MODELLING OF GAS FLOW IN THE UNDERGROUND COAL GASIFICATION PROCESS AND ITS INTERACTIONS WITH THE ROCK ENVIRONMENT

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Abstract
The main goal of this study was the analysis of gas flow in the underground coal gasification process and interactions with the surrounding rock mass. The article is a discussion of the assumptions for the geometric model and for the numerical method for its solution as well as assumptions for modelling the geochemical model of the interaction between gas-rock-water, in terms of equilibrium calculations, chemical and gas flow modelling in porous mediums. Ansys-Fluent software was used to describe the underground coal gasification process (UCG). The numerical solution was compared with experimental data. The PHREEQC program was used to describe the chemical reaction between the gaseous products of the UCG process and the rock strata in the presence of reservoir waters.

1. INTRODUCTION

Technology concerning underground coal gasification (UCG) is one of the most promising, innovative technologies connected to the exploitation of mineral deposits. Coal seams which are not available by conventional methods of exploitation can be converted into a syngas under the *in-situ* condition. The syngas can be processed by power plants or the chemical industry and can provide a basis for further chemical syntheses (Białecka 2008; Perkins 2005; Prabu, Jayanti 2011, 2012; Wachowicz, Janoszek, Iwaszenko 2010).

The UGC gaseous products may pose a potential threat to the environment by migrating to the surrounding geological structures. The syngas initiates a series of chemical reactions as a result of rock dissolution in the reservoir waters. The rate of chemical reactions depend on the mineral compositions of the rock strata, the chemical compositions of groundwater as well as the intensity of the flow of gaseous products into the rock environment (Motliński, Kowalczyk 2006).

In work (Białecka 2008) an analysis of the technological factors determining the proper conduct of the coal gasification process under the *in-situ* conditions were described and major issues in its implementation were identified. The author of the work (Białecka 2008) describes the negative impact of the UCG process on the environment, mainly on the groundwater, the results of studies on the pollution changes of groundwater were also presented. The geological aspects of gas migration were discussed in the work (Checko 2008). Based on the experimental analysis and modelling studies, the main parameters that determine the migration of gases in the rock mass were presented. The issue of modelling the process of underground coal gasification was discussed in (Hadi, Hafez 1986; Perkins 2005; Wachowicz, Janoszek, Iwaszenko 2010; Yang 2004, 2005). The author of the work (Hadi, Hafez 1986) presents the results of modelling studies concerning the process of coal gasification, using the finite element method, in order to predict changes of temperature, gas composition, pressure and coal consumption. In the work (Wachowicz, Janoszek, Iwaszenko 2010) the energy balance of thermal phenomena accompanying the coal gasification process were done in order to predict any changes to the chemical composition of the syngas. The results of the modelling studies were compared with the results of the experimental studies. In (Yang 2004, 2005) the results of the research model of the gasification process were presented in order to predict the changes of the chemical composition of the syngas and the temperature of the process. The results of the modelling studies were compared with the results of the experimental studies.

The ability to predict the chemical reactions, triggered by the transport phenomena of gases in the rock mass, seem to be necessary to increase the efficiency of the UCG process under *in-situ* conditions and to minimize the negative influence on the widely understood groundwater environment. The numerical model of the underground coal gasification process was developed thanks to Ansys-Fluent software. The geochemical model of the groundwater environment was developed thanks to PHREQQC software.

Ansys-Fluent is software that uses computational fluid dynamics (CFD), modelling phenomena associated with fluid flows (combustion, turbulence, multiphase flows, chemical reactions, heat conduction, convection, etc.) including fluid flow through porous media is possible thanks to it (ANSYS FLUENT… 2009). PHREEQC is a program created to undertake hydrogeochemical calculations (Appelo, Postma 2005; Motliński, Kowalczyk 2006).

The modelling of gas flow in the underground coal gasification process and its interactions with the rock mass can provide information regarding physical and chemical phenomena which occur under the conditions of temperature and pressure prevalent in the fixed bed.

2. SCHEME OF MODEL TESTS

The scheme of the model tests were divided into two main stages:

1. The modelling of underground coal gasification using Ansys-Fluent software is achieved by determining (Khadse et al. 2006; Białecka 2008; Hadi, Hafez 1986; Jaworski 2005; Perkins 2005; Wachowicz, Janoszek, Iwaszenko 2010; Yang, Liu 2003; Yang 2004, 2005):
● the geometry of the object
● the model grid
● the physical properties of the gasification agent
● boundary conditions
● the physical and chemical properties of coal

The developed numerical model of the UCG process provided information regarding the mass fraction of syngas components and the temperature in different rock layers.

2. The modelling of the geochemical model concerning the interaction syngas water rock using PHREQQC software is found by determining (Appelo, Postma 2005; Motliński, Kowalczyk 2006):
● the chemical composition of the groundwater
● the mineral composition of the rock strata

The developed geochemical model provides information concerning changes in the chemical composition of groundwater thanks to interaction with rock strata due to changes of partial pressure of syngas components during gasification run time.

3. MODEL DESCRIPTION AND SIMULATION METHODOLOGY

A simulation of the underground coal gasification process was developed based on reactive fluid flow along the gasification channel with the given geometry. Simulations of physical phenomena are related to the transport of mass and energy and chemical reactions (including the effect of energy). The Probabilistic Density Function (PDF) method was used to model the chemical reactions of the coal gasification process. This method facilitates obtaining the solution of the transport equation for mixture fractions, which is a conserved scalar. The PDF model reduced the gasification process into a mixing problem. The coal volatiles and char are delivered into the reaction zone (gasification channel) in the form of a single fuel stream and reacts with a gasification agent (a mixture of oxygen and steam). The equilibrium chemistry

equation was used to calculate the gas composition (ANSYS FLUENT… 2009; Jaworski 2005). The coal seam and rock strata are treated as a homogeneous solid body with variable parameters of porous medium and effective thermal conductivity. Due to the complexity of the equations and the complexity of the numerical methods, the Ansys-Fluent code was used to perform the numerical calculations of the UCG process.

3.1. Georeactor model

Figure 1 presents the geometric model of the rock strata surrounding the georeactor. The georeactor is located in the coal seam of group 610 of the Upper Silesian Coal Basin (USCB) (Bukowska 2005).
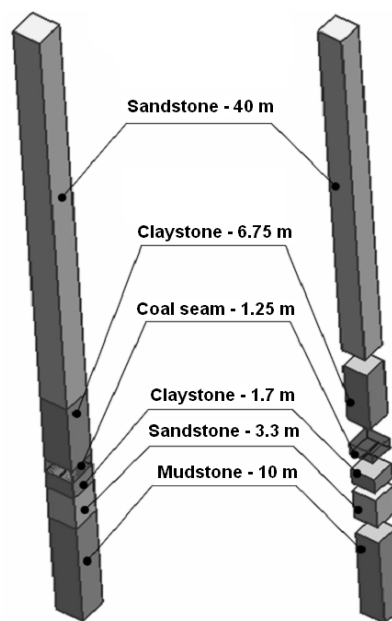

Fig. 1. The geometric model of the rock strata surrounding the georeactor developed for the simulation of the UCG process

The characteristics of individual fractions of minerals forming the rock strata were presented in Figure 2. The results were taken from (Strzyszcz, Harabin 2004). The results shown in Figure 2 were implemented as a model of mineral matrices in a geochemical model on the PHREEQC software.

The sandstone layer is formed by quartz and chalcedony, volume fraction of which is 35% (Fig. 2a), the claystone layer is made up of illite in amounts of up to 64% (Fig. 2b), the mudstones layer is formed by fractions of kaolinite and illite, in an amount up to 30% (Fig. 2c) (Strzyszcz, Harabin 2004).

The rock strata in the region of the georeactor in seam 610 are formed by the following geological structures, namely (Bukowska 2005; Strzyszcz, Harabin 2004):
● a sandstone layer with a thickness from 3.3 m to 40 m (Fig. 1), with significant amounts of quartz and chalcedony (Fig. 2a)
● a claystone layer with a thickness from 1.7 m to 6.75 m (Fig. 1), with significant amounts of illite (Fig. 2b)
● a mudstone layer with a thickness 10 m (Fig. 2), with significant amounts of kaolinite and illite (Fig. 2c)
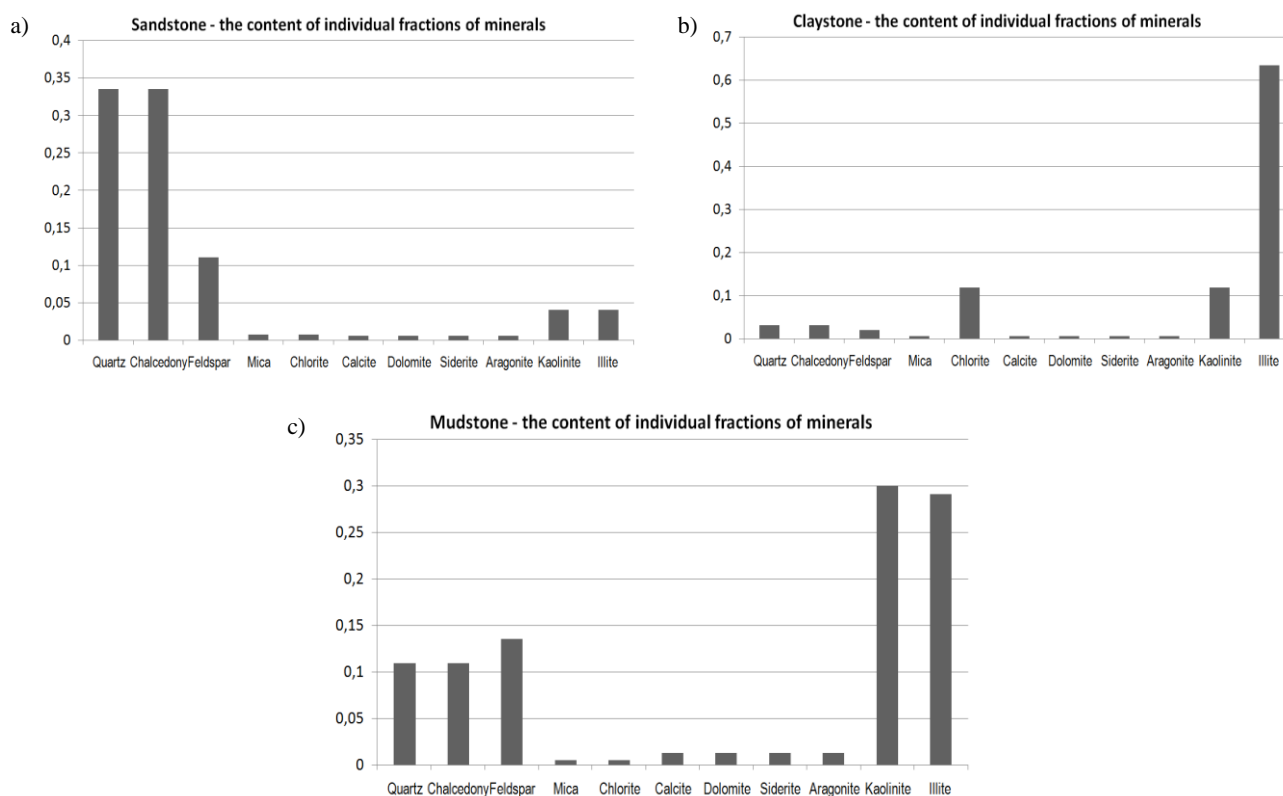
a)

b)

c)

Fig. 2. Characteristics of minerals fraction forming rock strata: a) sandstone, b) claystone, c) mudstone

The geometry of the georeactor was determined, based on the following assumptions (Fig. 1) (15, 16):

- solid model of the georeactor – 2.5 m × 2.5 m × 1.25 m
- solid model of mudstone – 2.5 m × 2.5 m × 10 m
- solid model of sandstone – 2.5 m × 2.5 m × 3.3 m and 2.5 m × 2.5 m × 40 m
- solid model of claystone – 2.5 m × 2.5 m × 1.7 m and 2.5 m × 2.5 m × 6.75 m

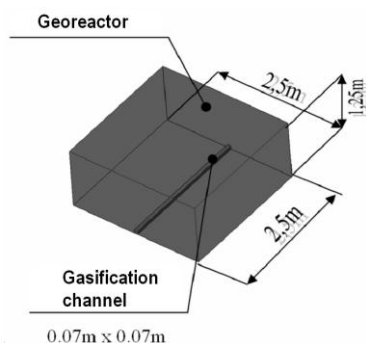The geometric model of the georeactor is presented in Fig. 3 (Stańczyk et al. 2009, 2010).

Fig. 3. The geometric model of the georeactor

Figure 1 and Figure 3 present the results of geometric modelling, developed in order to identify:

- the average temperature of the rock strata
- the average concentration of gas components in the rock strata

3.2. Discretization

The next step after preparing a solid model of a georeactor is discretization. Discretization is the process of creating a numerical area of the solution (Jaworski 2005). The model grids of the numerical solution are presented in Figure 4.

The following types of numerical grids were generated:

- the sandstone layer (with a thickness 40 m), created from 1725 nodes and 1088 wireframe elements, reflecting the solid model occupied by the solid (volume 250 m^3) – Fig. 4a
- the claystone layer (with a thickness 6.75 m), created from 35 712 nodes and 32 269 wireframe elements, reflecting the solid model occupied by the solid (volume 42.18 m^3) – Fig. 4b
- the coal seam (with a thickness 1.25 m), created from 53 016 nodes and 48 622 wireframe elements, reflecting the solid model occupied by the solid body (volume 7.80 m^3) – Fig. 4c
- the gasification channel, created from 621 nodes and 272 wireframe elements, reflecting the solid model occupied by the fluid (volume 0.012 m^3) – Fig. 5d
- the claystone layer (with a thickness 1.7 m), created from 62 775 nodes and 58 080 wireframe elements, reflecting the solid model occupied by the solid body (volume 10.625 m^3) – Fig. 4e
- the sandstone layer (with a thickness 3.3 m), created from 62 208 nodes and 57 575 wireframe elements, reflecting the solid model occupied by the solid body (volume 20.625 m^3) – Fig. 4f
- the mudstone layer (with a thickness 10 m), created from 19 074 nodes and 16640 wireframe elements, reflecting the solid model occupied by the solid body (volume 62.5 m^3) – Fig. 4g
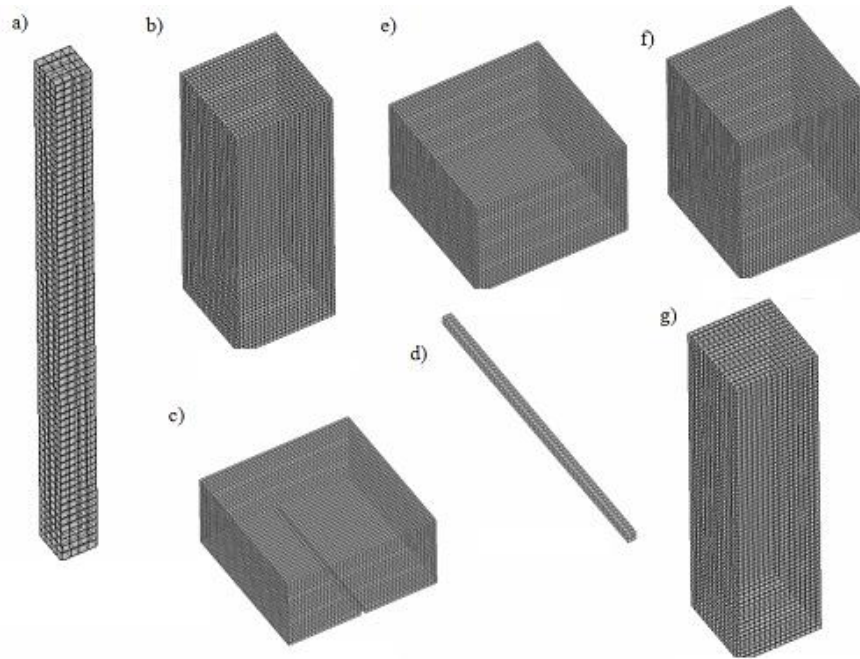
Fig. 4. Numerical grid of the georeactor and the rock strata: a) 40 m sandstone layer, b) 6.75m claystone layer, c) 1.25 m coal seam, d) gasification channel, e) 1.7 m claystone layer, f) 3.3 m sandstone layer, g) 10 m mudstone layer

3.3. Boundary conditions

After defining the area of the numerical solution, the next important step was to define the initial and boundary conditions. The analysis included the model of the gasification channel (fluid), the model of the georeactor (porous medium) and the model of the rock strata (porous medium), for which the boundary conditions were calculated, enabling the verification of the experimental results by means of the developed mathematical models and the numerical method of CFD calculation. Figure 5 shows the measurement system of the gas composition process (CH_4, CO_2, CO, H_2), which was located at the reactor outlet (point 1 to 5) (Stańczyk et al. 2009, 2010).
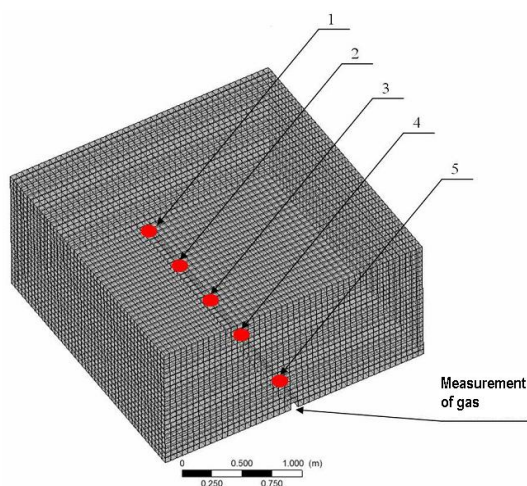

Fig. 5. The measuring system of the selected parameters developed thanks to the Ansys-Fluent software

The measurement of changes of the temperature profile were monitored along with the gasification channel in five measurement points, at different distances from the inlet of the georeactor, in the following manner (Fig. 5), namely (Stańczyk et al. 2009, 2010):

- point 1 – 0.3 [m]
- point 2 – 0.8 [m]
- point 3 – 1.3 [m]
- point 4 – 1.8 [m]
- point 5 – 2.3 [m]

The following initial and boundary conditions for each of the areas of discretization were examined:
1. The gasification channel (fluid):
   - the temperature and mass flux O_2 – 25 [°C] and from the expression

$$\dot{m} = \dot{m}_0 + 5\sin(4t) \quad (\dot{m}_0 - \text{initial mass flux}, \; t - \text{time step})$$

(Stańczyk et al. 2009, 2010)
   - the specific heat of oxygen O_2 cp_{O2} (ANSYS FLUENT… 2009) – cp_{O2} = 834.826 + 0.292T – 0.0001495T^2 + 3.41e – 07T^3 – 2.27·10 – 10T^4 [J·kg^{-1}·K^{-1}]
   - the temperature and mass flux H_2O–100 [°C] and from the expression

$$\dot{m} = \dot{m}_0 + 5\sin(4t) \quad (\dot{m}_0 - \text{initial mass flux}, \; t - \text{time step})$$

(Stańczyk et al. 2009, 2010)
   - the specific heat of steam H_2O cp_{H2O} from the expression (ANSYS FLUENT… 2009) – cp_{H2O} = 1563.08 + 1.60T – 0.0029332794T^2 + 3.21·10 – 6T^3 –1.15·10 – 9T^4 [J·kg^{-1}·K^{-1}]
   - the thermal conductivity of the oxygen-steam mixture – 0.0454 [W·m^{-1}·K^{-1}] (ANSYS FLUENT… 2009)
   - the dynamic viscosity of the oxygen-steam mixture – 1.72e–^{05} [kg·m^{-1}·s^{-1}] (ANSYS FLUENT… 2009).

2. The coal seam (porous medium):
   - mass loss rate of coal – 4 [kg·h^{-1}] (Stańczyk et al. 2009, 2010)
   - density – 1400 [kg·m^{-3}] (Perkins 2005)
   - the porosity of coal from the expression

$\varphi = 0.2286 + 0.01041T + 0.00001786T^2$ [%] (T – temperature [°C]) (Białecka 2008)

- permeability β – $1e^{-15}$ [m^2] (Chećko 2008)
- the specific heat of coal cp$_C$ from the expression (ANSYS FLUENT… 2009) – $cp_C = -464.18 + 4.97T - 0.003899261T^2 + 1.482 \cdot 10 - 6T^3 - 2.885 \cdot 10 - 10T^4$ [J·kg^{-1}·K^{-1}]
- initial temperature T – 298.15 [K],
- thermal conductivity – 0.9 [W·m^{-1}·K^{-1}] (Perkins 2005)
- ultimate/proximate analysis of the coal sample is presented in table 1:

Table 1. Ultimate/proximate analysis of the coal seam

Proximate Analysis	Fixed carbon	63.83%
	Volatiles matter	32.41%
	Ash	2.21%
	Moisture	1.55%
Ultimate Analysis	Carbon (C)	83.84%
	Hydrogen (H)	4.94%
	Oxygen (O)	9.79%
	Nitrogen (N)	1.15%
	Sulphur (S)	0.28%
Heat of combustion		3.54e^{+7} [J·kg^{-1}]

3. The sandstone layer (porous medium):
- density – 2690 [kg·m^{-3}] (Chećko 2008)
- porosity – 0.6 [%] (Chećko 2008)
- permeability β – $1e^{-14}$ [m^2] (Chećko 2008)
- specific heat – 1320 [J·kg^{-1}·K^{-1}] (Chećko 2008)
- initial temperature T – 298.15 [K] (Stańczyk et al. 2009, 2010)
- thermal conductivity from the expression (Jian et al. 2011) – $\lambda = 1.34053 - 0.00106T + 5.48226 \cdot 10^{-7}T^2$ [W·m^{-1}·K^{-1}]

4. The claystone layer (porous medium):
- density – 2790 [kg·m^{-3}] (Chećko 2008)
- porosity – 2.6 [%] (Chećko 2008)
- permeability β – $1e^{-15}$ [m^2] (Chećko 2008)
- the specific heat – 800 [J·kg^{-1}·K^{-1}] (Chećko 2008)
- initial temperature T – 298.15 [K] (Stańczyk et al. 2009, 2010)
- thermal conductivity from the expression (Jian et al. 2011) – $\lambda = 1.18965 - 0.0006007T + 3.41831 \cdot 10^{-7}T^2$ [W·m^{-1}·K^{-1}]

5. The mudstone layer (porous medium):
- density – 2600 [kg·m^{-3}] (Chećko 2008)
- porosity – 5 [%] (Chećko 2008)

- permeability β – $2e^{-15}$ [m^2] (Chećko 2008)
- specific heat – 1000 [J·kg^{-1}·K^{-1}] (Chećko 2008)
- initial temperature T – 298.15 [K]
- thermal conductivity from the expression (Jian et al. 2011) – $\lambda = 1.23052 - 0.00066644T + 2.54137 \cdot 10^{-7}T^2$ [W·m^{-1}·K^{-1}]

The following global settings in the ANSYS-Fluent software were considered, namely:
- transient
- the pressure of gasification – 101 325 [Pa]
- the model of turbulence – standard k-ε
- the gasification reaction model – model *PDF*
- the heat transfer model – model *Discrete Ordinate* (*DO*)
- gravity acceleration – 9.81 [m·s^{-2}]
- the gasification agent used in calculations is a mixture of oxygen and steam, treated as ideal gas
- time scale phenomena – 252 000 seconds (70 hours)
- the relative roughness of the gasification channel – 0.1 m
- convergence – $1 \cdot 10^{-4}$

4. RESULTS OF THE UCG SIMULATION

The changes of values in the volume fractions of CH$_4$, CO$_2$, CO and H$_2$ and the temperature profile obtained based on the experimental data and from the numerical model are presented in Figures 6 and 7. The results presented in Figure 6 were obtained during the measurement of syngas at the reactor outlet. The results presented in Figure 7 were obtained during the measurement along the gasification channel, in the five measurement points, at different distances from the inlet of the reactor with the use of the five thermocouples, deployed at 0.5m along the axis of the gasification channel.

The large amount of hydrogen, observed in figure 6c), is probably the effect of water intrusion from the surrounding rocks.

4.1. Results of syngas flow in rock mass

In Figures 8–12 the changes of the average concentration of syngas components and the temperature obtained from solutions of the numerical model CFD are displayed.

The rapid or sudden changes in the concentrations in Figures 8 to 12 are associated with the initiation of the ignition process and its stability which is observed at the beginning of the process.
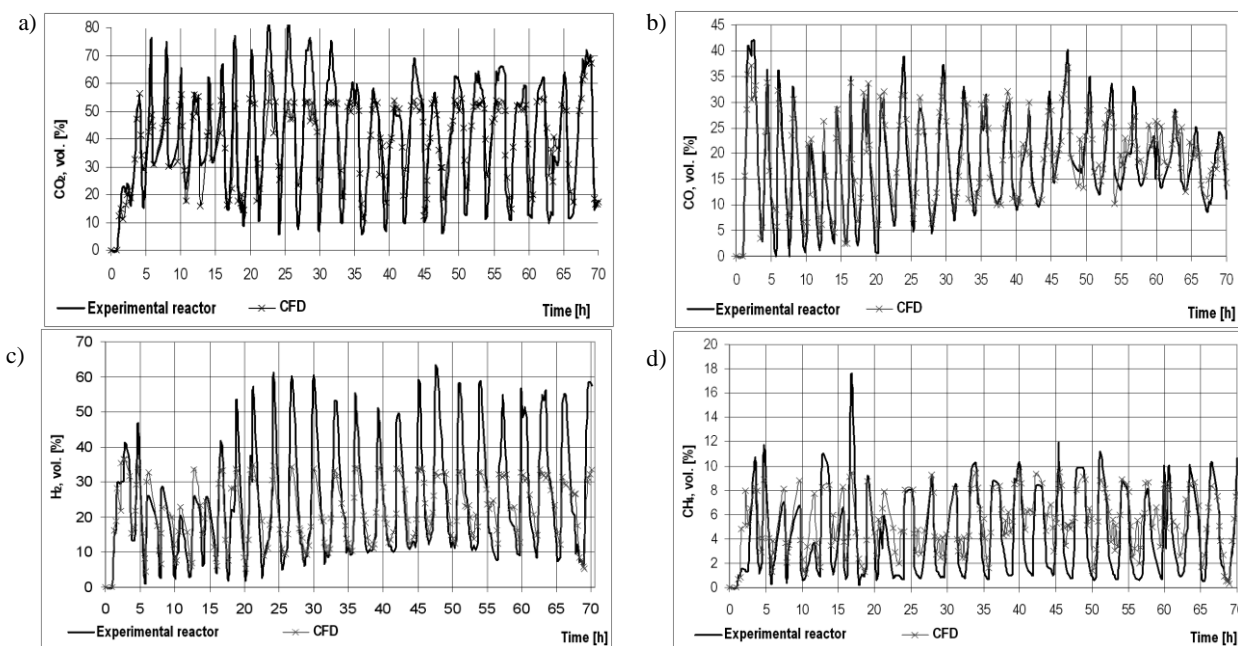
Fig. 6. The volume fraction changes of the syngas components during a time interval of 70 hours, based on the values measured in the reactor and from the CFD model:
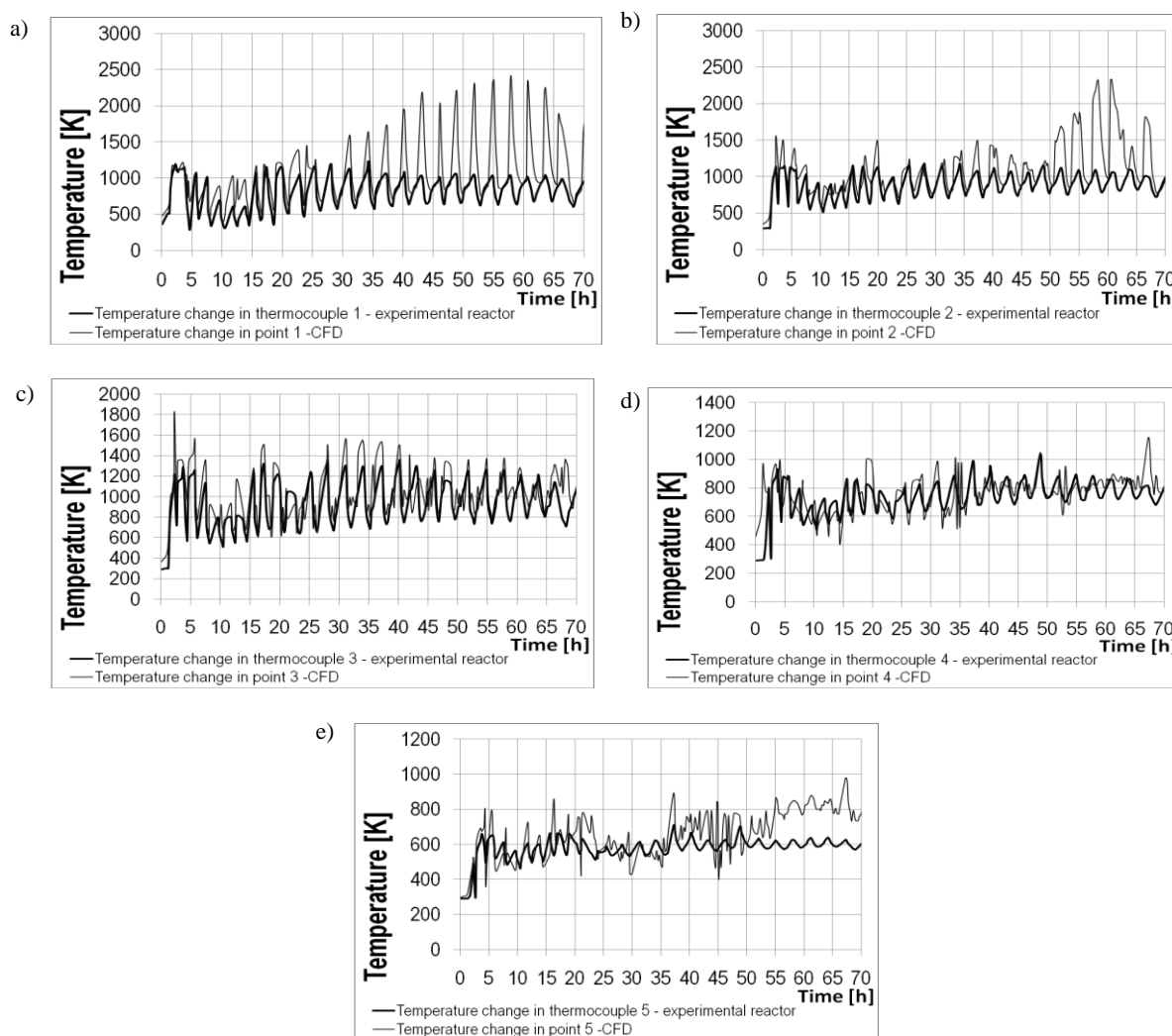a) CO_2, b) CO, c) H_2, d) CH_4 (Stańczyk et al. 2009, 2010)

Fig. 7. Change of temperature registered in thermocouple 1 (Fig. 7a), 2 (Fig. 7b), 3 (Fig. 7c), 4 (Fig. 7d) and 5 (Fig. 7e), obtained from the experimental reactor
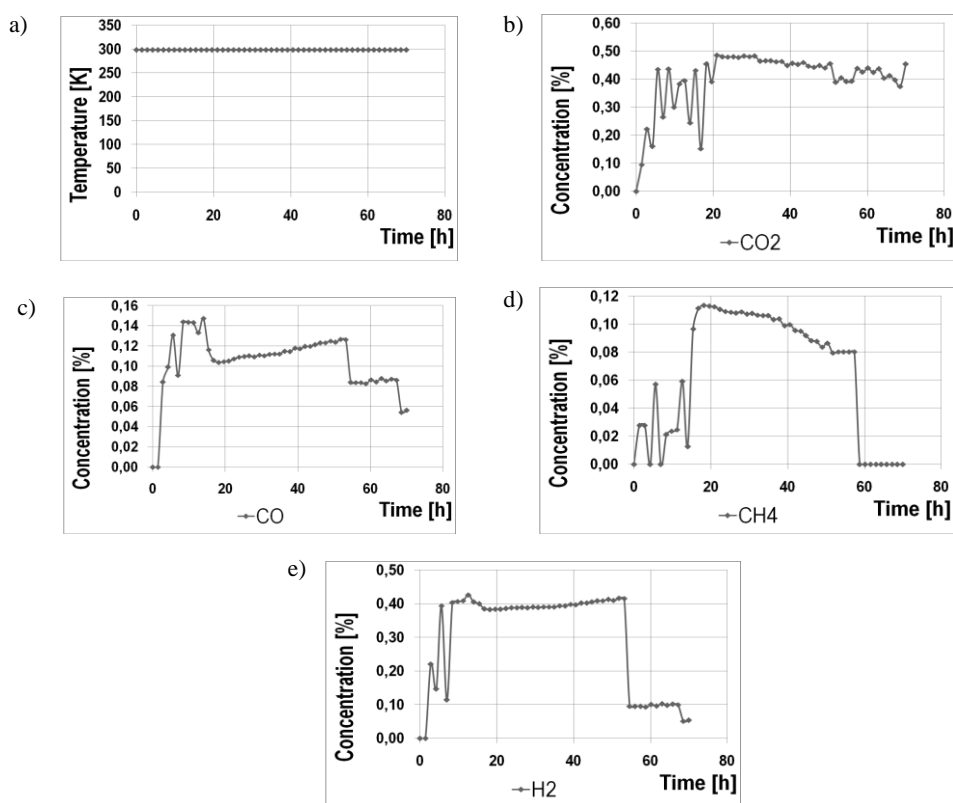and the CFD model (Stańczyk et al. 2009, 2010)

Fig. 8. Quantitative analysis of the average temperature and concentration of gas components in a layer of sandstone with a thickness of 40m during a time interval of 70 hours: a) temperature, b) CO_2, c) CO, d) CH_4, e) H_2
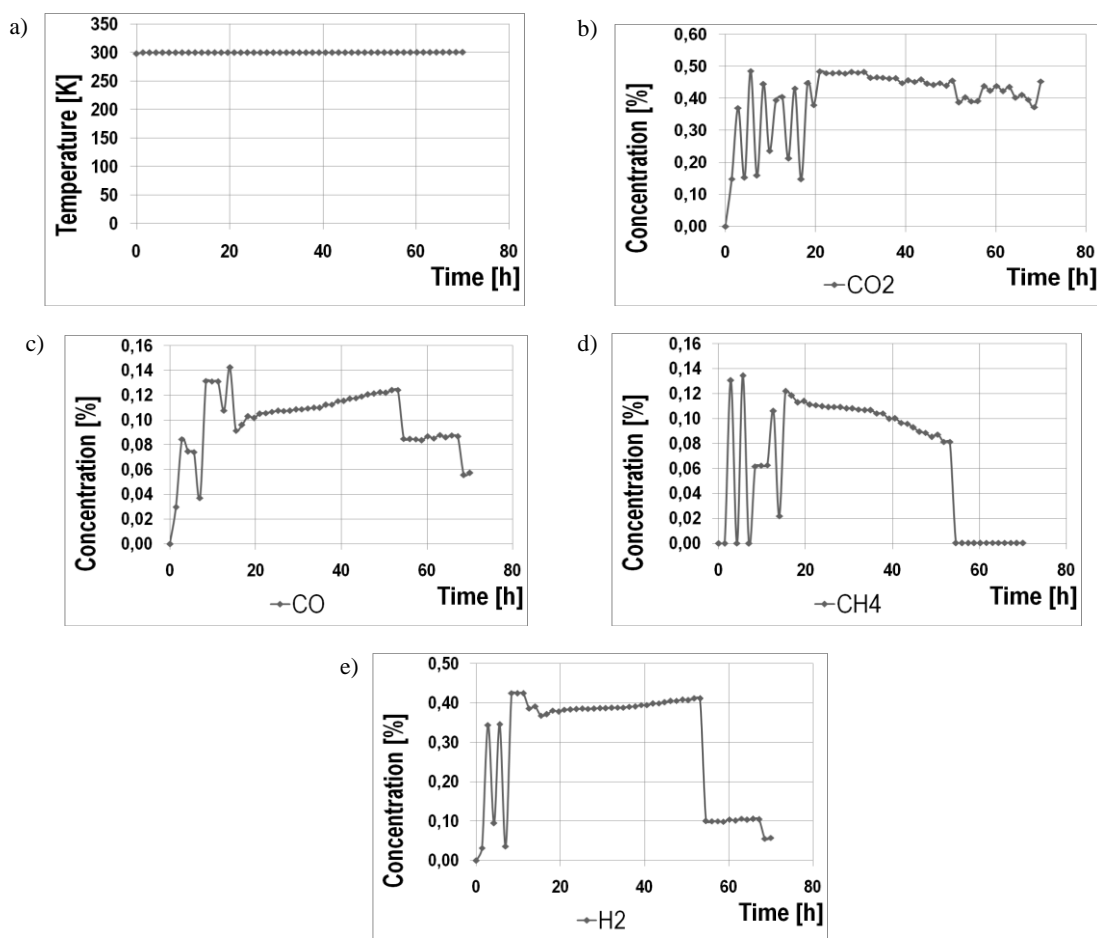

Fig. 9. Quantitative analysis of the average temperature and concentration of gas components in a layer of claystone with a thickness of 6.75m during a time interval of 70 hours: a) temperature, b) CO_2, c) CO, d) CH_4, e) H_2
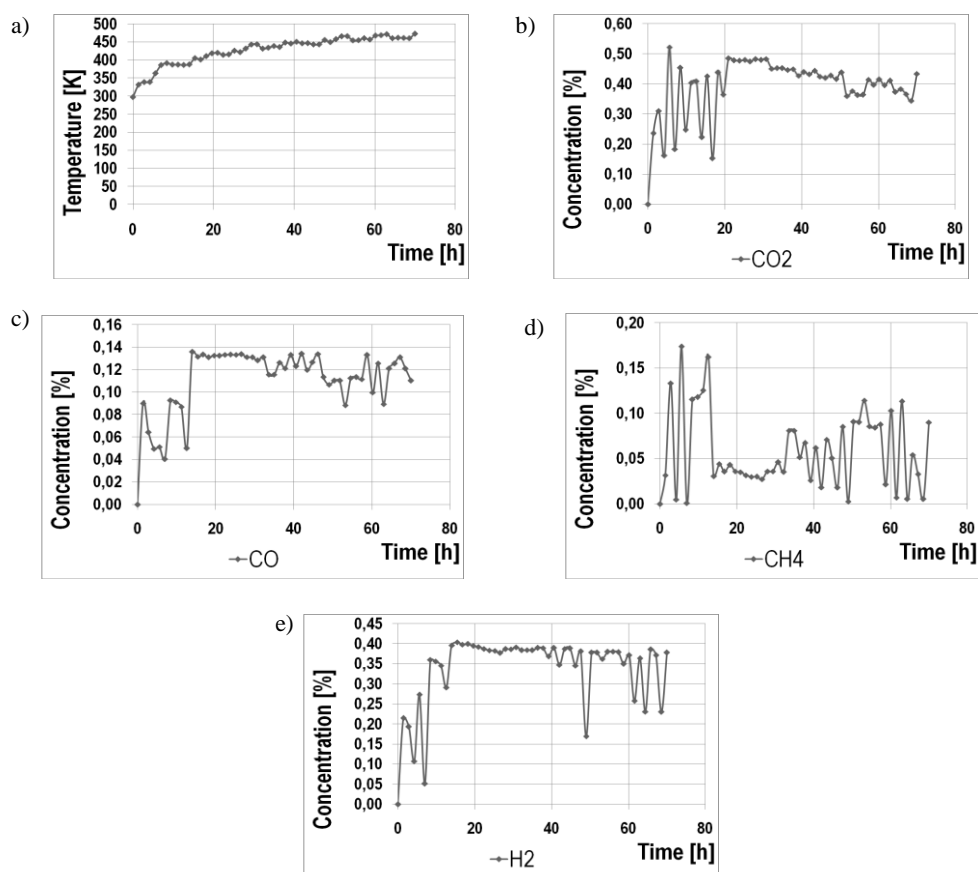
Fig. 10. Quantitative analysis of the average temperature and concentration of gas components in a layer of claystone with a thickness of 1.7m during a time interval of 70 hours: a) temperature, b) CO_2, c) CO, d) CH_4, e) H_2
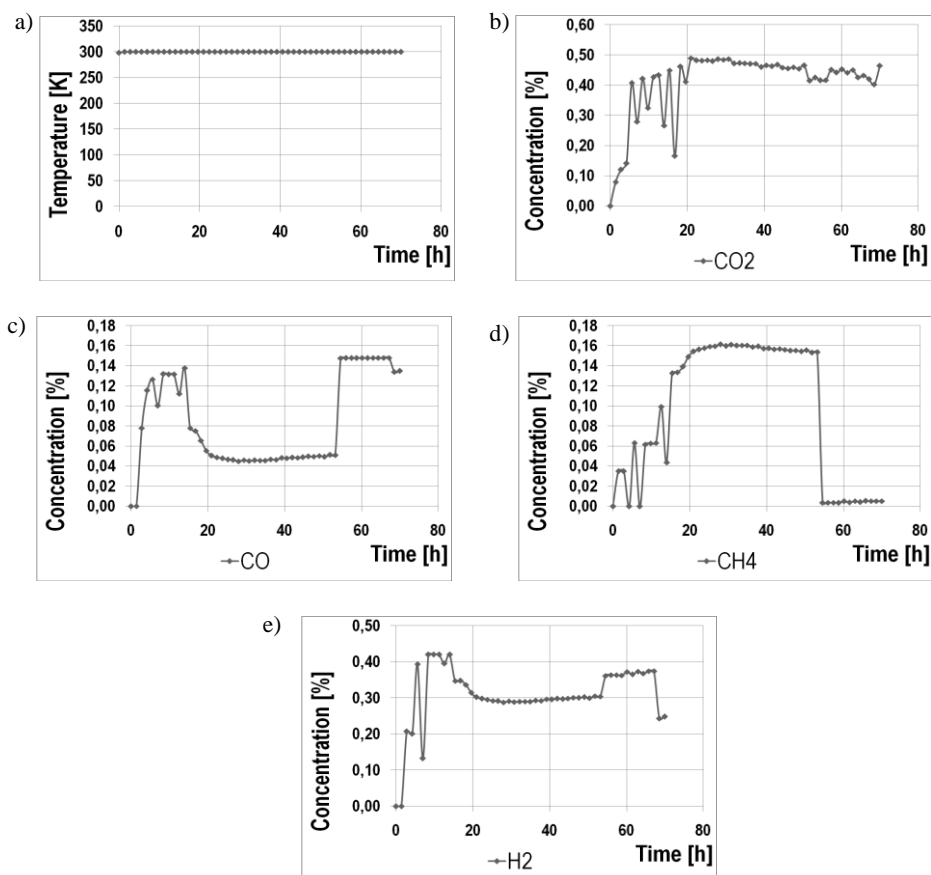

Fig. 11. Quantitative analysis of the average temperature and concentration of gas components in a layer of mudstone with a thickness of 10m during a time interval of 70 hours: a) temperature, b) CO_2, c) CO, d) CH_4, e) H_2
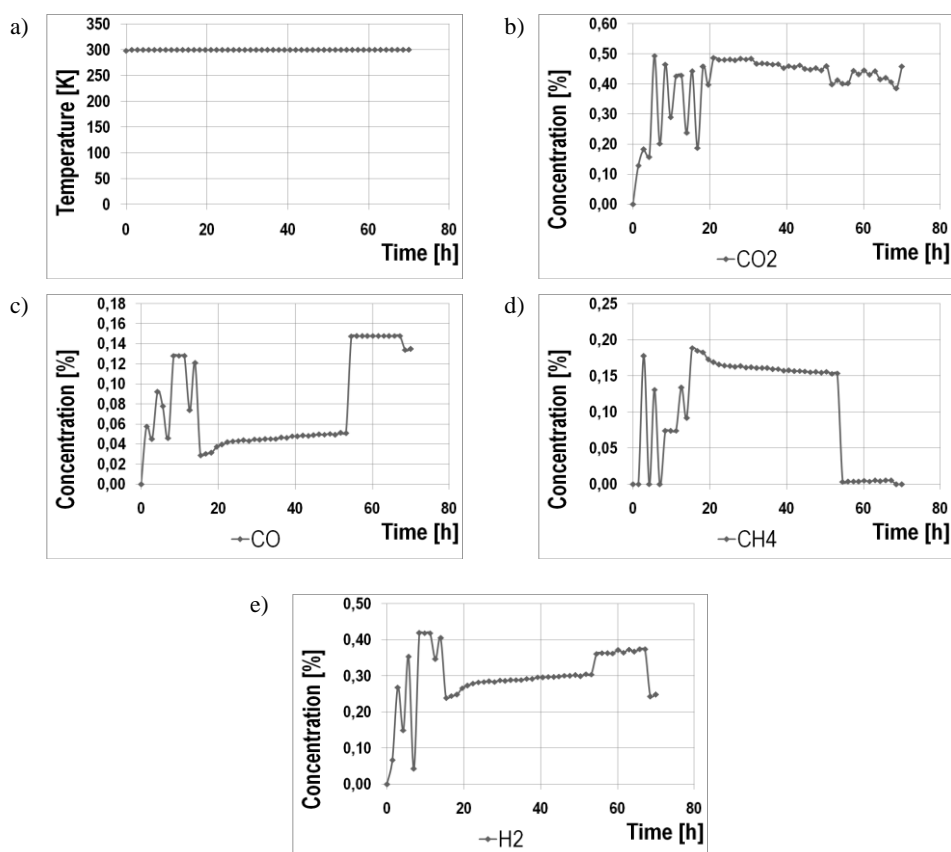
Fig. 12. Quantitative analysis of the average temperature and concentration of gas components in a layer of mudstone with a thickness of 3.3m during a time interval of 70 hours: a) temperature, b) CO_2, c) CO, d) CH_4, e) H_2

5. MODELLING OF THE GEOCHEMICAL INTERACTION OF ROCK-WATER-GAS

The analysis of the chemical reactions between the rock mass, the groundwater and the syngas were developed using PHREEQC software. The software facilitates performing a series of calculations and simulations, i.e. the distribution of the speciation and saturation index, the reaction of dissolution and the precipitation of minerals, ion exchange, surface complexation, kinetic processes, one-dimensional transport and inverse modelling (Appelo, Postma 2005; Motliński, Kowalczyk 2006).

5.1. Chemical composition of pore water

The following average concentrations of major components of groundwater were identified in the region of coal seam 610, namely (Pluta 2005):

- 2.0 mg dm^{-3} (1.85e^{-4} mol·dm^{-3}) of boron (B)
- 0.15 mg dm^{-3} (1.13e^{-6} mol·dm^{-3}) of barium (Ba)
- 27724.25 mg dm^{-3} (7.82e^{-1} mol·dm^{-3}) of chloride ion (Cl$^-$)
- 4.67 mg dm^{-3} (8.37e^{-5} mol·dm^{-3}) of iron ion (Fe^{2+}),
- 157.72 mg dm^{-3} (4.03e^{-3} mol·dm^{-3}) of potassium ion (K$^+$)
- 18132.21 mg dm^{-3} (7.89e^{-1} mol·dm^{-3}) of sodium ion (Na$^+$)
- 175.50 mg dm^{-3} (5.47e^{-3} mol·dm^{-3}) of sulphate ion (SO$_4^{2-}$)

The values were implemented as a model of the chemical composition of pore waters in the PHREEQC software geochemical model. The results were taken from (Pluta 2005).

The mineral composition of the rock strata is shown in Table 2 (Strzyszcz, Harabin 2004). The values were implemented as a model of mineral matrices in the PHREEQC software geochemical model.

Figures 13–17 show the change of pore water compositions in conditions of thermodynamic equilibrium, disturbed as a result of entering the reactive components of process gas as a mixture of CH_4, CO_2, CO, H_2 to rock mass.

The results of the numerical solution show a significant deterioration in the chemical status of the groundwater. The following markers were exceeded, namely:

- pH
- ion concentration of K$^+$ and Fe^{2+} – observed in the sandstone (Fig. 13 and Fig. 15) and claystone layer (Fig. 14)
- ion concentration of SO$_4^{2-}$ observed in sandstone layer of (Fig. 13 and Fig. 15)
- ion concentration of Cl$^-$ and Na$^+$ observed in all layers

The increase of the concentration of SO$_4^{2-}$, Cl$^-$ and Na$^+$ ions will result in the deterioration of groundwater quality by the salinity as well as create conditions for the formation of groundwater with a high concentration of sulphate ions.

A significant increase in the concentration of iron ions in groundwater, observed mainly in the claystone layer (Fig. 14), is the result of the weathering of rocks, which contain iron (siderite $FeCO_3$).

Table 2. The mineral composition of rock layers surrounding the georeactor

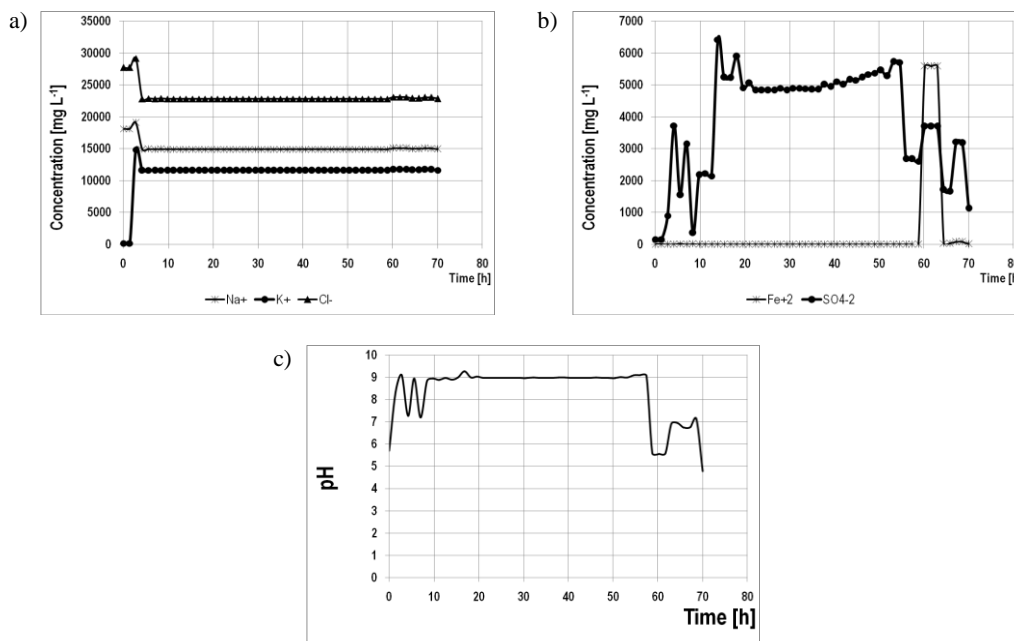| Layer	Concentration [mol·L^{-1}]										
	Quartz	Chalcedony	Feldspars	Micas	Chlorites	Calcite	Dolomite	Siderite	Aragonite	Kaolinite	Illite
Sandstone	15	15	1.063	0.047	0.034	0.146	0.079	0.126	0.146	0.432	0.144
Claystone	1.440	1.440	0.2	0.035	0.595	0.153	0.083	0.132	0.153	1.281	2.276
Mudstone	4.73	4.73	1.266	0.034	0.025	0.325	0.189	0.301	0.348	3.021	0.974

Fig. 13. Quantitative analysis change of pH and of groundwater components as a result of syngas migration into sandstone layer with a thickness of 40m during a time interval of 70 hours: a) Na$^+$, K$^+$ and Cl$^-$, b) Fe^{2+} and SO$_4^{2-}$, c) pH
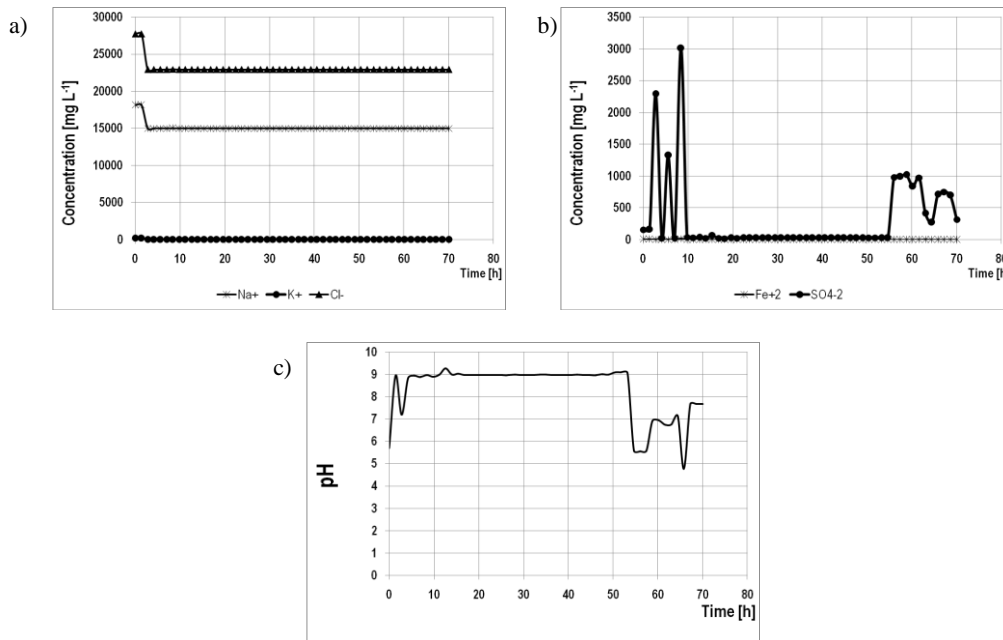

Fig. 14. Quantitative analysis change of pH and of groundwater components as a result of syngas migration into claystone layer with a thickness of 6.75m during a time interval of 70 hours: a) Na$^+$, K$^+$ and Cl$^-$, b) Fe^{2+} and SO$_4^{2-}$, c) pH
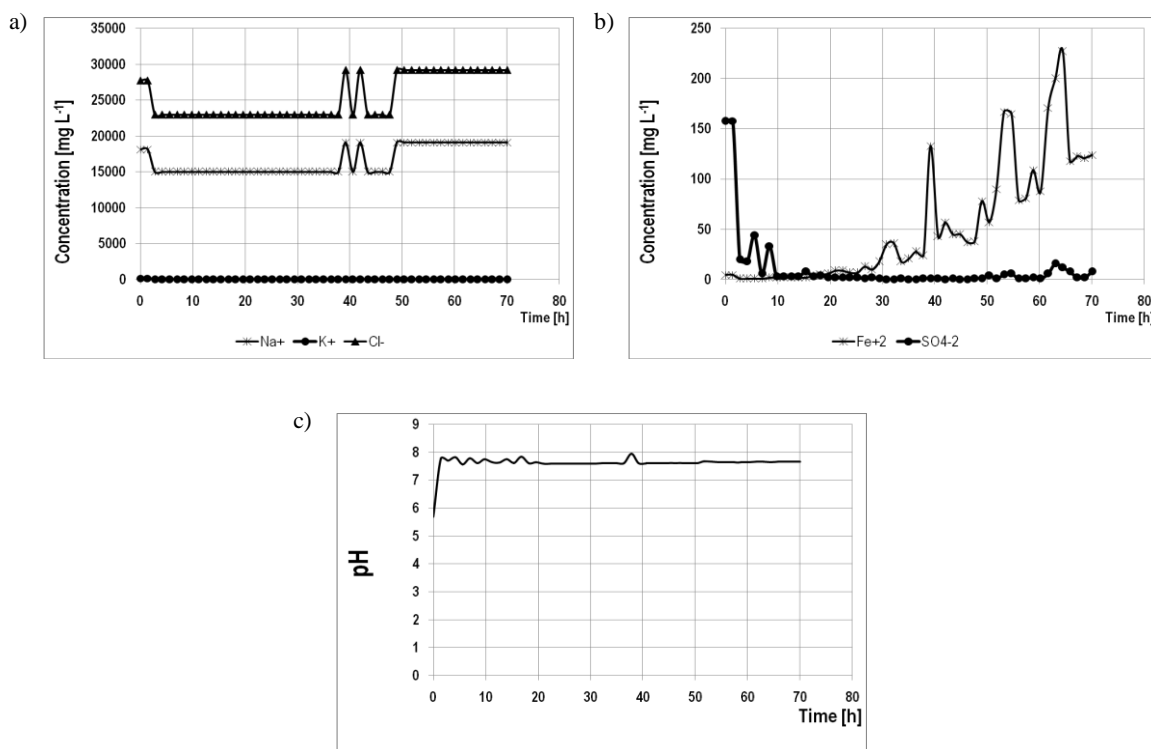
Fig. 15. Quantitative analysis change of pH and of groundwater components as a result of syngas migration into claystone layer with a thickness of 1.75m during a time interval of 70 hours: a) Na^+, K^+ and Cl^-, b) Fe^{2+} and SO_4^{2-}, c) pH
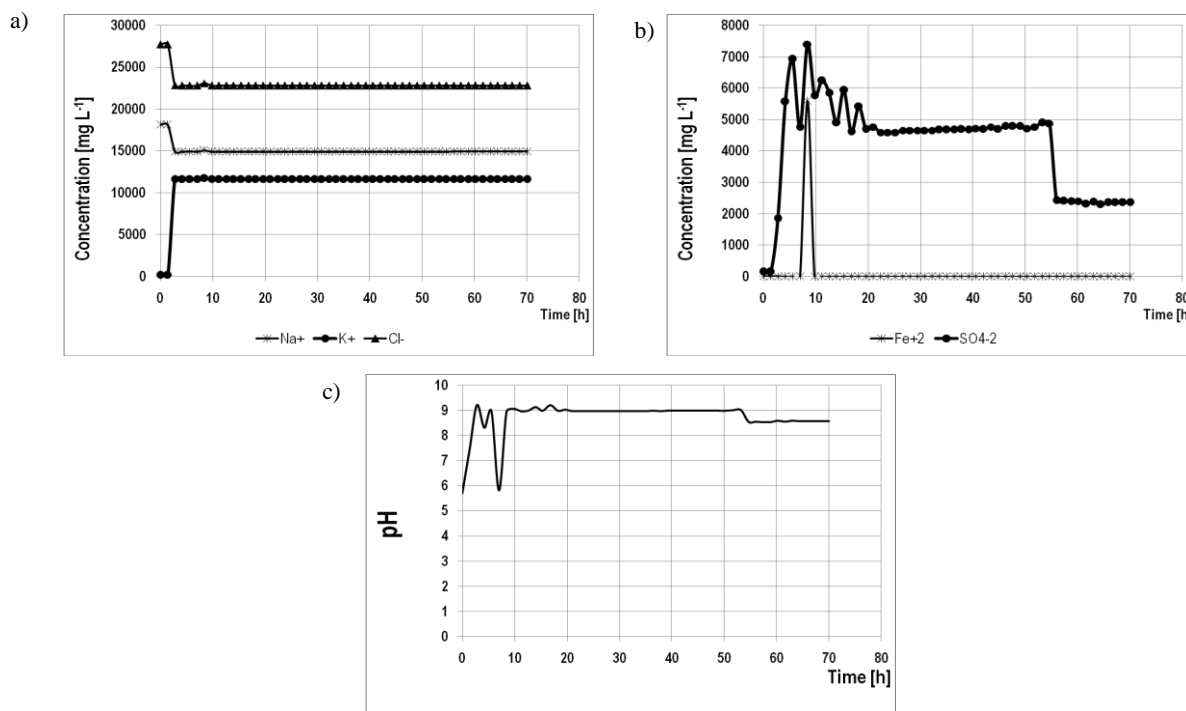

Fig. 16. Quantitative analysis change of pH and of groundwater components as a result of syngas migration into sandstone layer with a thickness of 3.3m, during a time interval of 70 hours: a) Na^+, K^+ and Cl^-, b) Fe^{2+} and SO_4^{2-}, c) pH
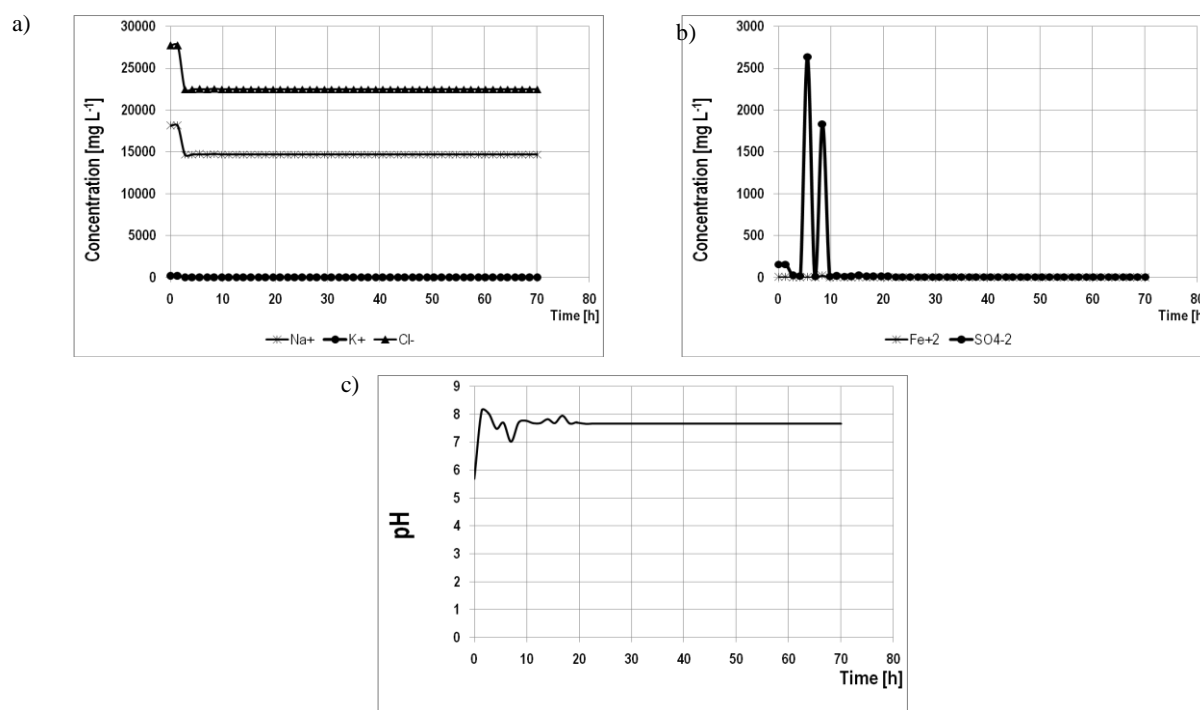
Fig. 17. Quantitative analysis change of pH and of groundwater components as a result of syngas migration into mudstone layer with a thickness of 10m during a time interval of 70 hours: a) Na^+, K^+ and Cl^-, b) Fe^{2+} and SO_4^{2-}, c) pH

6. SUMMARY AND CONCLUSIONS

The model of the georeactor and the rock strata was developed using the functionality of the design software Ansys-DesignModeler. The three-dimensional model was imported with Ansys-Fluent software. Based on the 3D model, the discretization area was developed. The numerical model which predicts parameters of the underground coal gasification process was formulated based on the discretization area. Data obtained from the numerical model were compared with the experimental results and statistically analysed. The geochemical model which predicts the chemical change of the groundwater environment was developed with the PHREEQC software.

The following conclusions were formulated:

1. Chemical reactions between the pore water and the syngas dissolution and the precipitation of minerals from the rock strata were observed. The chemical reactions that occur in the groundwater environment depend on mineral composition, the texture of rocks, filtration properties, temperature, the concentration of syngas components, the flow rate of syngas and the chemical composition of groundwater.
2. The Ansys-Fluent software is a useful tool for creating models of the coal gasification process.
3. Obtained parameters from the numerical solution facilitated developing the geochemical model of the reaction and transport of syngas migration into surrounding rocks thanks to the PHREEQC software.

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