

Żogała, A. (2014). Equilibrium simulations of coal gasification – factors affecting syngas composition. *Journal of Sustainable Mining*, 13(2), 30–38. doi:10.7424/jsm140205

## ORIGINAL PAPER

Received: 23 May 2014 | Revised: 20 July 2014 | Published online: 11 August 2014

# EQUILIBRIUM SIMULATIONS OF COAL GASIFICATION – FACTORS AFFECTING SYNGAS COMPOSITION

Alina Żogała

*Interdisciplinary PhD Studies in Field of Clean Coal Technologies, Central Mining Institute (Katowice, Poland)*

*Corresponding author: e-mail: azogala@autograf.pl, tel.: +48 503 161 360*

## ABSTRACT

<b>Purpose</b>	Coal gasification is complex technology, which results depend on many variables, connected among others with fuel, the converting agent and the process itself. The paper aims to analyze, by means of simulations, the influence of the following factors – temperature, pressure, characteristic parameters of coal and gasifying agent, on the composition and heating value of the obtained syngas. The other aim of this paper is the determination of gasification efficiency (based on the definition of cold gas efficiency) for various process conditions.
<b>Methods</b>	Computer simulations were used as the research method for the work presented. An equilibrium model, based on the stoichiometric method with four independent reactions, was formulated and used in this paper. This model was implemented in <i>Mathematica</i> software. The influence of temperature (in a range from 500 to 1500°C), pressure (changed from atmospheric to 35 atm), three types of gasifying agent (mixtures of air, pure oxygen and steam) and the composition of four Polish coals (lignite and three hard-coals) on syngas parameters were analyzed in this paper.
<b>Results</b>	Concentrations of CO <sub>2</sub> , CO, CH <sub>4</sub> , H <sub>2</sub> O, H <sub>2</sub> , N <sub>2</sub> in the equilibrium syngas, for the chosen temperature, pressure and parameters of the fuel and converting agent were the results of the simulations carried out. Subsequently, the lower heating value and process efficiency for each syngas composition was calculated.
<b>Practical implications</b>	The simulations indicated the thermodynamic limits of gasification and allowed for the formulation of the general principles ruling this process. Results presented in this paper may be useful in the preliminary optimization and analysis of coal gasification. They also can be a point of reference for more advanced simulations.
<b>Originality/value</b>	This paper presents own results obtained from equilibrium simulations of coal gasification. The author implemented a mathematical model, based on the method of Deringer and Traustel, presented earlier in literature, to carry out the calculations.

## Keywords

*coal gasification, equilibrium, syngas composition, heating value*

## 1. INTRODUCTION

Gasification is defined as the conversion of solid fuels into a gaseous product (called “syngas”) in the presence of a gasifying medium, such as: oxygen, air, steam, carbon dioxide or their combinations in different proportions. The gas obtained in this process is a mixture of combustible components (CO, H<sub>2</sub>, CH<sub>4</sub>) and other, noncombustible constituents (especially H<sub>2</sub>O, CO<sub>2</sub>, N<sub>2</sub>). The scope of potential applications of syngas may be very wide – it covers numerous chemical processes (synthesis of H<sub>2</sub>, NH<sub>3</sub>, CH<sub>3</sub>OH, SNG, Fischer-Tropsch process etc.) and the production of energy – provided that the

requirements of chemical composition and the heating value of this gas will be achieved (Petela, 1969; Wasilewski & Kobel-Najzarek, 1980).

In practice it is not an easy issue – the parameters of syngas mentioned above depend on many factors – the composition of the gasifying agent, the properties of the fuel, the pressure and temperature in the reactor. In the case of gasification carried out directly in a coal seam, geomechanical and geological aspects should also be taken into account. Determination of the importance of these factors is very complicated. What is more, they may positively affect some features

of the process, but negatively affect other ones (Żogała, Kabiesz, & Iwaszenko, 2013).

Therefore the management and running of a coal gasification process is very complicated. In such case it is necessary to create appropriate mathematical models, which simplify finding a solution to this problem.

There are a lot of different models of coal gasification, dedicated to calculate syngas composition. The simplest of them (because of the relatively uncomplicated mathematical formulation, the short time needed to achieve convergence and the small demand for computational power) are based on thermodynamic considerations and are called equilibrium models (Golec & Ilmurzyńska, 2008). An example of this kind of model is presented in this paper.

## 2. EQUILIBRIUM MODELING OF COAL GASIFICATION

Equilibrium models are based on the assumption that the rate of the particular reactions is infinitely high (or process time appropriately long) which allows the equilibrium state to be reached by the analyzed system. This premise is often acceptable in the case of real reactors, when gasification is carried out in conditions of high temperature (which ensures a fast rate of reactions) and intensive mixing (which enhances mass and heat exchange and thereby allows kinetic limitations and diffusion effects to be neglected).

There are two general approaches used in the equilibrium modeling of gasification: stoichiometric and non-stoichiometric. The first method is based on the mass-action law and knowledge about equilibrium constants of all the reactions considered, the second – minimizes Gibbs free energy of the analyzed system. The non-stoichiometric method is more universal (there is no need to determine chemical reactions and their equilibrium constants), but requires more time for computations. The stoichiometric method is appropriate only for one defined set of chemical reactions (when a new component must be included in the reacting mixture then the algorithm of the solution is changed), but the time of simulation is relatively short (Golec & Ilmurzyńska, 2008; Kozaczka, 1994). In the work presented a stoichiometric model of coal gasification is developed.

## 3. THE MODEL AND GASIFICATION SYSTEM DESCRIPTION

Although over one hundred chemical compounds take part in the gasification process (Golec & Ilmurzyńska, 2008), in the presented model only eight substances are considered – C, CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, CH<sub>4</sub>, O<sub>2</sub> and N<sub>2</sub>. Nitrogen is treated as inert, so seven compounds, formed from three elements, participate in conversions. Therefore the model was determined by four independent reactions. Usually the following reactions are used in equilibrium simulations (Higman & Van der Burgt, 2008; Kozaczka, 1994):

- the Boudouard reaction:  

$$\text{C} + \text{CO}_2 \leftrightarrow 2\text{CO} \quad +172 \text{ MJ/kmol} \quad (1)$$
- the water gas reaction:  

$$\text{C} + \text{H}_2\text{O} \leftrightarrow \text{CO} + \text{H}_2 \quad +131 \text{ MJ/kmol} \quad (2)$$
- the methanation reaction:  

$$\text{C} + 2\text{H}_2 \leftrightarrow \text{CH}_4 \quad -75 \text{ MJ/kmol} \quad (3)$$

- the water gas shift reaction:  

$$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \quad -41 \text{ MJ/kmol} \quad (4)$$

Equilibrium calculations were carried out based on the method of Deringer and Traustel, which was described in: (Kozaczka, 1994). This method assumes that the final gas consists of six compounds (CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>) and requires determination of the following inputs:

- process parameters (pressure and temperature),
- fuel composition,
- composition of the gasifying agent.

Other assumptions connected with the equilibrium model were:

- temperature was uniform for the whole reactor (oxidation, reduction and drying and pyrolysis zone were treated as one zone),
- the model was zero dimensional (geometry of the reactor was not considered),
- temperature did not change during the process (the influence of the heat of the reaction was not taken into account),
- tar formation was not simulated,
- the presence of sulfur and ashes was ignored.

Equations of the model, presented in: (Kozaczka, 1994), were implemented in the commercial computation software *Mathematica*.

### 3.1. Parameters of the process

Simulations were carried out for pressures from 1 atm to 35 atm<sup>1</sup> and for temperatures ranging from 500°C to 1500°C.

Values of equilibrium constants of reactions (1) – (4) as a function of temperature were determined from approximate equations proposed by Gumz (Kozaczka, 1994):

$$\log K_1 = 3.26730 - \frac{8820690}{T} - 1.208714 \cdot 10^{-3} T + 0.153734 \cdot 10^{-6} T^2 + 2.295483 \log T \quad (5)$$

$$\log K_2 = 0.8255488 \cdot 10^{-6} T^2 + 14.515760 \log T - \frac{4825968}{T} - 5.671122 \cdot 10^{-3} T - 33.45778 \quad (6)$$

$$\log K_3 = \frac{466280}{T} - 2.09594 \cdot 10^{-3} T + 0.38620 \cdot 10^{-6} T^2 + 3.034338 \log T - 13.06361 \quad (7)$$

$$\log K_4 = -36.72508 + \frac{3994704}{T} - 4.462408 \cdot 10^{-3} T + 0.671814 \cdot 10^{-6} T^2 + 12.220277 \log T \quad (8)$$

Changes of these *K* – values, in the analyzed temperature scope, are presented in figure 1.

<sup>1</sup> Maximal pressure used in the model was equal to 35 atm because similar values of this parameter are applied in moving bed reactors (Wasilewski & Kobel-Najzarek, 1980). Also two other, presented earlier in literature, equilibrium calculations of coal (Wasilewski & Kobel-Najzarek, 1980) and biomass gasification (Sharma, 2008) used maximum pressure values of approximately 35 atm.

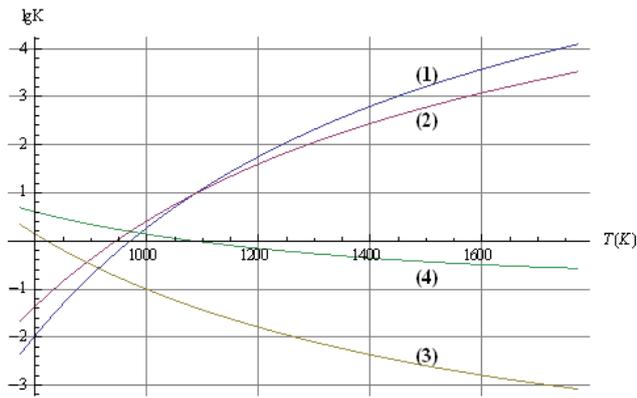


Figure 1. Values of equilibrium constants of reactions (1), (2), (3) and (4) in the analyzed temperature scope

### 3.2. Fuel composition

The gasification processes of four Polish coals – lignite from open cast Belchatów and hard coals from Bielszowice, Ziemowit and Bobrek coal mines were simulated. Samples of these fuels were analyzed earlier and presented in: (Stańczyk et al., 2011; Smoliński, Stańczyk, Kapusta, & Howaniec, 2012). Results of the ultimate and proximate analysis of these coals are given in table 1.

Table 1. Results of analysis of coal samples examined in simulations

Parameter	Coal sample from mine:			
	Belchatów	Ziemowit	Bobrek	Bielszowice
	<i>As received</i>			
Total moisture, $W^r$ (%)	53.0	9.0	4.0	1.6
Ash, $A^r$ (%)	4.7	5.4	10.0	2.2
Total sulfur, $S^r$ (%)	1.1	0.6	1.0	0.28
Calorific value, $LHV^r$ (kJ/kg)	9,316	26,969	28,611	33,370
	<i>Analytical</i>			
Moisture, $W^a$ (%)	14.5	6.8	2.1	1.5
Ash, $A^a$ (%)	8.6	5.5	10.2	2.2
Volatiles, $V^a$ (%)	42.8	35.9	33.2	32.4
Heat of combustion, $HHV^a$ (kJ/kg)	20,161	28,782	30,327	34,572
Calorific value, $LHV^a$ (kJ/kg)	18,955	27,581	29,242	33,399
Sulfur, $S^a$ (%)	1.9	0.6	1.0	0.28
Carbon, $C^a$ (%)	50.7	69.6	73.6	83.8
Hydrogen, $H^a$ (%)	3.9	4.6	4.7	4.9
Nitrogen, $N^a$ (%)	1.3	0.9	1.2	1.2
Oxygen, $O^a$ (%)	19.1	12	7.2	6.12
Reference	(Stańczyk et al., 2011)	(Smoliński, Stańczyk, Kapusta, & Howaniec, 2012)	(Stańczyk et al., 2011)	(Stańczyk et al., 2011)

\* Oxygen is calculated as:

$$(O^a) = 100 - (W^a) - (A^a) - (C^a) - (H^a) - (S^a) - (N^a) (\%)$$

### 3.3. The composition of the gasifying agent

The influence of different gasifying agent compositions on syngas parameters was examined in the work presented. Three types of converting medium, with changed proportion of components, were used:

- mixtures of steam and pure oxygen,
- mixtures of steam and air,
- mixtures of air and pure oxygen.

It was decided, that air, steam and oxygen would play the role of gasifying agents in the work presented, because these substances are mostly used in practical experiments.

## 4. RESULTS AND DISCUSSION

As a result of simulations, concentrations of  $CO_2$ ,  $CO$ ,  $CH_4$ ,  $H_2O$ ,  $H_2$ ,  $N_2$  in equilibrium syngas for the assumed values of temperature and pressure and the parameters of the gasifying agent and fuel were obtained. Subsequently, for each composition of product gas, the lower heating value (LHV) was calculated from the relation given below (Tomeczek, 1991):

$$LHV = \sum_{i=1}^n x_i LHV_i \quad (9)$$

where  $x_i$  is the mole fraction of the combustible component  $i$  ( $CO$ ,  $CH_4$ ,  $H_2$ ) in syngas,  $LHV_i$  – lower heating value of this component  $i$ ,  $n$  – number of combustible components in syngas (equal to three in the given case).

The efficiency of the gasification process was determined based on the definition of cold gas efficiency  $\eta$  (Higman & Van der Burgt, 2008):

$$\eta = \frac{LHV_{\text{syngas}}}{LHV_{\text{fuel}}} = \frac{x_{H_2} LHV_{H_2} + x_{CO} LHV_{CO} + x_{CH_4} LHV_{CH_4}}{LHV_{\text{fuel}}} \quad (10)$$

### 4.1. Temperature

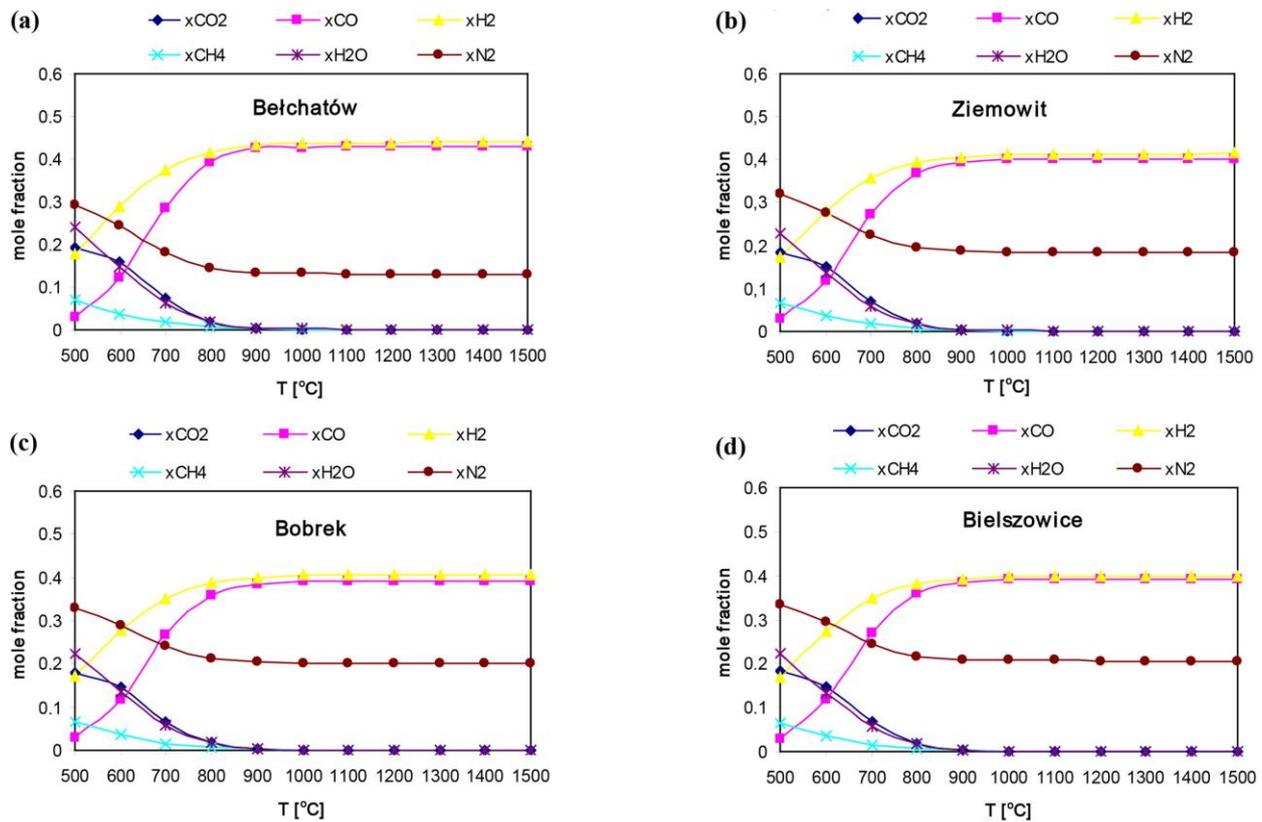
The effect of gasification temperature on syngas composition, calorific value of the product and process efficiency was investigated for atmospheric pressure and for conversion in a mixture of steam and air (in a ratio of 1:1).

In figure 2 changes in the mole fractions of the constituents of the final gas (calculated for each of the analyzed coals), as a function of temperature in the reactor were presented.

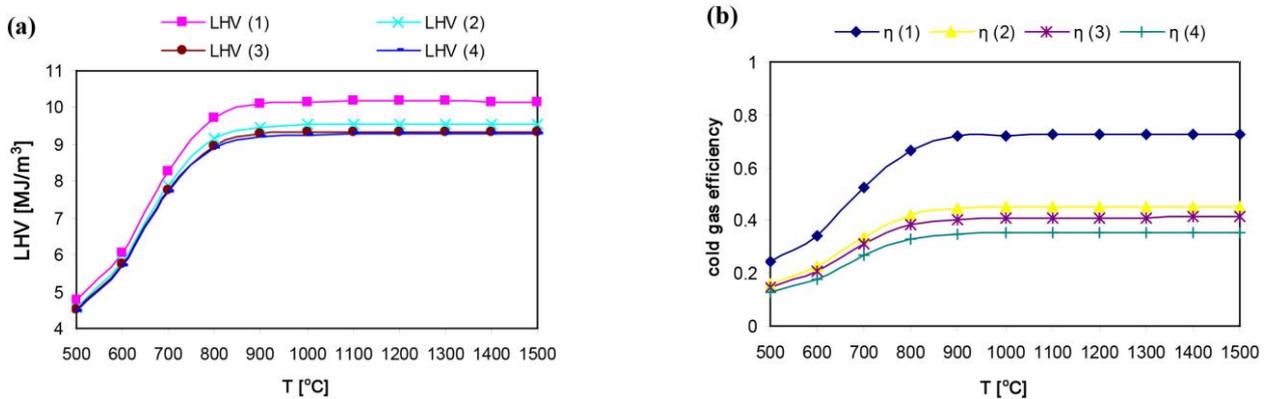
It could be observed, that the contents of  $CO_2$ ,  $N_2$ ,  $H_2O$ ,  $CH_4$  in syngas, decrease when the temperature of gasification grows, while the concentrations of  $CO$  and  $H_2$  in the product increase. The results obtained are in agreement with Le Chatelier's principle. This rule expresses the effect of a disturbance on an equilibrium state: the system reacts in such a way that the disturbance is counteracted (Atkins, 2001). This means, that temperature increase shifts the equilibrium of endothermic reactions (1) and (2) in the direction of the product formation ( $CO$  and  $H_2$ ), while the equilibrium of exothermic reactions (3) and (4) is moved in the direction of the reactants (mainly  $H_2$ ). Therefore the raising of the temperature of the gasification process is not beneficial to the generation of methane.

The effect of temperature in the reactor on the lower heating value of the syngas and the process efficiency was shown in figure 3. Syngas's calorificity grows with the increasing of temperature, which is due to boosting the amounts of  $CO$  and  $H_2$  in the process<sup>2</sup>. Because the heating value of the product increases, the cold gas efficiency improves significantly (from about 25% to 70% in the case of lignite, and from about 15% to approximately 40% for hard coals).

<sup>2</sup> Methane is produced in small amounts and has no significant influence on the syngas's calorific value.



**Figure 2.** Effect of temperature on syngas composition – results of simulations obtained for gasification in a mixture of air and steam (in a ratio of 1:1) of coal from mines: (a) – Belchatów, (b) – Ziemowit, (c) – Bobrek, (d) – Bielszowice



**Figure 3.** The effect of temperature on the lower heating value of syngas (a) and cold gas efficiency (b) – results of simulations obtained for gasification in a mixture of air and steam (in a ratio of 1:1) of coal from mines: (1) – Belchatów, (2) – Ziemowit, (3) – Bobrek, (4) – Bielszowice

## 4.2. Pressure

The role of pressure on the concentrations of syngas compounds, the lower heating value of product gas and process efficiency was examined for a temperature equal to 700°C<sup>3</sup> and for conversion with a mixture of steam and air (in a ratio of 1:1).

In figure 4 changes of syngas composition as a function of growing pressure in the reactor are given. It can be observed

<sup>3</sup> Rate of gasification depends on the transport of reactants and products and the rate of chemical reactions. Above 700°C the rate of chemical reactions begins to play a dominant role in this combination of processes (Petela, 1969). It is also a temperature observed in the reduction zone in the UCG reactor (Bhutto, Bazmi, & Zahedi, 2013) where reactions provided to obtain H<sub>2</sub> and CO take place.

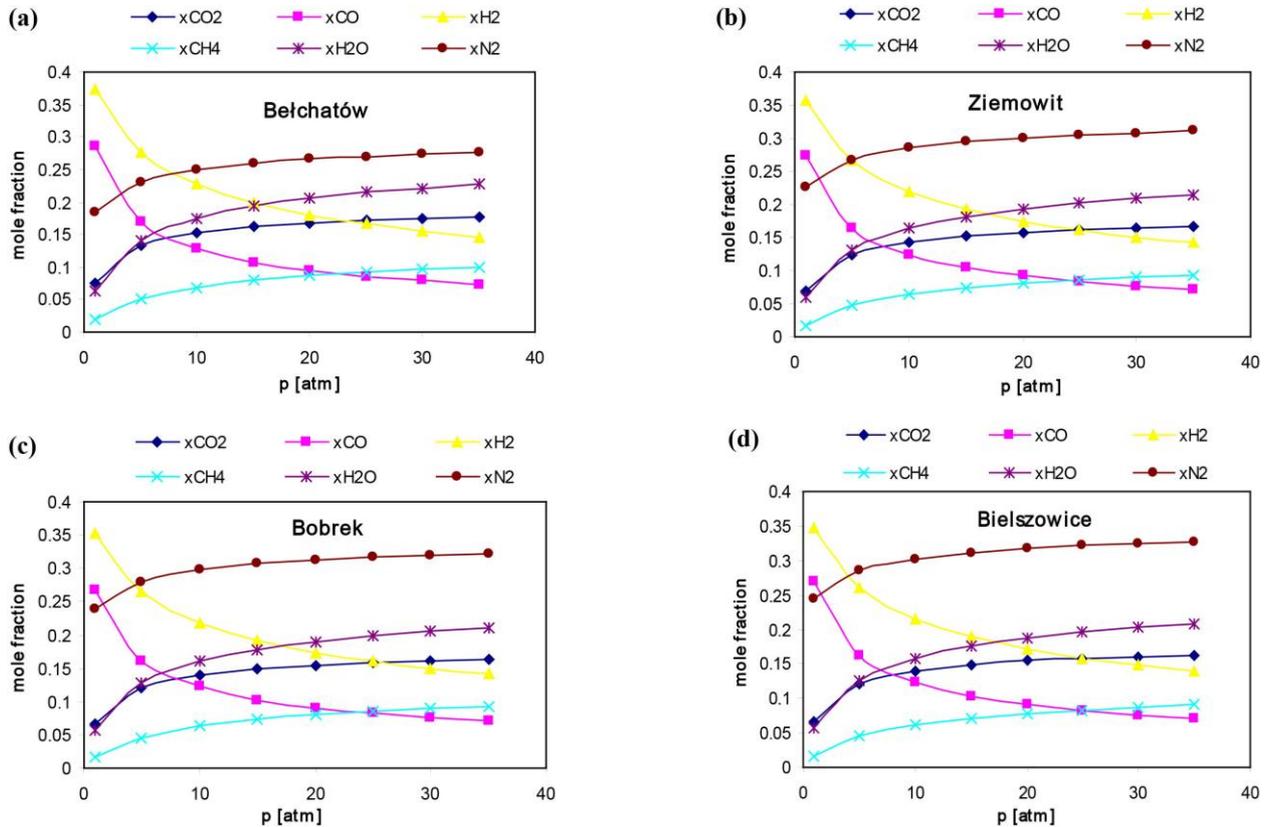
that, the concentrations of CO and H<sub>2</sub> in the final product decrease as the pressure increases, while the contents of other compounds (CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub>) in the produced gas boost. These changes are also compatible with conclusions from Le Chatelier's principle. Reaction (1), (2) and (3) have non – equal amounts of gaseous molecules<sup>4</sup> on the left and right side. Therefore pressure increase in the system promotes the formation of CO<sub>2</sub> and H<sub>2</sub>O in reactions (1) and (2), where the number of gaseous moles is smaller on the left and the production of CH<sub>4</sub> in reaction (3) with a smaller amount of gaseous molecules on the right.

In figure 5 the effect of pressure on the calorificity of the product gas and cold gas efficiency was illustrated. Because

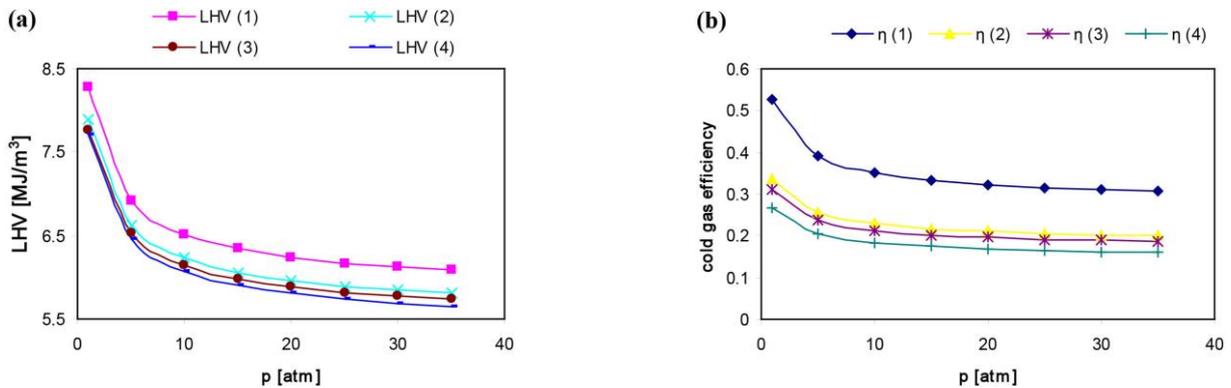
<sup>4</sup> Solid carbon is not taken into account in these considerations.

the value of the first of these parameters decreases with increasing pressure (which is due to the declining amounts of CO and H<sub>2</sub> in the syngas, CH<sub>4</sub> is produced in small amounts in comparison to the previously mentioned compounds), also

the cold gas efficiency of the process reduces (from above 50% to about 30% in the case of lignite gasification and from approximately 30% to about 20% for conversion of hard coals).



**Figure 4.** Effect of pressure on syngas composition – results of simulations obtained for gasification at a temperature of 700°C and using a mixture of air and steam (in a ratio of 1:1) of coal from mines: (a) – Bełchatów, (b) – Ziemowit, (c) – Bobrek, (d) – Bielszowice



**Figure 5.** Effect of pressure on the lower heating value of syngas (a) and cold gas efficiency (b) – results of simulations obtained for gasification at a temperature of 700°C and using a mixture of air and steam (in a ratio of 1:1) of coal from mines: (1) – Bełchatów, (2) – Ziemowit, (3) – Bobrek, (4) – Bielszowice

### 4.3. Gasifying agent

The influence of the gasifying medium on syngas composition and other process indicators was investigated for atmospheric pressure and a temperature equal to 700°C. Three types of converting agent were taken into account in the simulations: a mixture of steam and oxygen, a mixture of steam and air and a mixture of oxygen and air.

In figures 6 and 7 the parameters of the final gas and gasification process were plotted against the moisture concentration in the gasifying medium, which was a mixture of air and

steam. It has been observed that with the increasing content of steam in the converting agent, the concentrations of almost all syngas components (CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, CH<sub>4</sub>) boost, only the content of N<sub>2</sub> reduces. Therefore the lower heating value of the obtained gas and the process efficiency also improves. Admittedly, the concentrations of noncombustible components (CO<sub>2</sub>, H<sub>2</sub>O) in syngas increase with boosting the content of steam in the gasifying medium, but they are formed in small amounts when compared to the amount of CO and H<sub>2</sub>, so their changes have no significant influence on the gas's calorificity.

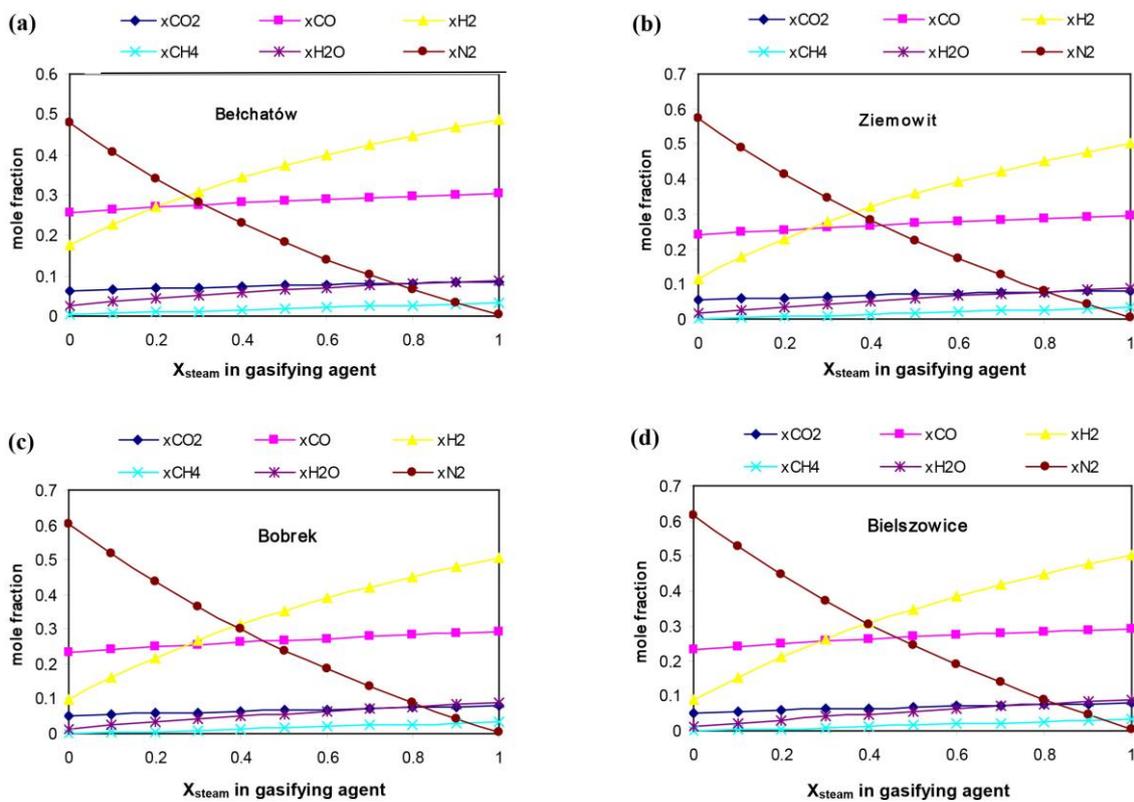
A slightly different situation is observed in the case of gasification in a mixture of steam and pure oxygen (fig. 8). Concentrations of compounds including hydrogen ( $H_2O$ ,  $H_2$ ,  $CH_4$ ) increase when moisture content in the gasifying agent is boosted, while the contents of carbon oxides ( $CO$ ,  $CO_2$ ) drop (the amount of nitrogen, present in the process, in comparison to the other produced substances is negligible). Despite this fact, both the calorificity of the obtained gas and the cold gas efficiency improves (fig. 9), because the drop in carbon monoxide concentration is compensated by the increase in hydrogen concentration. Nevertheless, the enhancement of syngas's lower heating value, which is due to the increase of moisture content in the converting agent, is more significant in the case of gasification in a mixture of steam and air (from about  $4 \text{ MJ/m}^3$  to  $10,5 \text{ MJ/m}^3$ ) than when the process is carried out in an atmosphere of steam and pure oxygen (from about  $8,5 \text{ MJ/m}^3$  to  $10,5 \text{ MJ/m}^3$ ).

In practice, the process of coal gasification carried out in steam is significantly more complicated than can be observed from the isothermal equilibrium model. Water gas reaction (2) is strongly endothermic, absorbing considerable amounts of heat and leading to a reduction of temperature in the reactor. Therefore gasification in a steam environment has to be carried out with continuous heat delivery to the reacting system (Bialecka, 2008).

Air enriched in oxygen is another important medium applied in coal gasification. Changes of syngas composition and process parameters, as a function of increasing concentration of oxygen in air, were shown in figures 10 and 11. It could be

observed that, when the content of  $O_2$  in the gasifying agent is enhanced, the concentrations of  $CO$ ,  $CO_2$ ,  $H_2O$ ,  $H_2$  in syngas increase while the concentration of  $N_2$  naturally decreases. Changes in  $CH_4$  content in the gas obtained are negligibly small. Because the amount of combustible components boosts, also the calorificity of the product gas and the cold gas efficiency enhances. The increase in the amount of  $H_2O$  in the final gas could probably be explained by the enhanced number of oxygen molecules added to the reacting system. Changes of  $H_2$  concentration in the product gas are likely to be a result of the reaction (4), between  $CO$  formed in the process (in increasing amounts) and the moisture included in the fuel (it can be observed that for coal with higher moisture content more  $H_2$  is formed).

To summarize the considerations presented above, it should be indicated, that air is the least effective agent applied in coal gasification. The heating value of syngas, obtained via coal conversion carried out in unenriched air, is low and amounts to about  $4\text{--}5 \text{ MJ/m}^3$ , while the calorificity of the product from gasification conducted in pure steam or pure oxygen was calculated, respectively, for about  $10\text{--}10,5 \text{ MJ/m}^3$  and  $8,5\text{--}9 \text{ MJ/m}^3$ . The efficiency of gasification in a pure air atmosphere is also very low – approximately 10% for hard coals and about 25% for lignite. In comparison, the efficiency of gasification in steam amounts to about 80% for lignite, 45–55% for hard coals, while the gasification efficiency in pure oxygen is 50% for lignite and 20–30% for hard coals. Therefore, in order to obtain an appropriately high caloric product gas, it is necessary to reduce the amount of nitrogen in the applied gasifying agent<sup>5</sup>.



**Figure 6.** Effect of steam concentration in air used as gasifying medium on syngas composition – results of simulations obtained for gasification at a temperature of  $700^\circ\text{C}$  of coal from mines: (a) – Belchatów, (b) – Ziemowit, (c) – Bobrek, (d) – Bielszowice

<sup>5</sup> Moreover, it should be said that nitrogen effects not only on product's heating value, but also reduces the partial pressure of oxygen and therefore the reaction with coal is more difficult and decrease temperature in the reactor (what may prevent steam dissociation).

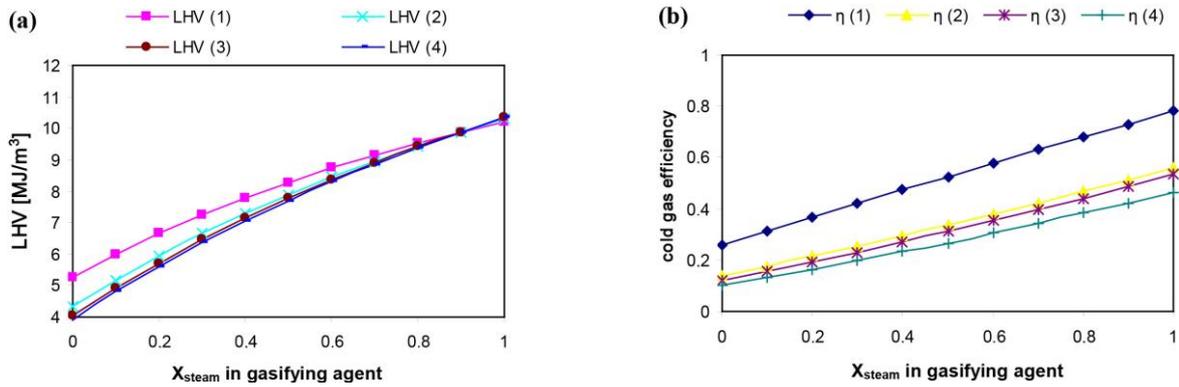


Figure 7. The effect of steam concentration in air used as a gasifying medium on lower heating value of syngas (a) and cold gas efficiency (b) – results of simulations obtained for gasification at a temperature of 700°C of coals from mine: (1) – Belchatów, (2) – Ziemowit, (3) – Bobrek, (4) – Bielszowice

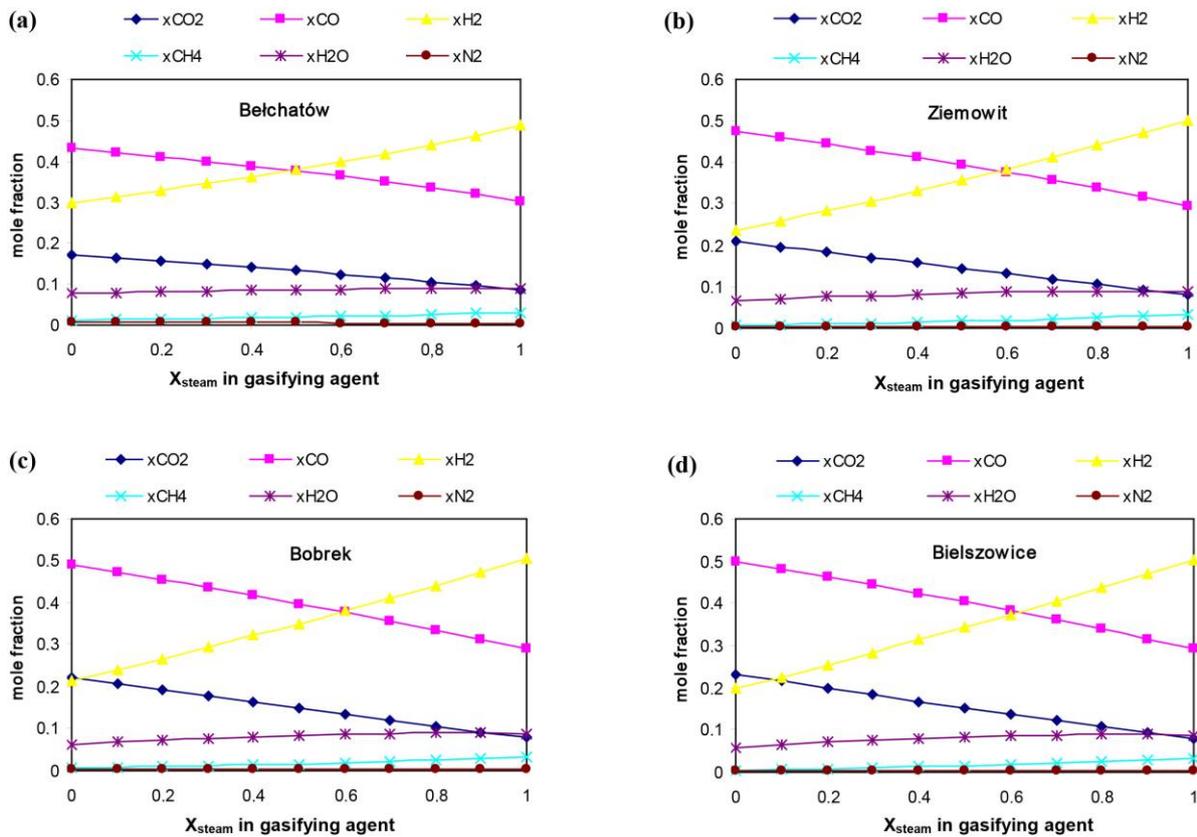


Figure 8. The effect of steam concentration in a mixture with oxygen used as a gasifying medium on syngas composition – results of simulations obtained for gasification at a temperature of 700°C of coal from mines: (a) – Belchatów, (b) – Ziemowit, (c) – Bobrek, (d) – Bielszowice

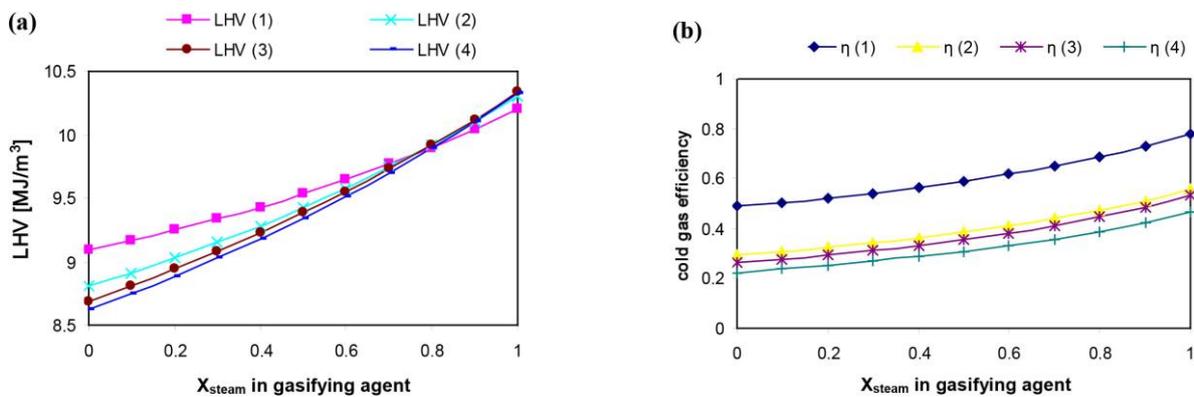


Figure 9. The effect of steam concentration in a mixture with oxygen used as a gasifying medium on a lower heating value of syngas (a) and cold gas efficiency (b) - results of simulations obtained for gasification at a temperature of 700°C of coal from mines: (1) – Belchatów, (2) – Ziemowit, (3) – Bobrek, (4) – Bielszowice

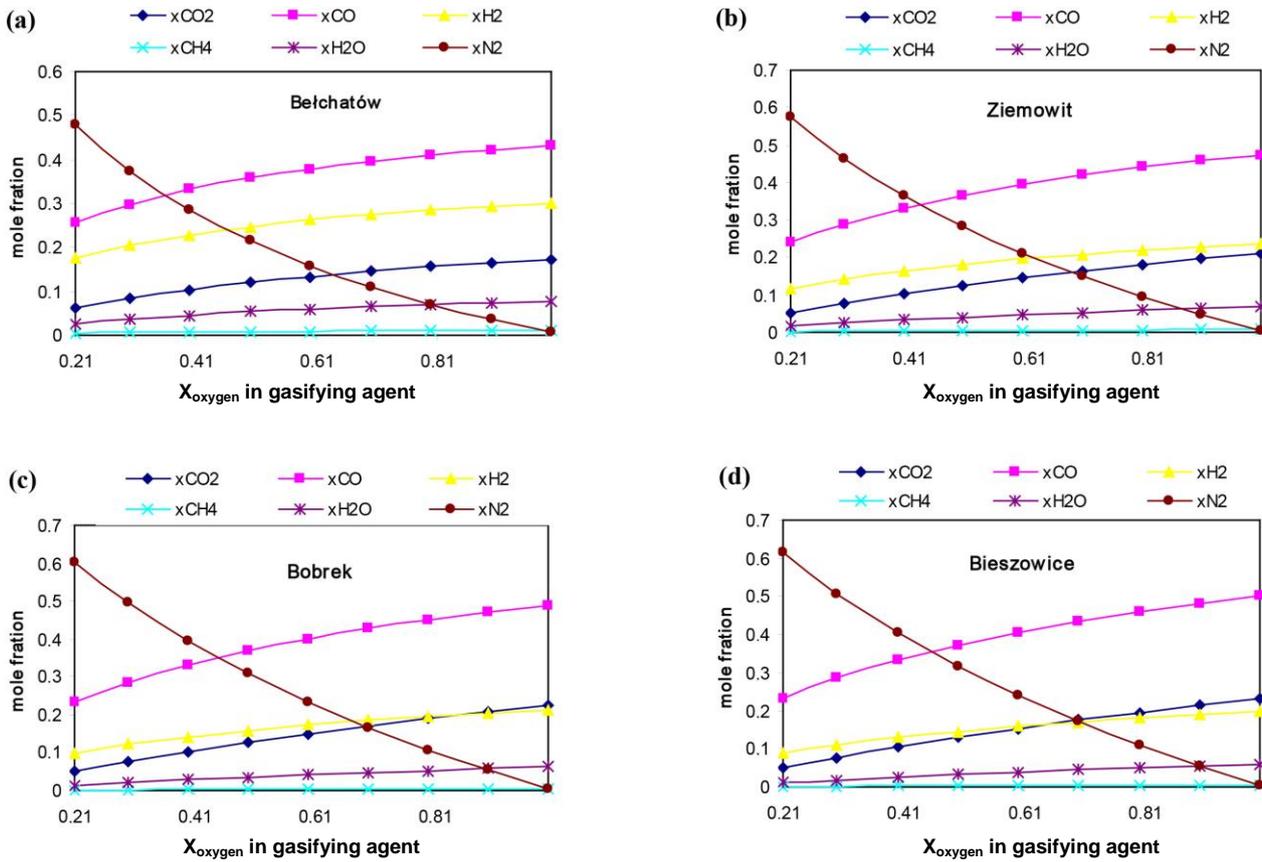


Figure 10. The effect of oxygen concentration in a mixture with air used as a gasifying medium on syngas composition – results of simulations obtained for gasification at a temperature of 700°C of coal from mines: (a) – Bełchatów, (b) – Ziemowit, (c) – Bobrek, (d) – Bielszowice

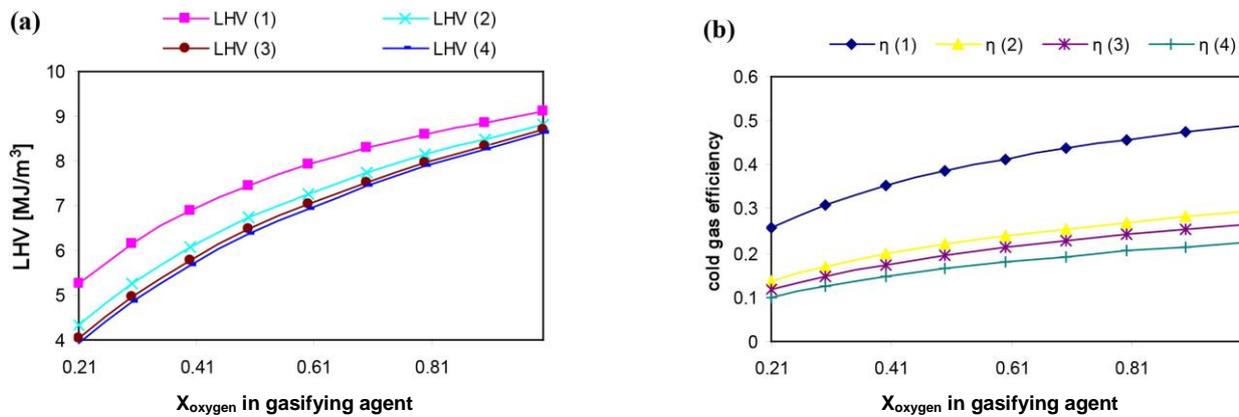


Figure 11. The effect of oxygen concentration in a mixture with air used as a gasifying medium on lower heating value of syngas (a) and cold gas efficiency (b) – results of simulations obtained for gasification at a temperature of 700°C of coal from mines: (1) – Bełchatów, (2) – Ziemowit, (3) – Bobrek, (4) – Bielszowice

#### 4.4. Fuel composition

The influence of fuel composition on syngas parameters is the best noticeable on graphs presenting changes in the calorific value of the product gas and cold gas efficiency (figures 3, 5, 7, 9 and 11) as a function of modified process parameters (temperature, pressure, converting agent composition). It is seen, that the lower heating value of produced gas depends on the rank of gasified coal– it is the highest for lignite (Bełchatów) and decreases with growing carbon content in the fuels analyzed. This relation could be easily explained – low-rank coals have a higher moisture content than hard coals. High moisture level in fuel promotes reac-

tions by which combustible components are formed. This applies especially to reaction (2), where CO and H<sub>2</sub> are produced.

Process efficiency is strictly connected, not only with syngas calorificity, but also with the lower heating value of the fuels. High-rank coals have a higher calorific value (which is due to having a higher carbon content). Therefore the best scope for high process efficiency was obtained for the gasification of lignite (the highest calorificity of syngas compared to the lowest calorificity of fuel). In the case of gasification in steam, the efficiency of lignite conversion was calculated to be about 80%, while the efficiency of conversion of hard coals was determined to be only 45–55%.

## 5. CONCLUSIONS

1. Coal gasification is a very complex and complicated technology – its final results (composition and calorific value of the obtained syngas) depend on many variables. The main factors that should be taken into account in the stage of process design and proceeding are:

- the temperature and pressure in the reactor,
- the composition of the converted fuel,
- the composition and type of the gasifying agent.

There are obviously other factors that affect coal gasification (for example the parameters of the coal seam in the case of UCG process). However, these issues were not a subject of the presented work.

2. Equilibrium models, based on thermodynamic considerations of the process, are the simplest models to be used in the analysis of coal gasification. These models are useful tools for the investigation of the thermodynamic limits of the process and may be applied to preliminary analysis and optimization. Simple mathematical formulation, good convergence and the lack of requirement of specialized software are the greatest advantages of equilibrium models.

3. Equilibrium calculations of coal gasification indicate a significant relationship between process parameters – temperature and pressure and syngas composition. The raising of temperature in the reactor leads to an increase of the H<sub>2</sub> and CO concentration in the product gas, while the boosting of pressure results in the enhancement of the content of other compounds (CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub>). Therefore processes oriented to obtain syngas with a high calorific value (or destined for various chemical syntheses) should be carried out at high temperature and under lower pressure. In contrast, when the production of CH<sub>4</sub> is the purpose of the process, a lower temperature and a higher pressure are more beneficial conditions.

4. The management and running of a coal gasification process is also possible via changes of the composition of the converting agent. Mixtures of air, pure oxygen and steam are mostly used in gasification processes. Increasing the moisture content in the converting medium (in mixtures of steam and air or oxygen) leads to an increase in the amount of combustible syngas components. Also, enriching air with oxygen results in obtaining a higher calorific gas. Therefore air is the least beneficial converting agent used in gasification processes.

5. Syngas composition and its calorific value also depend on the properties of the fuel used. Generally, the gasification of low-rank coals with higher moisture content leads to a higher calorific gas being obtained. Moreover, the efficiency of lignite gasification is better than the gasification efficiency of high-rank coals.

6. The model presented in this paper assumed a uniform temperature for the gasification process – which means that the initial temperature was also the temperature of the gas produced. In this case no temperature changes can occur as a consequence of exothermic and endothermic reactions.

Therefore the results presented in this study may significantly differ from values obtained in the case of a real reactors.

## Acknowledgements

The Polish Ministry of Science and Higher Education, Project No. 10150123, entitled “Computer simulation of influence of steam and oxygen in gasifying agent on syngas parameters” has supported the work presented in this paper.

## References

- Atkins, P. (2001). *Chemia fizyczna* [Physical chemistry]. Warszawa: PWN.
- Bhutto, A., Bazmi, A., & Zahedi, G. (2013). Underground coal gasification: From fundamentals to applications. *Progress in Energy and Combustion Science*, 39(1), 189–214. doi: 10.1016/j.pecs.2012.09.004
- Białecka, B. (2008). *Podziemne zgazowanie węgla: podstawy procesu decyzyjnego* [Underground coal gasification: basics of the decision-making process]. Katowice: Główny Instytut Górnictwa.
- Golec, T., & Ilmurzyńska, J. (2008). Modelowanie procesów zgazowania [Modeling of gasification process]. In T. Borowiecki, J. Kijeński, J. Machnikowski, M. Ściążko (Eds.), *Czysta energia, produkty chemiczne i paliwa z węgla – ocena potencjału rozwojowego* (pp. 170–187). Zabrze: Wydawnictwo Instytutu Chemicznej Przeróbki Węgla.
- Higman, C., & Van der Burgt, M. (2008). *Gasification* (2<sup>nd</sup> ed.). Elsevier.
- Kozaczka, J. (1994). *Procesy zgazowania, Inżynierskie metody obliczeń* [Gasification processes, engineering calculation methods]. Kraków: Wydaw. AGH.
- Petela, R. (1969). *Technologia paliw: odgazowanie, zgazowanie, spalanie dla kierunków energetycznych* [Fuels technology: devolatilization, gasification, combustion for energetic studies]. Gliwice: Wydaw. Politechniki Śląskiej.
- Sharma, A. (2008). Equilibrium modeling of global reduction reactions for a downdraft (biomass) gasifier. *Energy, Conversion & Management*, 49(4), 832–842. doi: 10.1016/j.enconman.2007.06.025
- Smoliński, A., Stańczyk, K., Kapusta, K., & Howaniec, N. (2012). Chemometric Study of the Ex Situ Underground Coal Gasification. *Wastewater Experimental Data. Water, Air and Soil Pollution*, 223(4), 5745–5758. doi: 10.1007/s11270-012-1311-5.
- Stańczyk, K., Howaniec, N., Smoliński, A., Świądrowski, J., Kapusta, K., Wiatowski, M., Grabowski, J., & Rogut, J. (2011). Gasification of lignite and hard coal with air and oxygen enriched air in a pilot scale ex situ reactor for underground coal gasification. *Fuel*, 90(5), 1953–1962. doi: 10.1016/j.fuel.2010.12.007.
- Tabiś, B. (2002). *Zasady inżynierii reaktorów chemicznych* [Principles of chemical reactors engineering]. Warszawa: WNT.
- Tomeczek, J. (1991). *Zgazowanie węgla* [Coal gasification]. Gliwice: Wydaw. Politechniki Śląskiej.
- Wasilewski, P., Kobel-Najzarek, E. (1980). *Chemia i technologia chemiczna węgla kamiennego* [Chemistry and chemical technology of hard coal]. Gliwice: Wydaw. Politechniki Śląskiej.
- Żogała, A., Kabiesz, J., & Iwaszenko, S. (2013). Czynniki wpływające na skład chemiczny i wartość opałową gazu uzyskiwanego w procesie podziemnego zgazowania węgla [Factors affecting chemical composition and heat value of syngas generated in the process of underground coal gasification]. *Przegląd Górniczy* 69(6), 89–95.