure 11. Control algorithm.

Figure 12 shows the behavior of CO after using the proposed control algorithm to prevent CO poisoning in a vulnerable place. Figure 12a shows the simulation results for the data from the third experiment and Figure 12b from the fourth experiment. For comparison, Figure 7c,d) show the behavior of CO without the proposed control (with a constant volume flow of air) for the third and fourth experiments.

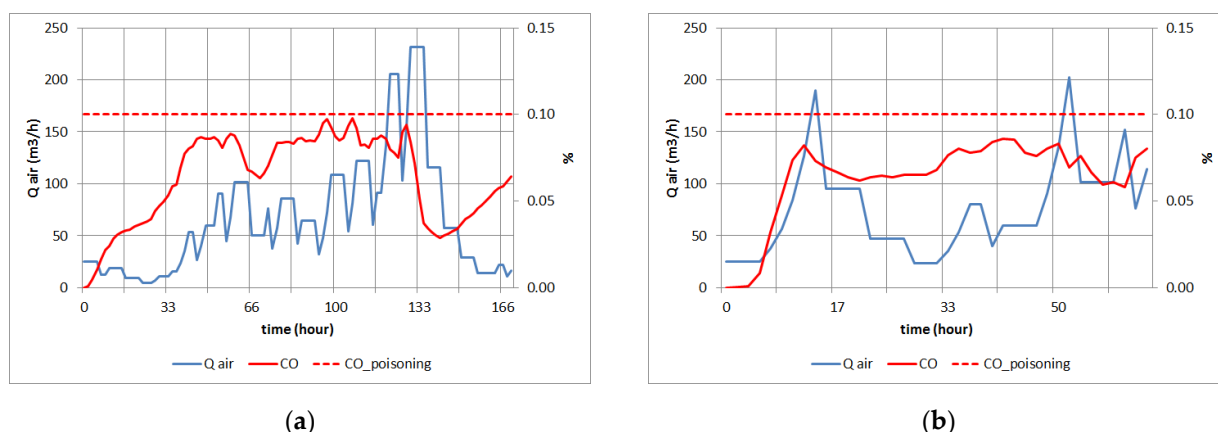


Figure 12. The behavior of CO with using control algorithm (a) experiment #3 (b) experiment #4.

4. Conclusions

The paper deals with the analysis of the UCG process in terms of negative impacts on the environment and process safety. The main product of UCG technology is gas (syngas), which must be safely brought to the surface using a production well. This gas can be dangerous under certain conditions (e.g., cracks in the rock mass, defect in the syngas pipe) and can cause an explosion in areas where the technology takes place or poisoning the personnel who provide it. The essential means for verifying safety in terms of possible gas explosion or CO poisoning was a mathematical model of mixing gases. The subject of the investigation of the syngas leak from the UCG process was a vulnerable area, i.e., mining shafts or populated areas near the UCG process. Data from four laboratory experiments were used for simulation studies and analysis. Based on the material balance of these experiments, we determined so-called losses or syngas leak during the experiment. The composition of syngas was also known from the experiments.

The performed simulation studies demonstrated that the explosive components didn't achieve limit values in any of the experiments in terms of the explosion. From this point of view, the process is safe. However, from the results of simulations focused on the possibility of CO poisoning in areas close to the UCG process, it can be seen that under certain conditions, a dangerous concentration of gas can occur in these areas. Important parameters by which we can influence the CO content in the vulnerable space include the volume flow of the supplied fresh air, the volume of the space into which the syngas can escape, the composition, and the volume flow of the syngas leaking. Based on these parameters, a static model was proposed and verified, which predicts the critical time of CO poisoning. The critical time is the time during which the concentration of gas in the monitored space can occur, which can cause CO poisoning. The task of this model is to determine the flow of the supplied air into the space in which the syngas leaking can mix with the air, at a known size of the space and the composition of the syngas. The second proposal for reducing the risk of CO poisoning is dynamic control of the process, the task of which is to set the flow of supplied air so that the limit of CO in the vulnerable space is not exceeded and the value of the critical time for CO poisoning was long as possible. Both proposed models could have practical significance as prevention against CO poisoning in vulnerability zones near to the real UCG process.

Author Contributions: Conceptualization, M.L. and M.D.; data curation, M.D.; formal analysis, P.F. and M.B.; methodology, J.K. and M.L.; software, M.L. and J.K.; project administration, M.L.; resources, M.D. and P.F.; supervision, M.D. and P.F.; validation, P.F. and J.K.; writing—original draft preparation, M.L. and M.D.; writing—review and editing M.D. and M.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by project COGAR RFCR-CT-2013-00002, Slovak Research and Development Agency under contracts No. APVV-18-0526 and No. APVV-14-0892. The APC was funded by APVV-18-0526.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: No new data were created or analyzed in this study. Data sharing is not applicable to this article.

Acknowledgments: This work was supported by the Slovak Research and Development Agency under contract No. APVV-18-0526 and APVV-14-0892.

Conflicts of Interest: The authors declare no conflict of interest.

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