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MODELLING OF UNDERGROUND COAL GASIFICATION PROCESS USING CFD METHODS

MODELOWANIE PROCESU PODZIEMNEGO ZGAZOWANIA WĘGLA KAMIENNEGO Z ZASTOSOWANIEM METOD CFD

The results of model studies involving numerical simulation of underground coal gasification process are presented. For the purpose of the study, the software of computational fluid dynamics (CFD) was selected for simulation of underground coal gasification. Based on the review of the literature, it was decided that ANSYS-Fluent will be used as software for the performance of model studies. The ANSYS--Fluent software was used for numerical calculations in order to identify the distribution of changes in the concentration of syngas components as a function of duration of coal gasification process. The nature of the calculations was predictive.

A geometric model has been developed based on construction data of the georeactor used during the researches in Experimental Mine "Barbara" and Coal Mine "Wieczorek" and it was prepared by generating a numerical grid. Data concerning the georeactor power supply method and the parameters maintained during the process used to define the numerical model. Some part of data was supplemented based on the literature sources.

The main assumption was to base the simulation of the georeactor operation on a mathematical models describing reactive fluid flow. Components of the process gas and the gasification agent move along the gasification channel and simulate physicochemical phenomena associated with the transfer of mass and energy as well as chemical reactions (together with the energy effect). Chemical reactions of the gasification process are based on a kinetic equation which determines the course of a particular type of equation of chemical coal gasification. The interaction of gas with the surrounding coal layer has also been described as a part of the model. The description concerned the transport of thermal energy. The coal seam and the mass rock are treated as a homogeneous body.

Modelling studies assumed the coal gasification process is carried out with the participation of separately oxygen and air as a gasification agent, under the specific conditions of the georeactor operations within the time interval of 100 hours and 305 hours. The results of the numerical solution have been compared with the results of experimental results under *in-situ* conditions.

Keywords: coal gasification, computational fluid dynamics, modelling, experiment

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Zaprezentowano wyniki badań modelowych polegających na numerycznej symulacji procesu podziemnego zgazowania węgla. Dla potrzeb realizowanej pracy dokonano wyboru oprogramowania wykorzystywanego do symulacji procesu podziemnego zgazowania węgla. Na podstawie przeglądu literatury zdecydowano, że oprogramowaniem, za pomocą, którego będą realizowane badania modelowe, będzie oprogramowanie informatyczne ANSYS-Fluent. Za jego pomocą przeprowadzano obliczenia numeryczne z zamiarem zidentyfikowania rozkładu zmian stężenia składników gazu procesowego w funkcji czasu trwania procesu zgazowania węgla. Przeprowadzone obliczenia miały charakter predykcji.

W oparciu o dane konstrukcyjne georeaktora stosowanego podczas badań na KD Barbara oraz KWK Wieczorek, opracowano model geometryczny oraz wykonano jego dyskretyzację poprzez wygenerowanie odpowiedniej siatki numerycznej w oparciu, o którą wykonywane są obliczenia. Dane dotyczące sposobu zasilania georeaktora oraz parametrów utrzymywanych podczas procesu wykorzystano do definiowania modelu numerycznego. Część danych została uzupełniona w oparciu o źródła literaturowe.

Głównym przyjętym założeniem było oparcie symulacji pracy georeaktora o modele opisujące reaktywny przepływ płynu. Składniki gazu procesowego oraz czynnik zgazowujący przemieszczają się wzdłuż kanału zgazowującego symulując zjawiska fizykochemiczne związane z transportem masy i energii oraz zachodzące reakcje chemiczne (wraz z efektem energetycznym). Chemizm procesu zgazowania oparto o równanie kinetyczne, które determinuje przebieg danego typu równania chemicznego zgazowania węgla. W ramach modelu opisano też interakcję gazu z otaczającą warstwą węgla. Opis ten dotyczył transportu energii cieplnej. Warstwę węgla oraz warstwy geologiczne otaczające georeaktor traktuje się jako ciało jednorodne.

Badania modelowe zakładały prowadzenie procesu zgazowania calizny węglowej przy udziale, osobno tlenu i powietrza, jako czynnika zgazowującego, w warunkach ustalonych pracy georeaktora w przedziale czasu 100 godzin i 305 godzin. Uzyskane wyniki rozwiązania numerycznego zestawiono z wynikami badań eksperymentalnych w warunkach *in-situ*.

Słowa kluczowe: zgazowanie węgla, numeryczna mechanika płynów, modelowanie, eksperyment

1. Introduction

Certain ecological effects are associated with the use of coal in the economy. Coal combustion for energy purposes is connected with emissions of large amounts of pollutants into the atmosphere (dust, carbon dioxide, nitrogen oxides, sulphur oxides). Environmental policy of the European Union assumes gradual limitation of emissions of these pollutants and it is particularly important in the countries where energy economy is based on coal. The direction releasing the environment of coal pollutants is to develop coal processing technologies which allow for limitation of its environmental impact. Coal gasification constitutes an example of such technology (*Clean Coal Technologies*, 2012; Społeczna Rada..., 2010).

Coal gasification is a complex sequence of thermochemical transformations taking place at elevated temperature between the organic part of the coal substance and the gasification agent such as oxygen, vapour, air or carbon dioxide. The aim of the process is to produce a synthetic gas which is widely used for industrial purposes. The composition and energy properties of the resulting gas are affected mainly by the gasification agent used and process parameters, such as: temperature and pressure (Smoliński, 2010; Rauk, 1981).

This process is currently carried out either in ground reactors (technologies of GE Energy/Texaco, Shell, SFG) or directly under the ground. Underground coal gasification (UCG) is an extremely complex process and it is not as well-known as gasification which has been carried out in ground reactors for years (Chmielniak et al., 2008; Younger, 2011).

Development of advanced industrial UCG technologies requires a thorough understanding of mechanisms which control the course of this process. Development of mathematical models describing the UCG process would be helpful in understanding the essence of it (Golec & Ilmurzyńska, 2008), thus a significant number of publications concerning partial process models can be found in the source literature, e.g. a pyrolysis model (Urych, 2014), cavity growth model (Nurzyńska et al., 2014; Sarraf et al., 2011; Perkins, 2005) as well as complex models of georeactor operations (Wachowicz et al., 2013; Seifi et al., 2011).

Particular difficulties during modelling of underground coal gasification process occur mainly due to the inability to clearly identify the characteristics of coal and gasification products. Depending on the type of coal and its resulting natural properties, the technological usefulness of coal to subject it to the gasification process is various. This is because the composition, mechanical and physicochemical properties of coal has a significant impact on the direction and reaction kinetics of the coal gasification process. A considerable amount of chemical compounds which are created during the process complicates the operations related to the development of the model, which induces to assume a number of simplifications and to determine basic chemical reactions and gasification products taken into account during the development of the model (Golec & Ilmurzyńska, 2008).

There are several ways of solving the problems concerning modelling of coal gasification process: equilibrium models, kinetic models, grain models (Cempa-Balewicz et al., 2013; Żogała, 2014). The equilibrium models allow determining the composition of gas and coal conversion degree, without the kinetic and diffusion effects. Kinetic models take into account the rate of selected reactions. The grain model takes into account the stages of penetration of gas reagents which penetrate into the external surface of the grain as well as diffusion of gas reagents in the structure of the porous grain, surface phenomena and transport of gas products outside the grain zone (Golec & Ilmurzyńska, 2008).

The current computational capabilities of modern computers, makes it possible to develop the numerical models (including the theory of fluid dynamics or Crip method). The authors of models often use software dedicated to this type of simulation as for example Ansys-Fluent package (Wachowicz et al., 2010) or Star package (Seifi & others, 2011). The result of the simulation includes a profile of concentration, temperature and pressure in the reactor with a predetermined geometry as well as the shape of the cavity. Therefore, these models are useful for optimization of georeactor operations.

The primary advantage of using numerical simulations to study complex physicochemical processes which include, without a doubt, the underground coal gasification, is the possibility to forecast selected parameters of the process. It provides valuable information at the stage of design of future underground coal gasification installations. The possibility to predict the variability of process parameters provides a valuable supplementation in the scientific and research approach (Perkins, 2005; Wachowicz et al., 2010, 2013).

2. Description of UCG experiments

The assumptions to the numerical simulation of the UCG process have been determined on the basis of two experiments: a half-technical method for underground coal gasification carried out in the Experimental Mine (EM) "Barbara" of the Central Mining Institute as well as a pilot method for underground coal gasification carried out in the Coal Mine "Wieczorek".

Underground coal gasification attempt carried out in EM "Barbara"

A coal gasification generator reflected a part of the coal seam about a thickness of 1.5 m with a "V-shaped" gasification channel about a diameter of 140 mm and length of 2×17.3 m. Details about the construction of the installation and process are presented in the publication (Wiatowski et al., 2012). In Figure 1 is shown a geometric interpretation of gasification channels and in Figure 2 is shown a geometric model of the coal seam.

The experiment was divided into three stages:

I. 0-190 h: ignition and achieving conditions of stable operation with air and oxygen as a mixture,

II. 190-355 h (165 h): stable operation of the georeactor with oxygen,

III. 355-1315 h: damping the georeactor and completion of the experiment with the participation of nitrogen.

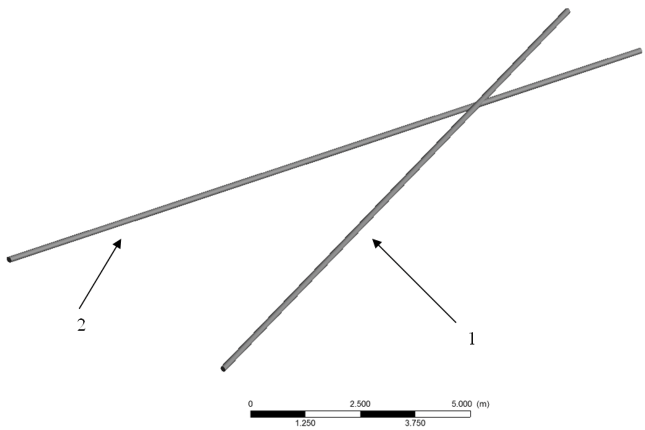


Fig. 1. View of a gasification channels: 1 – inlet gasification channel, 2 – outlet gasification channel

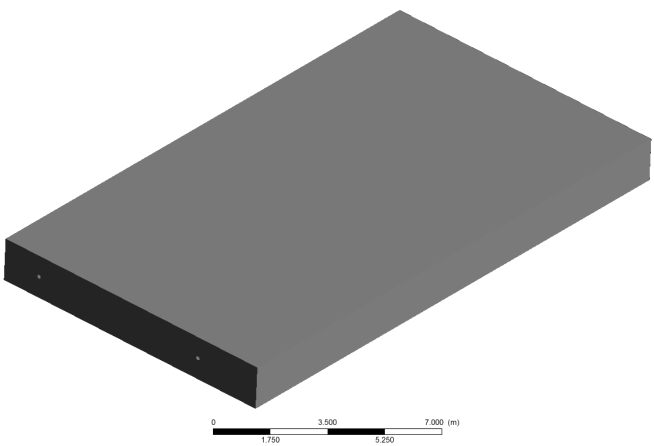


Fig. 2. View of coal seam

Underground coal gasification attempt carried out in Coal Mine "Wieczorek"

Coal gasification generator reflected a part of the coal seam 501 about a thickness of 5.0 m with a "V-shaped" gasification channel about a diameter of 200 mm (supply of the gasification agent) and 300 mm (output of gasification products), drilled in the mass rock and coal seam.

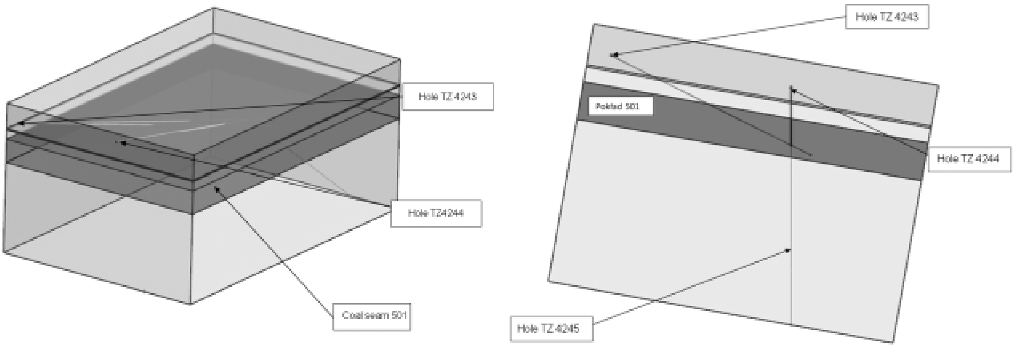


Fig. 3. View of the georeactor in the coal seam 501 of Coal Mine "Wieczorek"

The experiment was divided into several stages:

I. 0-193.5 h – ignition and the gasification with the participation of air and oxygen.
II. 193.5-336.5 h – hours – gasification with air,
III. 336.5-408 h – gasification with air and water,
IV. 408-888.5 h – gasification with air (including a technological break),
V. 336.5-408 h – gasification with air and carbon dioxide,
VI. 1008.5-1181.5 h – gasification with air.

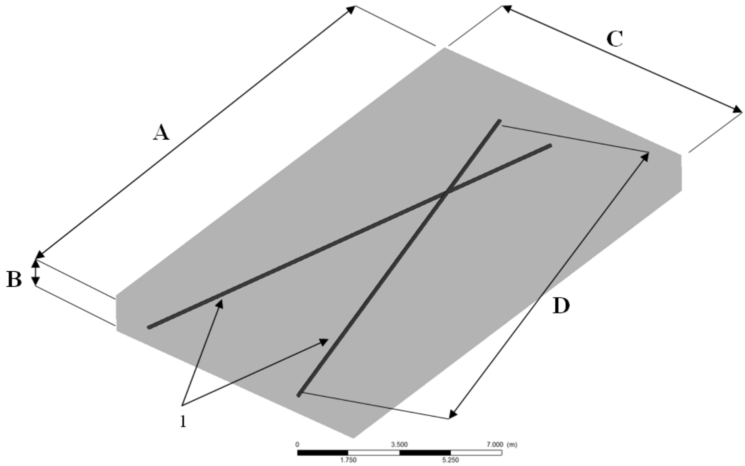
3. Numerical simulation

Based on data concerning the structure of the georeactor located within EM "Barbara" and Coal Mine "Wieczorek" and using Ansys-Fluent software, a numerical model was developed and discretized. A numerical grid was developed based on which a numerical simulation was carried out. Information about the georeactor supply method and parameters used during the real experiment was implemented into the software environment of Ansys-Fluent. Some part of data was supplemented based on the literature sources. The results of the numerical solution were compared with the experimental results.

A theoretical model of the georeactor was created based on the equations of fundamental chemical reactions which take place within the reaction space of the georeactor, taking into account the equations describing the kinetics of the process as well as equations of energy and mass transport which describe the processes occurring during coal gasification. The numerical analysis included a gasification channel model (fluid element) and coal seam model (porous medium). It was assumed that the numerical model will reflect the real experiment underground coal gasification. The final result of the model study is the identification of chemical composition of the synthesis gas at the outlet of the georeactor.

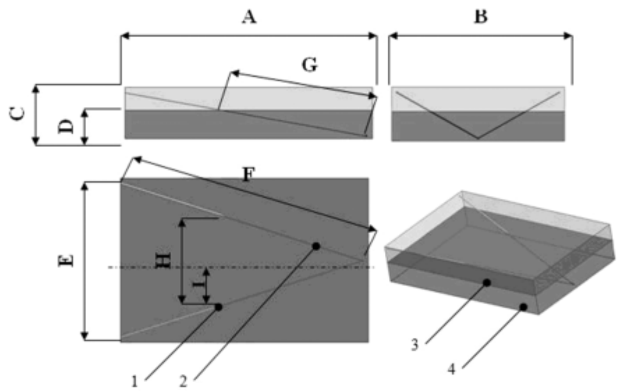
3.1. Geometry

A geometric interpretation of georeactor which constitute a reflection of real reactors (as specified in Chapter 2) is presented in Figure 4 and Figure 5. The geometric models will be used to define the area of the numerical solution of the analysed issue.



Lp.	A [m]	B [m]	C [m]	D [m]
1.	18.2	1.5	10.3	17.3

Fig. 4. The georeactor in EM "Barbara": 1 – gasification channel Ø140 mm



Lp.	A [m]	B [m]	C [m]	D [m]	E [m]	F [m]	G [m]	(F-G) [m]
1.	48	32	10	5.5	30	50	30	20

Fig. 5. The georeactor in the Coal Mine "Wieczorek": 1 – inlet channel Ø200 mm, 2 – outlet channel Ø300 mm, 3 – mass rock, 4 – coal seam

The presented models of the georeactor were developed in the order to predict the changes in concentration of the synthesis gas components, simulating particular conditions of coal gasification process in a certain period of time with the participation of oxygen (EM "Barbara") and air (Coal Mine "Wieczorek") as a gasification agent.

3.2. Numerical grid

Discretization area of the numerical solution, both for EM "Barbara" and Coal Mine "Wieczorek" includes a compilation of numerical grids presented in Figure 6 in the following form:

- a numerical grid of the gasification channel which reflects the reaction zone of the georeactor, formed of 8964 straight lines connected together in 12321 nodes (Fig. 6a),
- a numerical grid of the coal seam formed of 421283 straight lines connected with 75383 nodes, which is a reflection of the coal seam (Fig. 6b).

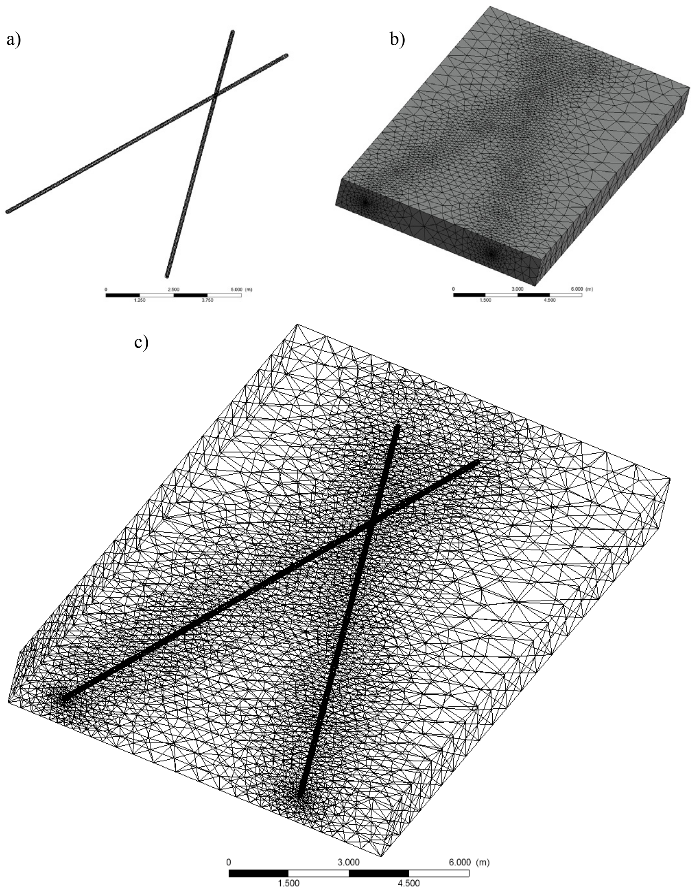


Fig. 6. The numerical grid of georeactor in EM "Barbara": a – the gasification channels, b – coal seam, c – a numerical grid of solution

The discretization area of the numerical solution shown in Figure 7 constitutes as follows:
- a numerical grid of the gasification channel which reflects the reaction zone of the georeactor, formed of 91046 straight lines connected together in 24584 nodes (Fig. 7a),
- a numerical grid of the coal seam formed of 124798 straight lines connected with 32261 nodes, which is a reflection of the coal seam (Fig. 7b).

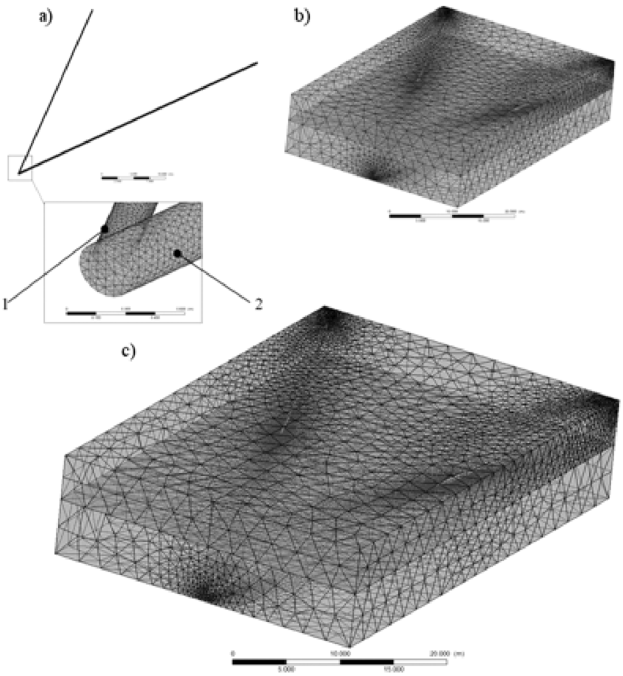


Fig. 7. The numerical grid of georeactor in Coal Mine "Wieczorek": a – a numerical grid of the gasification channels, b – a numerical grid of coal seam geometry, c – a numerical grid of solution

3.3. Chemical reactions

After determining the discretization area and coal gasification reactions, the next stage was to determine the initial conditions of the numerical solution. The following basic set of gasification chemical reactions for the analysed issue has been adopted for that purpose:

$$C + 0.5O_2 \xrightarrow{r_1} CO \tag{1}$$

$$C + O_2 \xrightarrow{r_2} CO_2 \tag{2}$$

$$C + H_2O \xrightarrow{r_2} CO + H_2 \tag{3}$$

$$C + 2H_2 \xrightarrow{r_4} CH_4 \tag{4}$$

$$CO_2 + H_2 \xrightarrow{r_5} CO + H_2O \quad (5)$$

$$CO + H_2O \xrightarrow{r_6} CO_2 + H_2 \quad (6)$$

The mechanism of the gasification process was expressed in form of the equation (Ansys, 2009):

$$k = AT^{\beta} e^{-E/RT} \quad (7)$$

where:

A — pre-exponential factor, [-],
T — temperature, [K],
β — temperature exponent, [-],
E — activation energy, [J kmol^{-1}],
R — universal gas constant, [J kmol^{-1} K^{-1}].

The parameter values adopted for the calculation of gasification reaction kinetics were listed respectively in Table 1.

TABLE 1

Parameters adopted for calculation of coal gasification chemical reactions

No.	Rate of reaction	EM "Barbara"			Coal Mine "Wieczorek"	
		β	A [1/s]	E [J/mol]	A [1/s]	E [J/mol]
1.	$^{**)}\, r_1 = k_1 \cdot C_{O2}$	0	0.89	$^{**)}\, 61.13 \cdot 10^{-3}$	0.89	$^{**)}\, 61.13 \cdot 10^{-3}$
2.	$^{**)}\, r_2 = k_2 \cdot C_{O2}$	0	0.84	$^{**)}\, 90.10 \cdot 10^{-3}$	0.84	$^{**)}\, 90.10 \cdot 10^{-3}$
3.	$^{**)}\, r_3 = k_3 \cdot C_{H2O}$	0	$5.96 \cdot 10^{-0.95}$	$^{**)}\, 208.3 \cdot 10^{-3}$	$5.96 \cdot 10^{-1.45}$	$^{**)}\, 208.3 \cdot 10^{-3}$
4.	$^{**)}\, r_4 = k_4 \cdot C_{H2}$	0	$6 \cdot 10^{-1.85}$	$^{**)}\, 7.53 \cdot 10^{-3}$	$6 \cdot 10^{-0.6}$	$^{**)}\, 7.53 \cdot 10^{-3}$
5.	$^{***)}\, r_5 = k_5 \cdot C_{CO2} \cdot C_{H2}$	0	$^{*)}$0.0265	$^{*)}$ 3960	$^{*)}$ 0.0265	$^{*)}$ 3960
6.	$^{***)}\, r_6 = k_6 \cdot C_{CO} \cdot C_{H2O}$	0	$^{*)}$2.75E^{+10}	$^{*)}$ 8.36E^{+07}	$^{*)}$ 2.75E^{+10}	$^{*)}$ 8.36E^{+07}

$^{*)}$ (Watanabe et al., 2006) cited with (Vikram, 2012); $^{**)}$ (Tomeczek, 1991); $^{***)}$ (Ansys, 2009)

The following local uniqueness conditions of the numerical solution were adopted for each numerical grid, respectively:

1. for numerical grid of gasification channel:
   - temperature of gasification agent (oxygen, air) – 298.15 K,
   - volume flow for oxygen (EM "Barbara") – 29 Nm$^3 \cdot$ h^{-1} and for air (Coal Mine "Wieczorek") 270 Nm$^3 \cdot$ h^{-1}
2. for numerical grid of coal seam:
   - density – 1450 kg $\cdot$ m^{-3},
   - porosity – 5% (Białecka, 2008),
   - permeability β – 1e^{-15} m^2 (Białecka, 2008),
   - specific heat (average value) c_{pC} 1300 J $\cdot$ kg $\cdot$ K^{-1} (Chmura, 1968),
   - temperature T – 298.15 K,
   - thermal conductivity coefficient (average value) – 0.535 W $\cdot$ m$^{-1} \cdot$ K^{-1} (Chmura, 1968).

The following global (system) settings in Ansys-Fluent were considered:
- gasification pressure – 101325 Pa,
- gravitational acceleration – 9.81 $m \cdot s^{-2}$,
- time scale– 100 hours (EM “Barbara”) and 305 hours (Coal Mine “Wieczorek”).

3.4. Result

Based on the assumptions of the numerical model in the CFD system, the characteristics of changes in the volume fraction of components of the process gas were obtained and compared with the experimental data. The results of changes in the concentration of sought process gas components obtained during the model tests are presented in Figures 8÷15. These results were compared with experimental data. In case of the experiment in Coal Mine “Wieczorek”, the results were presented within the time interval of 408.6-708.6 hour of the experiment which was considered as a steady state of the georeactor operation.

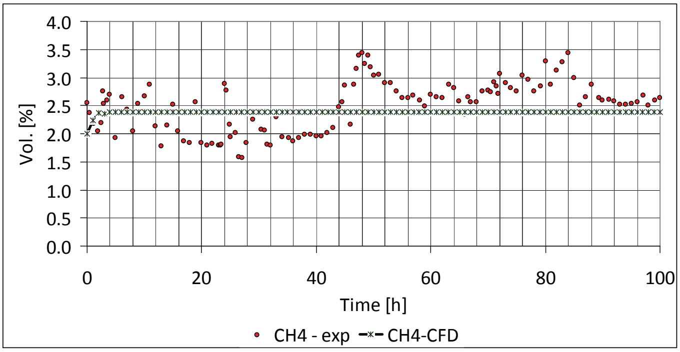


Fig. 8. Changes in the concentration of CH_4 in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in EM “Barbara”

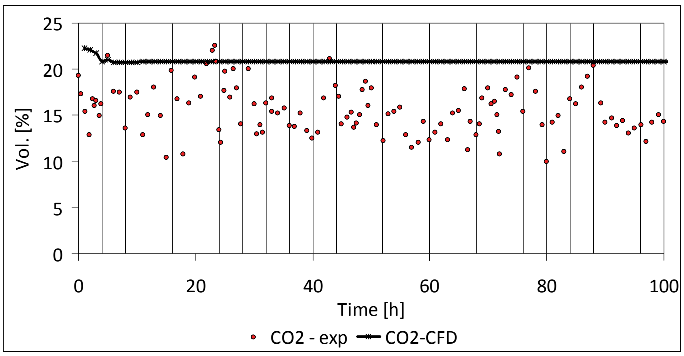


Fig. 9. Changes in the concentration of CO_2 in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in EM “Barbara”

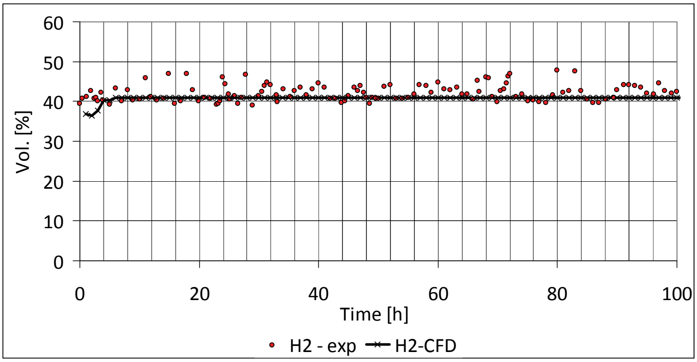


Fig. 10. Changes in the concentration of H_2 in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in EM "Barbara"

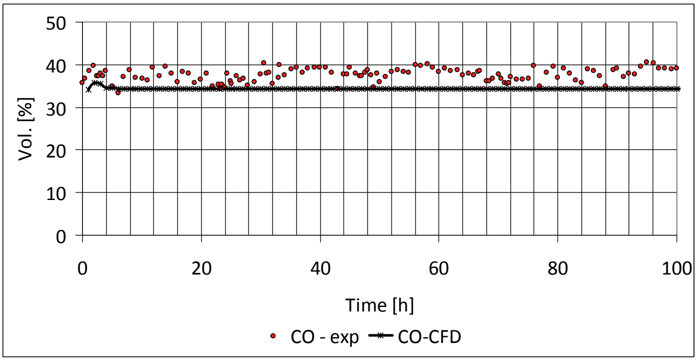


Fig. 11. Changes in the concentration of CO in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in EM "Barbara"

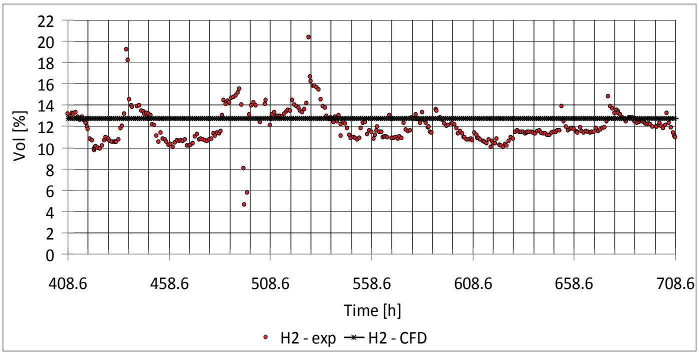


Fig. 12. Changes in the concentration of H_2 in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in Coal Mine "Wieczorek"

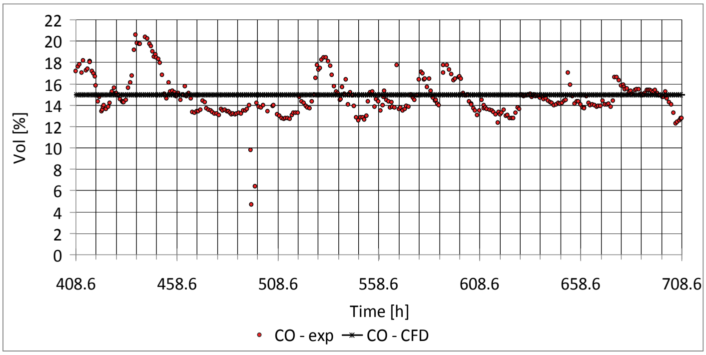


Fig. 13. Changes in the concentration of CO in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in Coal Mine "Wieczorek"

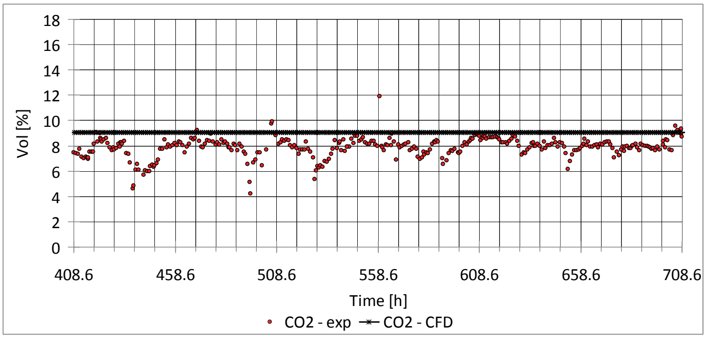


Fig. 14. Changes in the concentration of CO_2 in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in Coal Mine "Wieczorek"

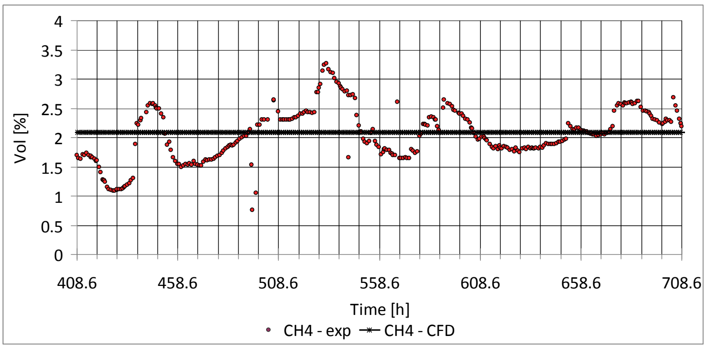


Fig. 15. Changes in the concentration of CH_4 in the time interval of 100 hours of coal gasification process, obtained from the solution of the CFD numerical model and measurements on the experimental model in Coal Mine "Wieczorek"

Comparison of results of the composition of coal gasification products obtained for the numerical model of the gasification process with the experimental data is shown in Table 2.

TABLE 2

The results of composition of gas obtained during coal gasification (average values)

Gas component	KD Barbara	CFD	KWK Wieczorek	CFD
	Concentration [%]		Concentration [%]	
H_2	42.16	40.82	12.03	12.72
CH_4	2.50	2.38	2.05	2.07
CO_2	15.62	20.83	7.89	9.02
CO	37.61	34.43	14.79	14.91

4. Summary and conclusions

The result of conducted works is the numerical model of underground coal gasification process (UCG) developed to predict the physicochemical phenomena occurring in the reaction zone of the gasification channel. The term UCG numerical model shall be understood as:

- an interpretation of the scope of physical and chemical phenomena defined by the model,
- selection of mathematical models determining the described phenomena,
- the methods of solving equations and tools dedicated for that purpose,
- implementation of the model for the coal gasification process with the assumed formal description and based on the selected IT tools.

The developed numerical model was compared with data obtained during the experiment in full scale. Consequently, an initial model for determination of operation parameters of the underground coal gasification generator which constitutes the basis for calculations and study of the coal gasification process using computer simulation has been defined.

The following conclusions can be formulated based on the conducted model studies:

- the obtained results of the numerical model of UCG process are comparable with the results obtained from measurements on the real object of the study,
- modelling the coal gasification process using computational fluid dynamics methods constitutes a valuable research tool at the stage of design of an underground coal gasification installation.

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