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EXERGY ANALYSIS OF THE COAL GASIFICATION PROCESS IN EX-SITU CONDITIONS

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Abstract

In this article the possibilities of implementing exergy analysis of coal gasification processes in ex-situ conditions was presented. The analysis was performed in order to detect the sources of exergy loss. The experimental results of the coal gasification process are also presented and was used as input data to perform the exergy analysis of the coal gasification process.

Keywords

coal gasification process, exergy analysis, fossil fuels.

1. INTRODUCTION

Coal gasification is the chemical processing of fossil fuels through the thermo-chemical conversion of coal seams to a syngas due to interaction with gasification agents (air, oxygen or a mixture of oxygen and steam) (Białecka 2008; Bielewicz, Prus, Honysz 1993; Stańczyk 2008). Syngas is a result of the thermo-chemical process (Białecka 2008; Stańczyk 2008; Stańczyk et al. 2012). Energy devaluation is mainly related to the occurrence of certain exergy value losses of the gasification reaction by-products that are apparently only dissipated in natural surrounding of the georeactor; in the analysed case in the rock mass (Łączny 2011).

The success and the commercialization of technology of underground coal gasification process (UCG) depend on the effective use of chemical energy accumulated in fossil fuels (Białecka 2008; Stańczyk 2008; Szargut, Guzik, Górnik 1979).

The main goal of the work is to detect the causes of reduction of the excellence of the UCG process in the form of the value of the exergy loss, and thus by obtaining information concerning the possibilities of its improvement (Szargut, Petela 1965; Szargut 2007; Szargut, Guzik, Górnik 1979; Szargut 1976).

Article presents the practical benefits of the implementation of exergy analysis for examining the coal gasification process under ex-situ conditions (Szargut, Petela 1965). The analysis is carried out in order to detect the main sources of exergy loss of the georeactor. The results of coal gasification process in ex-situ conditions were obtained and developed by the research employees of Department of Energy Saving and Air Protection of the Central Mining Institute (Stańczyk et al. 2012).

2. DESCRIPTION OF THE EX-SITU TESTS

The experiment was carried out in a block of coal, which was built to imitate the phenomena accompanying underground coal gasification process. The tests was carried out in the time interval of 170 hours. The main elements of the reactor were shown in Figure 1. The coal gasification process tests were realized under normal conditions 5.

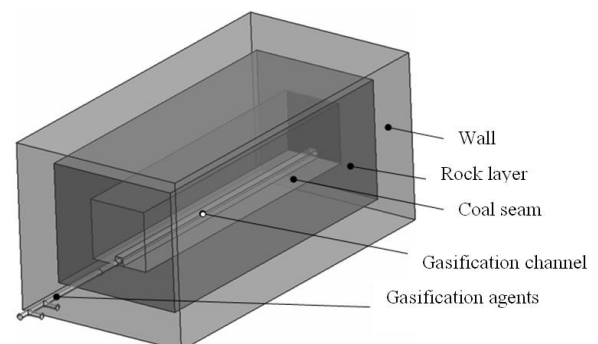


Fig. 1. Model of ex-situ reactor developed for simulation the gasification process

Along the gasification channel, about dimensions $0.1 \times 0.1 \times 2.5$ m, the coal gasification process was realized. The gasification channel was built along a solid block of coal about dimension $0.7 \times 0.7 \times 2.5$ m. Surrounding of the coal seam was a layer of rock. The rock layer was created to imitate the natural surrounding of the georeactor. The georeactor was insulated from the surrounding without the loss of gas. The chemical composition of syngas and temperature were measured at the outlet of the reactor. The pressure of gasification was equal to the ambient pressure (Stańczyk et al. 2012).

3. ANALYSIS OF THE GEOREACTOR

Exergy analysis describes the following equation (Szargut 2007; Szargut, Guzik, Górnik 1979; Szargut 1976):

$$B_d = \Delta B_u + B_{wuz} + L + \sum \Delta B_{cr} + \delta B \quad (1)$$

where:

- ΔB_u – system exergy [J]
- B_{wuz} – exergy of products [J]
- L – work performed by a system [J]
- $\sum \Delta B_{cr}$ – exergy of external heat source [J]
- δB – exergy loss [J]

For the purposes of tests was decided to divide the georeactor into two volumes. The results were shown in Figure 2.

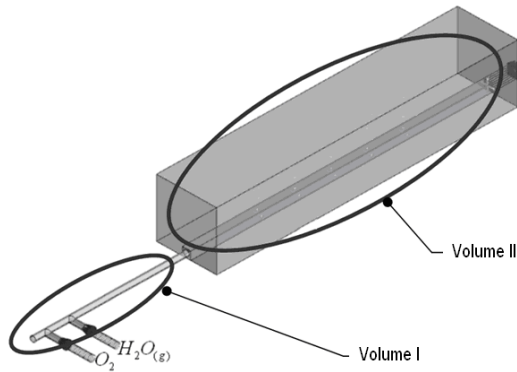


Fig. 2. View of the georeactor

3.1. Exergy analysis of the gasification agents

The equation (1) was adapted to the examined process conditions. In the first order, the process of mixing the gasification agents was analyzed. The components of the gasification agents delivered to the reactor were presented in Figure 3.

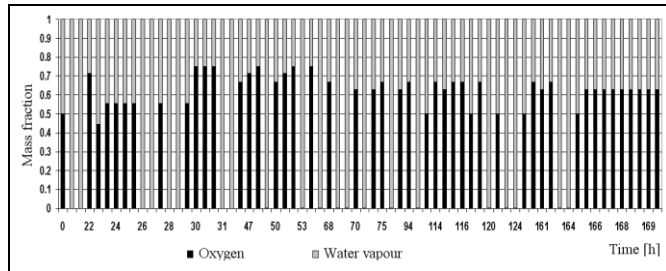


Fig. 3. Changes of the oxygen and water vapour volume fraction in the time interval of 170 hours (Stańczyk et al. 2012)

Change of the gasification agents were shown in Figure 4.

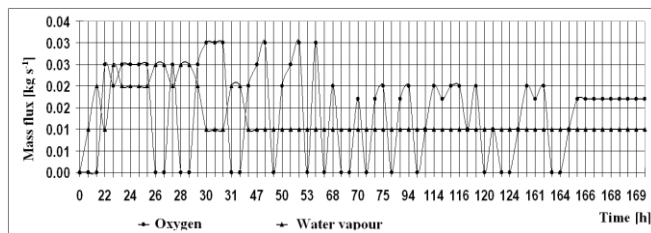


Fig. 4. Mass flow of a water vapour and oxygen in the time interval of 170 hours (Stańczyk et al. 2012)

In connection with the above, equation (1) can be formulated in the following form:

$$B_{O_2} + B_{H_2O} = B_w + \delta B_s = B_w + \delta B_{s_{oi}} + \delta B_{s_d} + \delta B_{s_r} \quad (2)$$

where:

- B_w – exergy of the gasification agents [J]
- $B_{O_2}; B_{H_2O}$ – exergy of the gasification medium components [J]
- δB – internal exergy losses [J]
- $\delta B_{s_{oi}}$ – exergy losses due to heat flux [J]
- δB_{s_d} – exergy losses due to diffusion [J]
- δB_{s_r} – exergy losses due to flow resistance [J]

The graphic interpretation of the exergy balance of analysed volume I was shown in Figure 5.

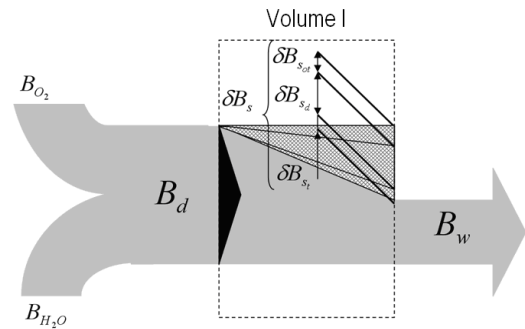


Fig. 5. Flow diagram of the volume I

The system, described in Figure 2 as volume I, is an open system, where mass and energy change enables to interpretate the equation (2) in the following form, namely

$$\frac{dB_{O_2}}{dt} + \frac{dB_{H_2O}}{dt} = \frac{dB_w}{dt} + \frac{dB_s}{dt} \quad (3)$$

where:

- $\frac{dB_{O_2}}{dt}; \frac{dB_{H_2O}}{dt}$ – change of exergy of components of the gasification agent [$J \cdot s^{-1}$]
- $\frac{dB_w}{dt}$ – change of exergy of mixture, [$J \cdot s^{-1}$]
- $\frac{dB_s}{dt}$ – change of exergy losses of mixture [$J \cdot s^{-1}$]

In accordance with the above, the internal exergy loss was formulated in the following form (4):

$$\delta B_s = B_{O_2} + B_{H_2O} - B_w \quad (4)$$

where:

- δB – change of internal exergy loss [$J \cdot s^{-1}$]
- $B_{O_2}; B_{H_2O}$ – change of exergy of components of gasification medium [$J \cdot s^{-1}$]
- B_w – change of exergy of products [$J \cdot s^{-1}$].

The exergy of components of the gasification agent were expressed in the following form of equation (5) based on work (Szargut 2007):

$$B_f = H - H_o - T_o(S - S_o) \quad (5)$$

where:

- H_o, S_o – enthalpy and entropy in the ambient pressure and temperature [J]

H, S – enthalpy and entropy [J]
 T_o – ambient temperature [K]

After the appropriate transformations, the following form of equation was developed based on work (Szargut 2007):

$$\delta \dot{B}_s = \dot{m}_{O_2} (h_{O_2} - h_{o_{O_2}} - T_o (s_{O_2} - s_{o_{O_2}})) + \dot{m}_{H_2O} (h_{H_2O} - h_{o_{H_2O}} - T_o (s_{H_2O} - s_{o_{H_2O}})) - \dot{m}_w (h_w - h_{o_M} - T_o (s_M - s_{o_M})) \quad (6)$$

where:

\dot{m}_{O_2} – mass flow of oxygen [$\text{kg}\cdot\text{s}^{-1}$]
 \dot{m}_{H_2O} – mass flow of water vapour [$\text{kg}\cdot\text{s}^{-1}$]
 \dot{m}_{H_2O} – mass flow of the mixture [$\text{kg}\cdot\text{s}^{-1}$]
 T_o – ambient temperature [K]
 h_{O_2} – enthalpy of oxygen [$\text{J}\cdot\text{kg}^{-1}$]
 h_{H_2O} – enthalpy of water vapour [$\text{J}\cdot\text{kg}^{-1}$]
 $h_{o_{O_2}}$ – enthalpy of oxygen under normal conditions [$\text{J}\cdot\text{kg}^{-1}$]
 $h_{o_{H_2O}}$ – enthalpy of water vapour under normal conditions [$\text{J}\cdot\text{kg}^{-1}$]
 s_{O_2} – entropy of oxygen [$\text{J}\cdot\text{kg}^{-1}$]
 s_{H_2O} – entropy of water vapour [$\text{J}\cdot\text{kg}^{-1}$]
 $s_{o_{O_2}}$ – entropy of oxygen under normal conditions [$\text{J}\cdot\text{kg}^{-1}$]
 $s_{o_{H_2O}}$ – entropy of water under normal conditions [$\text{J}\cdot\text{kg}^{-1}$]

Under the conditions of the process, the phenomenon of intensive mixing of gasification agent components occurs. This phenomenon is the result of an exergy loss due to the diffusion of mixture components. The exergy loss was estimated based on the following equation (7) given in work (Szargut 2007):

$$\delta \dot{B}_{sd} = RT_o \dot{n}_k \sum_i z_{ik} \ln \frac{z_{ik}}{z_{im}} \quad (7)$$

where:

$\delta \dot{B}_{sd}$ – exergy losses as a result of mixing of gasification agents [$\text{J}\cdot\text{s}^{-1}$]

\dot{n}_k – the moles of the k component of gasification agents [$\text{mole}\cdot\text{s}^{-1}$]

z_{ik} – initial mole fraction of the i component of the gasification agents [-]

z_{im} – the final molar fraction of the i component in the gasification agents [-]

The mixing process also includes an irreversible process due to the transport of heat into the surrounding area. The value of these losses was determined based on the following equation given in work (Szargut 2007):

$$\delta \dot{B}_{sw} = \left(1 - \frac{T_o}{T}\right) \dot{Q} \quad (8)$$

where:

$\delta \dot{B}_{sw}$ – exergy losses due to heat loss [$\text{J}\cdot\text{s}^{-1}$]
 T_o – ambient temperature [K]

T – temperature of the gasification agents [K]

\dot{Q} – heat loss [$\text{J}\cdot\text{s}^{-1}$]

The heat loss was estimated as the amount of heat lost by the gas in interaction with the surrounding. The exergy efficiency was expressed in the form of (9):

$$\eta = \frac{\dot{B}_w}{\dot{B}_{O_2} + \dot{B}_{H_2O}} \quad (9)$$

In Figures 6–9 the results of the analysis were presented.

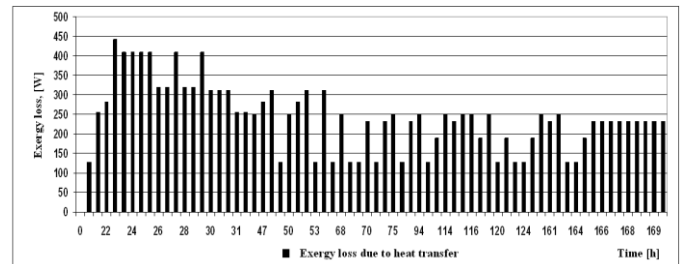


Fig. 6. The exergy loss due to heat transfer in a time interval of 170 hours

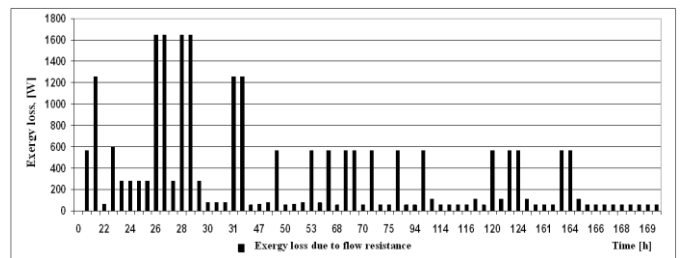


Fig. 7. The exergy loss due to flow resistance in the time interval of 170 hours

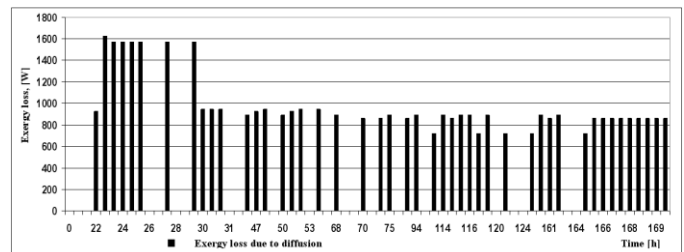


Fig. 8. The exergy loss due to diffusion in the time interval of 170 hours

The exergy efficiency of the gasification agents transport process was shown in Figure 9.

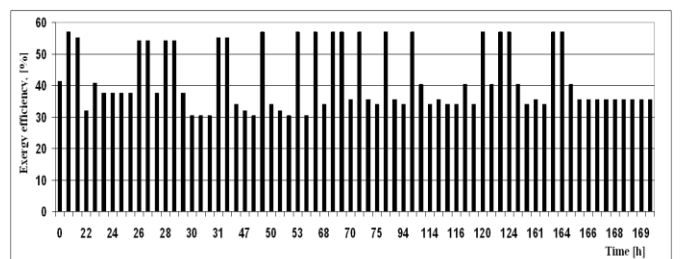


Fig. 9. Exergy efficiency of the gasification agent transport process in the time interval of 170 hours

The analysis shows that the primary sources of the exergy losses are phenomena of diffusion and dissipation in the first 30 hours of the process.

3.2. Exergy analysis of the reactor

Under the conditions of the UCG process along the gasification channel, three gasification reaction zones are separated, namely (Białecka 2008):

- oxidation zone
- reduction zone
- pyrolysis zone

The oxidation zone includes exothermic reactions between the gasification agent and the coal seam. The reduction zone includes endothermic reactions between products of the oxidation zone and the gasification agent. The pyrolysis zone includes the thermo-chemical processes in which gaseous and liquid products are produced (Białecka 2008; Stańczyk 2008). A graphic interpretation of the volume II was shown in Figure 10.

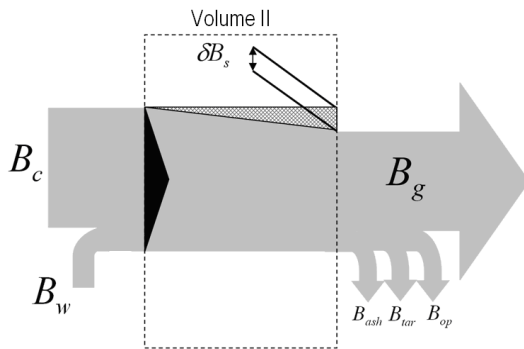


Fig. 10. Flow diagram of volume II

Exergy of the volume II was expressed in the following form of equation:

$$B_c + B_w = B_g + B_{ash} + B_{tar} + B_{op} + \delta B_s \quad (10)$$

The expression (10) is transformed to the following equation (11):

$$\dot{B}_c + \dot{B}_w = \dot{B}_g + \dot{B}_{ash} + \dot{B}_{tar} + \dot{B}_{op} + \delta \dot{B}_s \quad (11)$$

where:

- \dot{B}_w – exergy of gasification agent [$\text{J}\cdot\text{s}^{-1}$]
- \dot{B}_{ash} – exergy of ash [$\text{J}\cdot\text{s}^{-1}$]
- \dot{B}_c – exergy of the coal [$\text{J}\cdot\text{s}^{-1}$]
- \dot{B}_g – exergy of syngas [$\text{J}\cdot\text{s}^{-1}$]
- \dot{B}_{op} – exergy of liquid products, [$\text{J}\cdot\text{s}^{-1}$]
- \dot{B}_{tar} – exergy of tar [$\text{J}\cdot\text{s}^{-1}$]
- $\delta \dot{B}_s$ – exergy loss [$\text{J}\cdot\text{s}^{-1}$]

Hence, the internal exergy losses were estimated based on the following equation:

$$\delta \dot{B}_s = \dot{B}_c + \dot{B}_w - (\dot{B}_g + \dot{B}_{ash} + \dot{B}_{tar} + \dot{B}_{op}) \quad (12)$$

After the appropriate transformations, the following equation was obtained based on work (Szargut, Guzik, Górnik 1979):

$$\delta \dot{B}_s = \dot{B}_w + \dot{P} \left[W_d + r_n \cdot w \left(1.0437 + 0.1896 \frac{h}{c} + 0.0617 \frac{o}{c} + \left[\left(+0.0428 \frac{n}{c} \right) + (b_{chs} - W_{ds})s \right] - (\dot{B}_g + \dot{B}_{ash} + \dot{B}_{tar} + \dot{B}_{op}) \right) \quad (13)$$

where:

- \dot{B}_w – exergy of the gasification mixture [$\text{J}\cdot\text{s}^{-1}$]
- W_d – calorific value of wet coal ($W_d = 3.54e^{+07}$) [$\text{J}\cdot\text{kg}^{-1}$]
- r_n – heat of water vaporization [$\text{J}\cdot\text{kg}^{-1}$]
- w – moisture fraction ($w = 0.0115$)
- $\frac{h}{c}, \frac{o}{c}, \frac{n}{c}$ – mass fraction of hydrogen and carbon, oxygen and carbon as well as nitrogen and carbon
- b_{chs} – exergy of sulphur [$\text{J}\cdot\text{kg}^{-1}$]
- W_{ds} – sulphur calorific value [$\text{J}\cdot\text{kg}^{-1}$]
- s – mass fraction of sulphur ($s = 0.0028$)
- \dot{P} – mass loss rate of coal, [$\text{kg}\cdot\text{s}^{-1}$]

The moisture and sulphur mass fraction were taken based on the ultimate/proximate analysis of coal seam (Table 1) (Stańczyk et al. 2012).

Slag exergy was determined based on the following form of equation based on work (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{ash} = \dot{P} \frac{G_p c_p}{12} (Mb_{chn})_C \quad (14)$$

where:

- \dot{P} – mass loss rate of coal [$\text{kg}\cdot\text{s}^{-1}$]
- c_p – coal mass fraction ($c_p = 0.35$) [–]
- G_p – mass fraction of slag ($G_p = 0.045$ [$\text{kg}\cdot\text{kg}^{-1}$])
- $(Mb_{chn})_C$ – normal chemical exergy ($(Mb_{chn})_C = 410\,820$) [$\text{kJ}\cdot\text{kmole}^{-1}$]

The chemical composition of coal seam was shown in Table 1.

Table 1. Proximate and ultimate analysis of the coal seam (Stańczyk et al. 2012)

Proximate analysis	Fixed carbon	63.83%
	Volatile parts	32.41%
	Ash	2.21%
	Moisture	1.55%
Ultimate analysis	C	83.84%
	H	4.94%
	O	9.79%
	N	1.15%
	S	0.28%

The mass loss rate of coal was defined based on the equation (15) and shown in Figure 11:

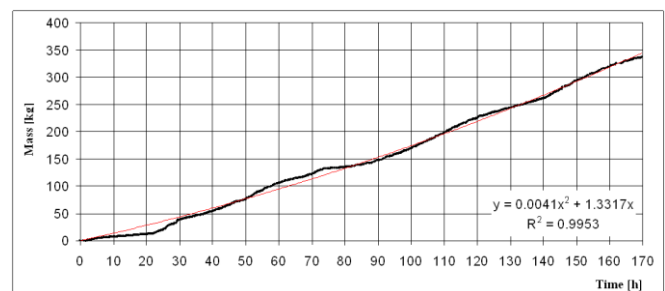


Fig. 11. The mass loss rate of the coal in the time interval of 170 hours

$$\dot{P} = 0.0082t \quad (15)$$

where t – time [s]

The amount of carbon converted was presented in Figure 11 and was calculated from the output data of the reactor.

Exergy of \dot{B}_g was estimated based on the following equation given in work (Szargut, Guzik, Górnik 1979):

$$\dot{B}_g = \dot{B}_{g_f} + \dot{B}_{g_{ch}} \quad (16)$$

where:

\dot{B}_{g_f} – physical part of exergy of gas component [$\text{J}\cdot\text{s}^{-1}$]

$\dot{B}_{g_{ch}}$ – chemical part of exergy of gas components [$\text{J}\cdot\text{s}^{-1}$]

Individual components of the equation (16) were defined based on the following expression given in work (Szargut, Guzik, Górnik 1979):

• physical part (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{g_f} = \sum_i \dot{n}_i \cdot (Mh_{f_d})_i - T_o \sum_i \dot{n}_i \cdot \Delta(Ms_p)_i \Big|_{T_o}^{T_g} \quad (17)$$

where:

\dot{n}_i – fraction of gas components [$\text{mole}\cdot\text{s}^{-1}$]

$(Mh_{f_d})_i$ – specific enthalpy of gas components (CO_2 , CO , CH_4 , H_2 , O_2 , N_2) [$\text{J}\cdot\text{mole}^{-1}$]

$\Delta(Ms_p)_i \Big|_{T_o}^{T_g}$ – specific entropy of gas components (CO_2 , CO , CH_4 , H_2 , O_2 , N_2), [$\text{J}\cdot\text{mole}^{-1}\cdot\text{K}^{-1}$]

• chemical part (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{g_{ch}} = \sum_i \dot{n}_i \cdot (Mb_{chn})_i - T_o (MR) \sum_i \dot{n}_i \ln z_i \quad (18)$$

where:

$(Mb_{chn})_i$ – specific exergy to gas components (CO_2 , CO , CH_4 , H_2 , O_2 , N_2 , C_2H_6), [$\text{J}\cdot\text{mole}^{-1}$]

$\ln z_i$ – mole fraction of the i -th component

The parameter values for the equation (17) and (18) are shown in Table 2.

Table 2. Average value of the enthalpy and entropy for $T_{g,ave} = 350$ [K] (Szargut, Guzik, Górnik 1979)

Component	$(Mh_{f_d})_i$ [kJ·kmol ⁻¹]	$\Delta(Ms_p)_i \Big _{T_o}^{T_g}$ [kJ·kmol ⁻¹]	$(Mb_{chn})_i$ [kJ·kmol ⁻¹]
CO	2243	6.93	275 430
CH ₄	2848	8.65	836 930
H ₂	2224	6.73	238 490
O ₂	2273	6.89	3970
CO ₂	2942	9.05	20 140
N ₂	2240	6.89	690

The composition of syngas was presented in Figure 12 and the mass flow was presented in Figure 13.

The tests also included the monitoring of temperature of the syngas at the outlet of the georeactor system. The measured parameter was shown in Figure 14.

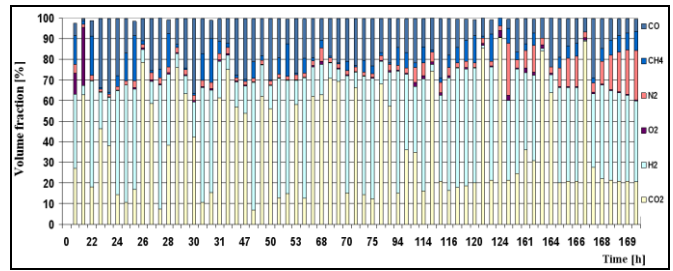


Fig. 12. The concentration of the syngas in the time interval of 170 hours (Stańczyk et al. 2012)

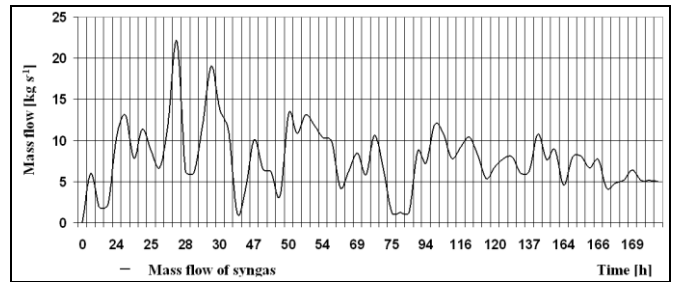


Fig. 13. The mass flow of the syngas in the time interval of 170 hours (Stańczyk et al. 2012)

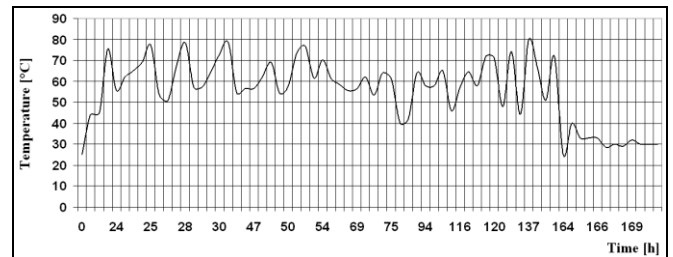


Fig. 14. Changes of the syngas temperature at the outlet of the gasification channel in the time interval of 170 hours (Stańczyk et al. 2012)

The tar exergy \dot{B}_{tar} was estimated based on the following equation (19) given in work (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{tar} = \dot{B}_{tar_f} + \dot{B}_{tar_{ch}} \quad (19)$$

where the physical part was calculated based on work (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{tar_f} = \dot{m}_{g_{uz}} \left(G_s C_{s_p} (T_g - T_o) - T_o G_s c_{sp} \ln \frac{T_g}{T_o} \right) \quad (20)$$

where:

$\dot{m}_{g_{uz}}$ – mass flow of syngas [$\text{kg}\cdot\text{s}^{-1}$]

G_s – mass fraction of tar ($G_s = 0.034$) [$\text{kg}\cdot\text{kg}^{-1}$]

C_{sp} – specific heat of tar ($c_{sp} = 0.8e^{+03}$) [$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$]

T_g – temperature of syngas [K]

and chemical part was calculated based on work (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{tar_{ch}} = \dot{m}_{g_{uz}} \sum_s \beta_s W_{d_s} \quad (21)$$

where:

$\dot{m}_{g_{uz}}$ – syngas mass flow [$\text{kg}\cdot\text{s}^{-1}$]

G_s – mass fraction of tar ($G_s = 0.034$) [$\text{kg}\cdot\text{kg}^{-1}$]

W_{d_s} – calorific value of tar ($W_{d_s} = 39\ 800e^{+03}$) [$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$]

The exergy of waste water was interpreted based on the following form of the expression given in work (Szargut, Guzik, Górnik 1979):

$$\dot{B}_{op} = \dot{m}_g c_w \left(T_g - T_o - T_o \ln \frac{T_g}{T_o} \right) \quad (22)$$

where:

T_g – temperature of syngas [K]

\dot{m}_g – syngas mass flow [$\text{kg}\cdot\text{s}^{-1}$]

c_w – specific heat of water [$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$]

The value of changes of internal exergy losses of the analysed thermal system, in the interval of 170 hours, is described in Figure 15.

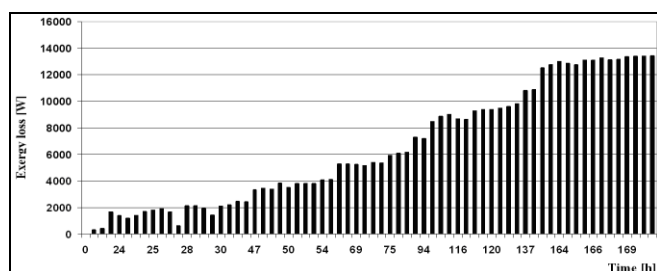


Fig. 15. Exergy losses of the coal gasification process in the time interval of 170 hours

4. DISCUSSION OF RESULTS

Within the framework of this work, an analysis of coal gasification process was carried out under ex-situ conditions. Model studies were based on performing an exergy analysis (a gasification agent and syngas) of two separate volumes. As input data for the analysis the results of ex-situ experimental tests were used, which included information regarding the changes of the temperature and chemical composition of the syngas, the mass flow and mass fraction of gasification agent components as well as the mass loss rate of coal.

The exergy analysis shows that the initial loss of exergy appears at the stage associated with supplying the gasification agent to the georeactor. Also the sources of loss are the phenomena of diffusion between the gasification agents.

The results of the research allow formulating the following conclusions:

1. Due to the losses of gasification factor exergy, it was better to create conditions in which the irreversible phenomena of diffusion and heat loss will be eliminated,
2. The exergy losses of liquid (tar) and solid (ash) products are determined by the value of chemical exergy.

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