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# CFD simulations of influence of steam in gasification agent on parameters of UCG process

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## ABSTRACT

Underground coal gasification (UCG) is considered to be a perspective and constantly developing technology. Nevertheless it is a very complex and technically difficult process, which results depend on many variables. Mathematical models enable detailed analysis of UCG process – for example – give possibility of prediction of syngas composition depending on applied gasification medium. In practice, mixtures of oxygen, air and steam are the most frequently used as converting agents. Steam is injected to the reactor in order to obtain combustible components. Nevertheless higher concentrations of steam create a problem of reduction of temperature in reactor. This issue of amount of steam in reacting system was analyzed in given paper. Computer simulations were used as test method applied in presented work. Calculations were carried by using Computational Fluid Dynamics (CFD) method and Ansys Fluent software. Changes in outlet concentrations of syngas components (CO, CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>O, H<sub>2</sub>), in relation with time of process, were presented. Composition of product gas, its heating value and temperature of process were also examined (on outlet of reactor) in function of content of steam in gasification agent (which was mixture of O<sub>2</sub> and H<sub>2</sub>O). Obtained results indicated a possibility of conduct of stable gasification process (with predictable characteristic of gas). The simulation also demonstrated a possibility of deterioration of conditions in real reactors as a results of applying of too high amounts of steam.

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## 1. Introduction

Underground coal gasification (UCG) is defined as thermochemical process, which aim is a production of gaseous fuel or gas for wide range of chemical syntheses, carried in presence of converting agent, directly in coal seam. Result of gasification, called “syngas” is mixture of combustible

components – CO, H<sub>2</sub>, CH<sub>4</sub>, with other, less desirable constituents – mainly CO<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub> (Białecka, 2008; Petela, 1969).

Gasification of coal (both surface and underground processes) is described by set of homogenous and heterogeneous reactions; the most important of them are collected in table below (Table 1).

UCG is a very promising technology – it is connected with many environmental and economic benefits, like:

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**Table 1 – Main reactions of gasification process (Higman & Van der Burgt, 2008).**

| No.  | Reaction name                    | Mechanism                             | Enthalpy of reaction           |
|------|----------------------------------|---------------------------------------|--------------------------------|
| (1)  | Reactions of combustion          | $C + 0.5O_2 \rightarrow CO$           | $\Delta H = -111\text{kJ/mol}$ |
| (2)  |                                  | $CO + 0.5O_2 \rightarrow CO_2$        | $\Delta H = -283\text{kJ/mol}$ |
| (3)  |                                  | $C + O_2 \rightarrow CO_2$            | $\Delta H = -393\text{kJ/mol}$ |
| (4)  |                                  | $H_2 + 0.5O_2 \rightarrow H_2O$       | $\Delta H = -242\text{kJ/mol}$ |
| (5)  | Boudouard reaction               | $C + CO_2 \rightarrow 2CO$            | $\Delta H = +172\text{kJ/mol}$ |
| (6)  | Water gas reaction               | $C + H_2O \rightarrow CO + H_2$       | $\Delta H = +131\text{kJ/mol}$ |
| (7)  | Water gas shift reaction         | $CO + H_2O \rightarrow CO_2 + H_2$    | $\Delta H = -41\text{kJ/mol}$  |
| (8)  | Methanation reaction             | $C + 2H_2 \rightarrow CH_4$           | $\Delta H = -75\text{kJ/mol}$  |
| (9)  | Reforming of methane with steam  | $CH_4 + H_2O \rightarrow CO + 3H_2$   | $\Delta H = +206\text{kJ/mol}$ |
| (10) | Partial oxidation of methane     | $CH_4 + 0.5O_2 \rightarrow CO + 2H_2$ | $\Delta H = -36\text{kJ/mol}$  |
| (11) | Reforming of methane with $CO_2$ | $CH_4 + CO_2 \rightarrow 2CO + 2H_2$  | $\Delta H = +247\text{kJ/mol}$ |

- possibility of utilization of that coal seams which are technically difficult to exploit (too thin, too deep, steeply-dipping, seams of low ranked coals),
- lower capital cost in comparison to surface gasification processes (UCG allows to avoid expenditures connected with mining, transport, storage of fuel and there is no need for construct a reactor),
- problem of ash is solved (it stays underground),
- UCG produces less greenhouse gases in comparison to conventional mining combined with combustion of coal,
- pollution of water, noise and visual impact on surface are lower in comparison to conventional mining,
- site for UCG processes can be potentially used for subsequent geological sequestration of  $CO_2$  (Bhutto, Bazmi, & Zahedi, 2013).

On the other hand UCG is a very complex and technically challenging process. Its results depend on many variables – characteristic of fuel, geomechanical and geological factors, physicochemical phenomena occurring in reactor (ex. turbulence), geometry and configuration of channel, applied parameters (temperature, pressure) and above all, type of gasification medium (Bialecka, 2008).

Design and analysis of UCG processes may be simplified when the support of computer simulations is provided. Currently, methods of computational fluid dynamics (CFD) are increasingly applied in works about underground coal conversion. CFD models of UCG presented earlier in literature were concerned, among others, on prediction of temperature, pressure and concentration fields in reactor (Yang, 2004a, 2004b, 2005), cavity growth (Lou, Coertzen, & Dumble, 2009), changes of temperature in rocks surrounding reaction space (Janoszek, Sygala, & Bukowska, 2013). Detailed CFD models (including among others problem of cavity, water income to reactor) were also developed by Perkins and co-workers (Perkins, 2005; Perkins, Saghafi, & Sahajwalla, 2003; Perkins & Sahajwalla, 2007).

However, there is still a need for theoretical modeling of UCG process, especially concerning on optimization of inlet parameters (Khadse, Qayyumi, Mahajani, & Aghalayam, 2007). Example of this kind of CFD model of UCG was developed in presented paper.

## 2. Gasification agents applied in UCG process

Processes of coal gasification are the most frequently carried out in atmosphere of oxygen, steam, air and their mixtures joined in different proportions. Depending on applied gasification agent, gas with different composition and calorific value is obtained. But not only composition of converting medium is important – its temperature, flow rate or way of injection (for example gasification may be carried in two stages – in the first step reactor is injected by air, in the second – by steam) also should be taken into account (Bialecka, 2008; Wang, Huang, Zhang, & Xin, 2011).

The simplest case of UCG process is described by conversion conducted in pure oxygen. CO and  $CO_2$  are main components of product gas, as a result of reactions (1), (2), (3) and (5). Gasification occurs on relatively short length of seam, because oxygen is the most intensive gasification agent and reacts with fuel the most rapidly (in comparison to other converting media). Unfortunately, production of pure oxygen is expensive, therefore gasification is often carried in air or oxygen – enriched air (Bialecka, 2008; Petela, 1969).

Air applied as gasification agent is not effective, what is connected with presence of nitrogen.  $N_2$  does not take part in reactions and, as non-combustible substance, decreases heating value of product gas. Moreover, flow of nitrogen through the gasifying channel causes reduction of temperature in system and makes a contact between oxygen and coal more difficult, consequently reactions are less intense (Bialecka, 2008; Wang et al., 2011). Therefore, the air playing role of converting agent is not considered in presented paper.

Steam is injected to the reactor in order to produce combustible components including hydrogen –  $H_2$  and  $CH_4$ . Theoretically, when the more amount of steam is delivered to reacting system then the more amounts of  $H_2$  and  $CH_4$  are produced in process and more calorific gas is obtained. This presumption is confirmed by calculation carried out with isothermal equilibrium model (Fig. 1). Nevertheless, in case of design of real processes (which conditions are not isothermal) temperature changes due to heat of chemical reactions (especially reactions of steam dissociation) should be taken into account (Petela, 1969; Żogała, 2014). This problem will be subject of presented work.

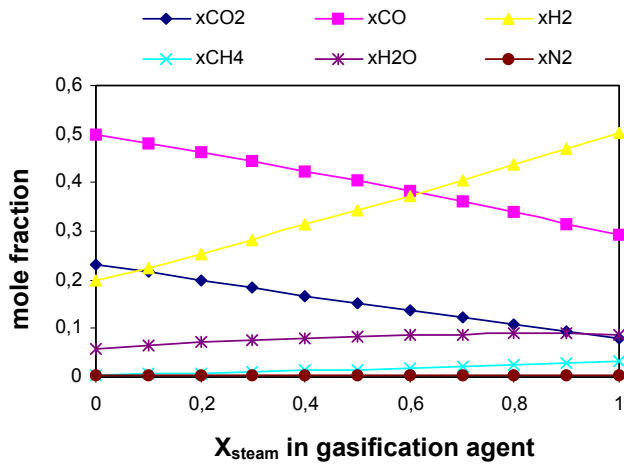


Fig. 1 – Effect of steam concentration in mixture with oxygen used as converting medium on syngas composition – results of equilibrium simulations obtained for coal from mine Bielszowice (Zogała, 2014).

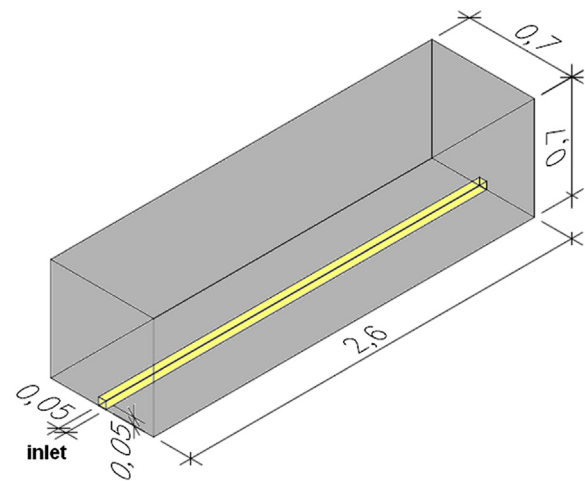


Fig. 2 – Geometrical model of examined reactor.

### 3. Model and gasification system description

The model of reactor of underground coal gasification, based on principles of computational fluid dynamics (CFD) was developed in presented work. This model was due to include (as completely as possible) complexity of phenomena connected with gasification – transport of mass, momentum and energy, turbulent mixing, flow through the porous medium, changes in concentration of components in way of chemical reactions. Ansys Fluent software was used to perform calculations.

The aim of simulations was analysis of influence of steam in gasification agent on parameters of UCG process – composition and heating value of product gas and temperature in reactor.

#### 3.1. Geometry of reactor and numerical grid

Georeactor was projected as system composed of coal block and straight gasifying channel (Fig. 2). Each dimensions of reactor are given in meters. Inlet and outlet were located on the opposite sides of reactor (inlet is indicated in the picture).

Presented space of reactor was subsequently undertaken a discretization process. Numerical grid was generated for two volumes (Fig. 3), sharing one contact surface:

- volume connected with channel (taken up by fluid), created from 219,840 tetragonal cells (Fig. 4),
- volume connected with solid (taken up by coal mass), created from 87,492 tetragonal cells (Fig. 5).

Quality of grid was checked by determination of value of aspect ratio  $a_R$ . Aspect ratio is a parameter, which describes stretching of cell. In practical applications values of  $a_R$  should be smaller than 100 (greater values of  $a_R$  are connected with round-off errors and difficulties with convergence). Aspect ratio of presented grid was equal to  $a_R = 20.7893$ , therefore it comprises in an acceptable range.

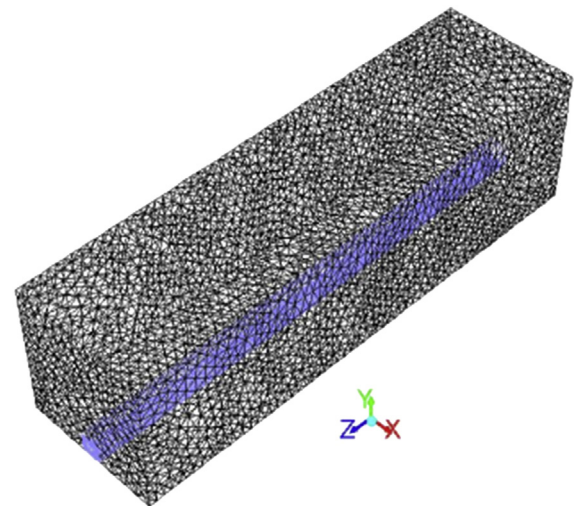


Fig. 3 – Numerical grid of whole examined reactor.

#### 3.2. Modeling of oxidizer's flow

Modeling of fluid flow through the gasifying channel is based on solving well-known transport differential equations, which description is given in the majority of elaborations concerning on fluid dynamics (for example, in handbook of Jaworski from 2005). This equations are also presented below:

- equation of the conservation of mass:

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \bar{u}) = S_m \quad (12)$$

- equation of the conservation of momentum:

$$\frac{\partial(\rho \bar{u})}{\partial t} + \text{div}(\rho \bar{u} \bar{u}) = \text{div}(\mu \text{grad} \bar{u}) + S_u \quad (13)$$

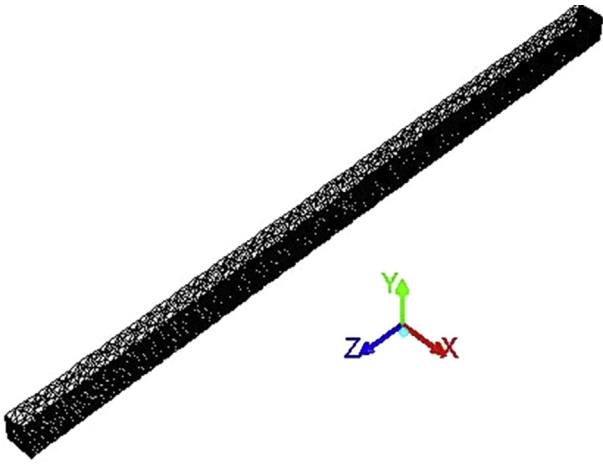


Fig. 4 – Numerical grid of gasification channel.

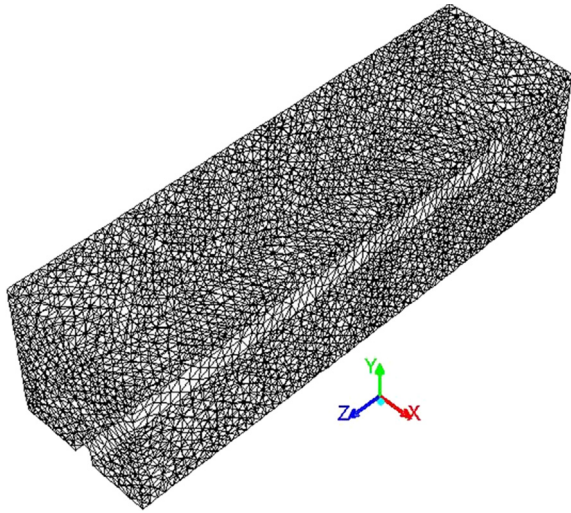


Fig. 5 – Numerical grid of coal mass.

- equation of the conservation of energy:

$$\frac{\partial(\rho e)}{\partial t} + \text{div}(\rho e \bar{u}) = \text{div}(\lambda \text{grad} T - p \bar{u}) + S_e \quad (14)$$

where:  $t$  – time, [s]

- $\rho$  – density of fluid, [kg/m<sup>3</sup>]
- $\bar{u}$  – velocity vector of fluid element, [m/s]
- $p$  – pressure of fluid, [Pa]
- $\mu$  – dynamic viscosity of fluid, [Pa·s]
- $e$  – total energy related to unit mass of fluid, [kJ/kg]
- $\lambda$  – thermal coefficient, [W/mK]
- $T$  – temperature of fluid, [K]
- $S_m$  – source term connected with mass exchange, [kg/m<sup>3</sup>·s]
- $S_u$  – source term connected with momentum exchange, [kg/m<sup>2</sup>·s<sup>2</sup>]
- $S_e$  – source term connected with energy exchange, [kJ/m<sup>3</sup>·s]

Different mixtures of oxygen and steam were used as gasification medium in presented work. Compositions of these mixtures are given in Table 2.

Besides, following parameters of converting agent were assumed:

- thermal coefficient of O<sub>2</sub> – H<sub>2</sub>O mixture (ANSYS, 2009):  
 $\lambda = 0.0454$  [W/m·K],
- dynamic viscosity of O<sub>2</sub> – H<sub>2</sub>O mixture (ANSYS, 2009):  
 $\mu = 1.72 \cdot 10^{-5}$  [kg/m·s],
- temperature of converting agent on inlet:  $T_{inl} = 420$  [K],
- specific heat of O<sub>2</sub> [J/kgK] (ANSYS, 2009):

$$c_{p_{O_2}} = 834.8264 + 0.292958 \cdot T - 0.0001495637 \cdot T^2 + 3.413885 \cdot 10^{-7} \cdot T^3 - 2.278358 \cdot 10^{-10} \cdot T^4$$

- specific heat of H<sub>2</sub>O [J/kgK] (ANSYS, 2009):

$$c_{p_{H_2O}} = 1563.082 + 1.60376 \cdot T - 0.002932794 \cdot T^2 + 3.216112 \cdot 10^{-6} \cdot T^3 - 1.156831 \cdot 10^{-9} \cdot T^4.$$

### 3.3. Modeling of turbulence

In description of gas flow through the gasifying channel it was necessary to include turbulence effect. In presented work standard  $k$ - $\epsilon$  model of turbulence was applied. This model is based on conception of turbulent viscosity  $\mu_t$  (which is used to closing Navier–Stokes equations), given by expression (Lauder & Spalding, 1972):

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (15)$$

where:  $k$  – turbulence kinetic energy, [m<sup>2</sup>/s<sup>2</sup>]

- $\epsilon$  – rate of turbulent energy dissipation, [m<sup>2</sup>/s<sup>3</sup>]
- $C_\mu$  – empiric constant,  $C_\mu = 0.09$

Therefore, two additional transport equations are solved during simulations (Lauder & Spalding, 1972):

- equation of turbulence kinetic energy  $k$ :

$$\frac{\partial(\rho k)}{\partial t} + \text{div}(\rho k \bar{u}) = \text{div}\left(\frac{\mu_t}{\sigma_k} \text{grad} k\right) + \rho P - \rho \epsilon \quad (16)$$

- equation of rate of turbulent energy dissipation  $\epsilon$ :

$$\frac{\partial(\rho \epsilon)}{\partial t} + \text{div}(\rho \epsilon \bar{u}) = \text{div}\left(\frac{\mu_t}{\sigma_\epsilon} \text{grad} \epsilon\right) + C_{1\epsilon} \frac{\rho P \epsilon}{k} - C_{2\epsilon} \rho \frac{\epsilon^2}{k} \quad (17)$$

where empirical constants take values given below:

$$C_{1\epsilon} = 1.44; \quad C_{2\epsilon} = 1.92; \quad \sigma_k = 1.0; \quad \sigma_\epsilon = 1.3,$$

**Table 2 – Compositions of examined mixtures of oxygen and steam.**

| No.                         | 1 | 2   | 3   | 4    | 5   | 6   | 7   | 8   | 9   | 10   | 11  | 12  | 13 |
|-----------------------------|---|-----|-----|------|-----|-----|-----|-----|-----|------|-----|-----|----|
| x <sub>O<sub>2</sub></sub>  | 1 | 0.9 | 0.8 | 0.75 | 0.7 | 0.6 | 0.5 | 0.4 | 0.3 | 0.25 | 0.2 | 0.1 | 0  |
| x <sub>H<sub>2</sub>O</sub> | 0 | 0.1 | 0.2 | 0.25 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.75 | 0.8 | 0.9 | 1  |

and  $P$  is local production of turbulence kinetic energy due to velocity gradient [ $\text{m}^2/\text{s}^3$ ].

### 3.4. Modeling of flow through the porous medium

Coal seam is a medium characterized by determined porosity  $\phi$ . Therefore fluid flows not only through the gasifying channel but also through the solid body. Consequently, this fact should be included in simulations.

The simplest model of the porous medium is based on Darcy law:

$$\nabla p = -\frac{\mu}{\alpha} \bar{u} \quad (18)$$

where  $\alpha$  – permeability of seam [ $\text{m}^2$ ].

That pressure gradient is added to momentum conservation Equation (13) in position of sources.

In presented model of coal gasification following parameters of fuel seam were assumed (Bialecka, 2008):

- porosity:  $\phi = 5$  [%],
- permeability:  $\alpha = 1 \cdot 10^{-15}$  [ $\text{m}^2$ ].

### 3.5. Modeling of process chemistry

Rate of each chemical processes depend on kinetics of chemical reactions and intensity of turbulent mixing. Provided that time of reactions is relatively short, rate of process is connected mainly with transport phenomena. For this kind of processes model with so-called “fast chemistry”, based on definition of mixture fraction  $f$ , is applied.

Mixture fraction is a scalar, defined by expression given below (Ansys, 2009; Sivathanu & Faeth, 1990):

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \quad (19)$$

where  $Z_i$  is the mass fraction of element  $i$ , subscripts **ox** and **fuel** represent respectively values of oxidizer stream and fuel stream on inlet.

Under assumption that diffusivities of each species are equal, all process chemistry could be reduced to one parameter – mixture fraction  $f$ . Therefore, modeling of chemical reaction is based on solving transport equation for mean mixture fraction (Ansys, 2009; Jones & Whitelaw, 1982):

$$\frac{\partial}{\partial t} (\rho \bar{f}) + \nabla \cdot (\rho \bar{u} \bar{f}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_t} \nabla \bar{f} \right) + S_f \quad (20)$$

and mixture fraction variance:

$$\frac{\partial}{\partial t} (\rho \overline{f'^2}) + \nabla \cdot (\rho \bar{u} \overline{f'^2}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_t} \nabla \overline{f'^2} \right) + C_g \mu_t (\nabla \bar{f})^2 - C_d \rho \frac{\epsilon}{k} \overline{f'^2} + S_f \quad (21)$$

where:

$\bar{f} = \overline{\rho f} / \bar{\rho}$  – Favre mean (density – averaged) mixture fraction, [–],

$\sigma_t$  – turbulent Prandtl number, [–]

$S_f$  – source term connected with mass exchange of products of reactions, [ $\text{kg}/\text{s} \cdot \text{m}^3$ ],

$f' = f - \bar{f}$ ,

and constants take following values:  $\sigma_t = 0.85$ ,  $C_g = 2.86$ ,  $C_d = 2.0$ .

Transport equations for individual species are not modeled. Instead of this, mole fractions of reactants (and other scalars as temperature or density) are computed from distribution of mixture fraction. Provided that reacting system reached equilibrium state, algorithm of calculations is based on Gibbs free energy minimization (Ansys, 2009; Kuo, 1986).

Influence of flow fluctuations on intensity of products formation in reactions is computed by using probability density function (PDF). PDF function allows to determine relations between probability of obtaining some parameters of distribution (ex. mean or variance) and independent variables, like time or position.

Shape of PDF is described the most frequently by  $\beta$ -function, given below (Ansys, 2009, Li & Toor, 1986):

$$p(f) = \frac{f^{\alpha-1} (1-f)^{\beta-1}}{\int_0^1 f^{\alpha-1} (1-f)^{\beta-1} df} \quad (22)$$

where:  $\alpha = \bar{f} \left[ \frac{\bar{f}(1-\bar{f})}{\bar{f}^2} - 1 \right]$ ,  $\beta = (1-\bar{f}) \left[ \frac{\bar{f}(1-\bar{f})}{\bar{f}^2} - 1 \right]$

### 3.6. Other process and model parameters

Simulations were carried for hard coal from mine Bielszowice. Parameters of this fuel are given in Table 3.

Additionally, the following parameters and assumptions were considered:

- transient state,
- pressure:  $p = 101,325$  [Pa],
- gravity acceleration:  $g = 9.81$  [ $\text{m}/\text{s}^2$ ],
- time step size: 612 [s],
- time scale of process: 170 [h],
- roughness of gasification channel: 0.1 [m],
- convergence:  $1 \cdot 10^{-4}$ .

**Table 3 – Proximate and ultimate analysis of examined coal (Stańczyk et al., 2011).**

|                    |              |                          |
|--------------------|--------------|--------------------------|
| Proximate analysis | Fixed carbon | 63.83 [%]                |
|                    | Volatiles    | 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 [%]                 |
| Heat of combustion |              | $3.34 \cdot 10^7$ [J/kg] |

#### 4. Results and discussion

Changes of process parameters in function of time of gasification are results of CFD simulations carried out. Exemplary time series for concentrations of species (CO<sub>2</sub>, CO, CH<sub>4</sub>, H<sub>2</sub>O, H<sub>2</sub>), analyzed on outlet of reactor, for chosen initial compositions of gasification agent (fractions of H<sub>2</sub>O and O<sub>2</sub> are given in mole percents) were presented in Figs. 6–10, together with calculated calorific value of product gas. The lower heating value (LHV) was determined from the relation given below:

$$LHV = \sum_{i=1}^n x_i LHV_i \quad (23)$$

where  $x_i$  is the mole fraction of combustible component  $i$  (CO, CH<sub>4</sub>, H<sub>2</sub>) of product gas,  $LHV_i$  – lower heating value of this component  $i$ ,  $n$  – number of combustible components in product (equal to three in given case).

It could be observed, that gasification process can be divided into two stages – stage of initialization and stabilization (when parameters of process change in significant scope) and stage of stable work of reactor (when concentrations of components remain in approximately constant level).

Presented diagrams also enable preliminary analysis of role of steam in gasification agent on syngas parameters. When the process is carried out in pure oxygen, CO is the main component of obtained product, fractions of other constitu-

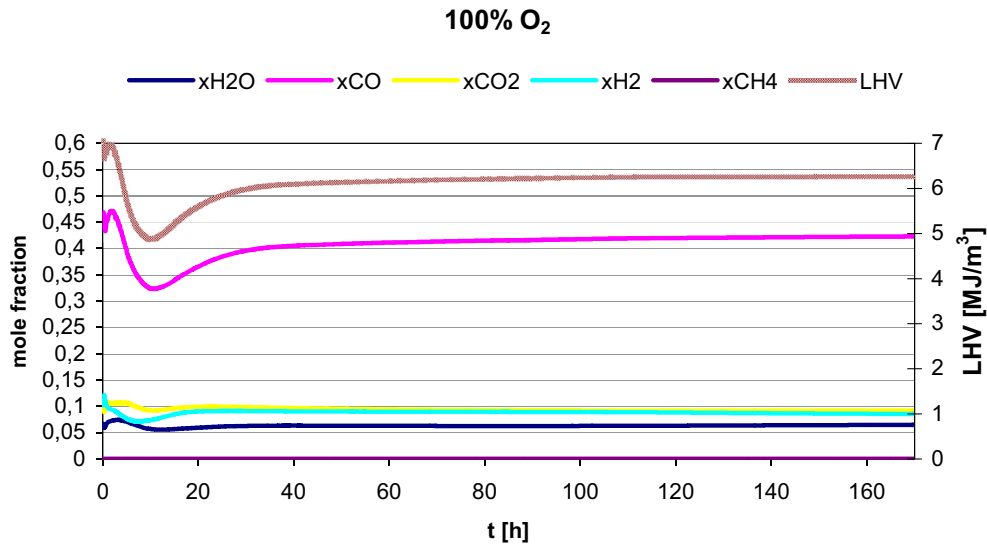


Fig. 6 – Changes of composition and heating value of syngas during 170 h – results of simulations obtained for gasification conducted in pure oxygen (100% O<sub>2</sub>).

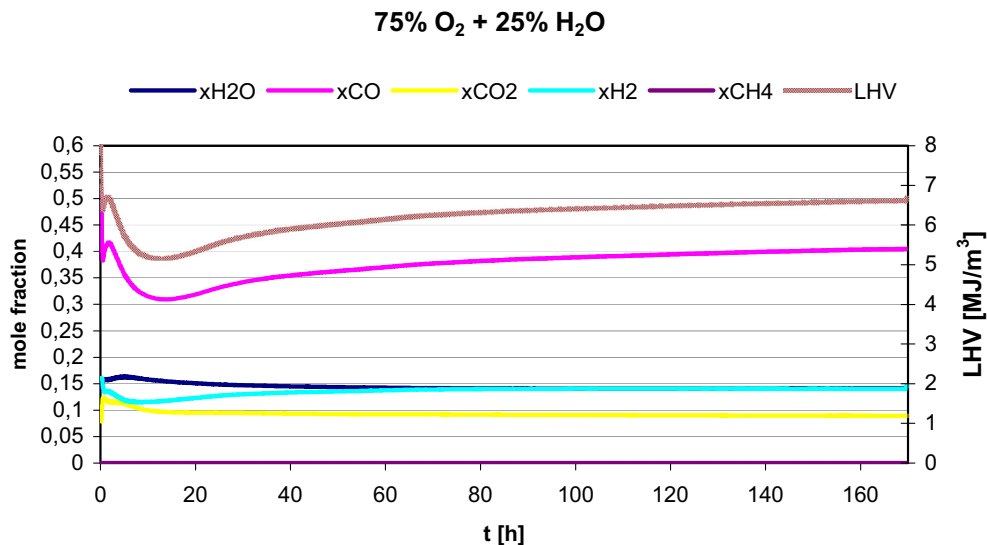
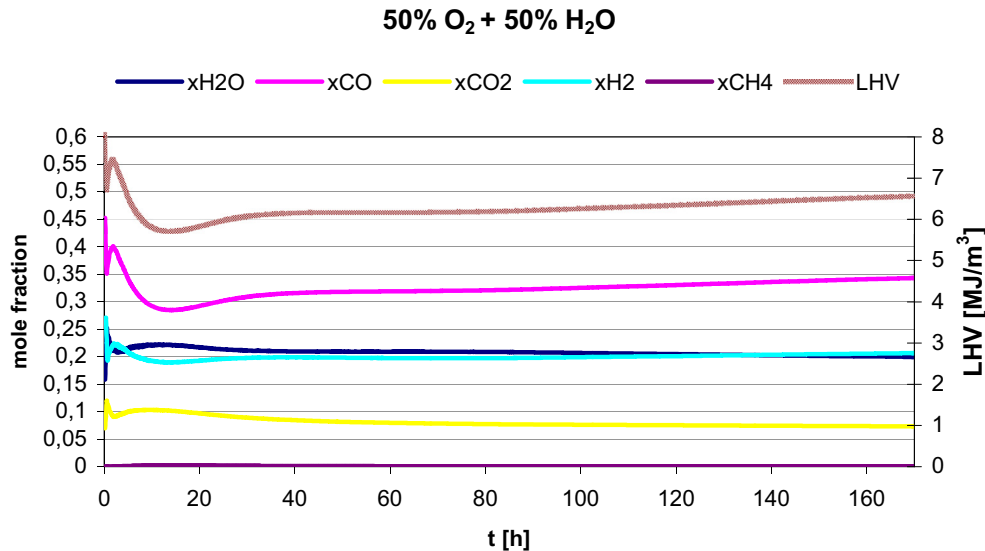


Fig. 7 – Changes of composition and heating value of syngas during 170 h – results of simulations obtained for gasification conducted in mixture of 75% O<sub>2</sub> + 25% H<sub>2</sub>O.



**Fig. 8** – Changes of composition and heating value of syngas during 170 h – results of simulations obtained for gasification conducted in mixture of 50% O<sub>2</sub> + 50% H<sub>2</sub>O.

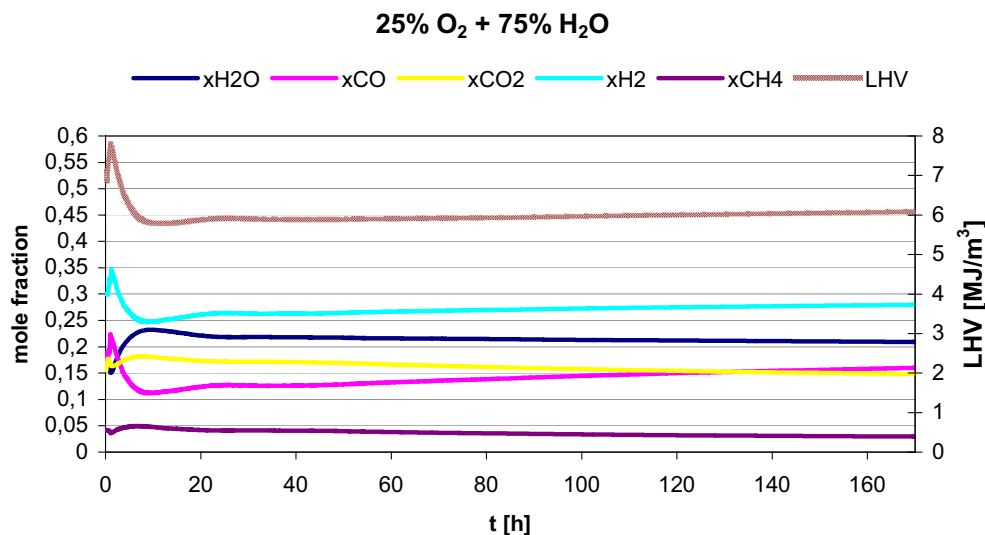
ents are considerably smaller. Together with increasing amount of steam in gasification medium concentrations of H<sub>2</sub> and H<sub>2</sub>O increase, content of CO and slightly content of CO<sub>2</sub> decrease.

When H<sub>2</sub>O is the basis component of converting agent, H<sub>2</sub> becomes the main constituent of obtained gas. Fractions of carbon oxides are smaller than fractions of H<sub>2</sub> and H<sub>2</sub>O. In this situation also some amounts of forming CH<sub>4</sub> are observed. Whereas gasification is conducted in atmosphere of pure steam, H<sub>2</sub>O is also a dominant component of product gas.

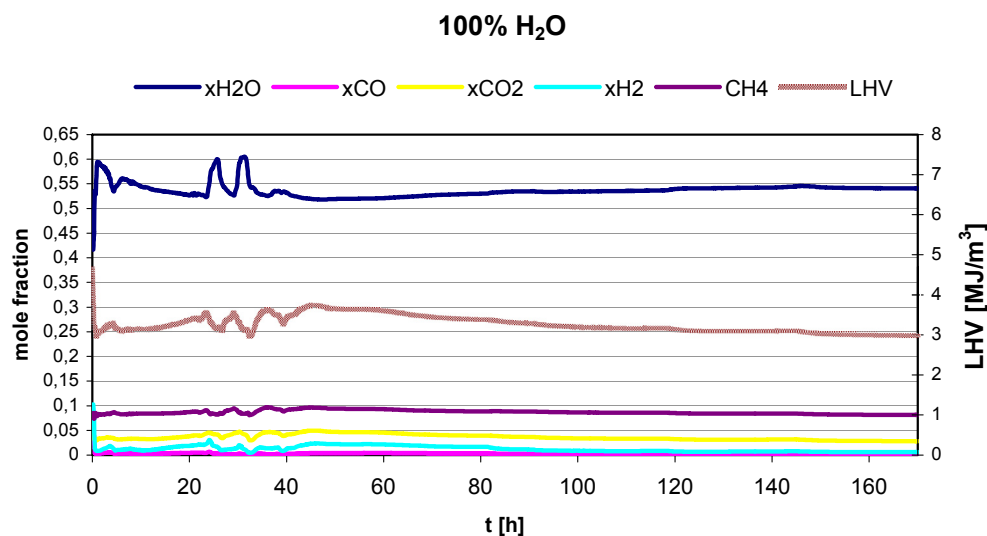
Influence of steam on parameters of gasification process is probably better to observe in Fig. 11, where composition and heating value of product gas, analyzed on outlet of reactor, were drawn against vapor concentration in gasification agent.

As the concentration of steam in converting agent grows, it could be seen that:

- amount of CO in product gas systematically decreases, and it is practically equal to zero in case of gasification in pure H<sub>2</sub>O,
- concentration of CH<sub>4</sub> increases (from negligibly small amount to about 10%),
- content of H<sub>2</sub>O in obtained gas steadily increases, but significant growth is observed when amount of steam in gasification agent exceeds 75%,
- concentration of H<sub>2</sub> in product initially grows, reaching maximum for 75% of steam in converting medium, subsequently sharply decreases,



**Fig. 9** – Changes of composition and heating value of syngas during 170 h – results of simulations obtained for gasification conducted in mixture of 25% O<sub>2</sub> + 75% H<sub>2</sub>O.



**Fig. 10 – Changes of composition and heating value of syngas during 170 h – results of simulations obtained for gasification conducted in steam (100% H<sub>2</sub>O).**

- amount of CO<sub>2</sub> in gas initially decreases (but slightly), subsequently increases (for about 75% of steam in oxidizer, similarly like in case of H<sub>2</sub>), finally decreases again,
- calorific value of product gas (when concentration of steam in gasification medium is smaller than 70–75%) reaches similar values (because drop of CO amount is compensated by growth of H<sub>2</sub> concentration), but while amount of steam on inlet exceeds 75% then calorific value of syngas sharply decreases (because both concentrations of H<sub>2</sub> and CO decline).

Meanwhile in Fig. 12, as function of increasing amount of steam in gasification agent, changes of temperature of product gas on outlet were presented. It could be seen, that this temperature reduces when concentration of H<sub>2</sub>O in oxidizer grows, from about 2800 K in case of gasification in pure oxygen to approximately 300 K for conversion carried out in steam only (process is practically turned off).

Above mentioned relations are strictly connected with thermal effects of chemical reactions. Reaction of water gas production (6) is strongly endothermic, consuming significant amount of heat. Consequently, if the more amount of steam is delivered to reacting system, then the more considerably reduction of temperature is observed (which explains changes presented in Fig. 12).

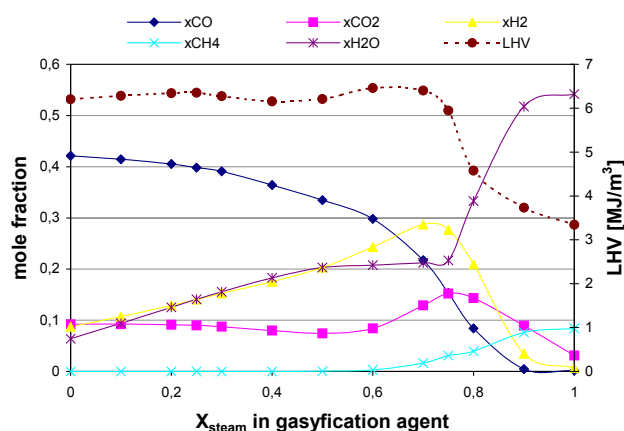
Observed in Fig. 11 sharp drop in produced amount of H<sub>2</sub>, joined with enhancement of H<sub>2</sub>O concentration in final gas, is probably connected with changes of thermal conditions occurring in reactor. Temperature of process is too low for ensure steam conversion (as a consequence, hydrogen could not be formed).

Low temperature, by contrast, promotes of CH<sub>4</sub> production due to exothermic methanation reaction (8). Therefore, relatively considerable amount of CH<sub>4</sub> in syngas is a result not only of increasing concentration of H<sub>2</sub>O in oxidizer, but also

a decreasing temperature in reactor (which is connected with too high concentration of steam in reacting system).

Initial drop of CO<sub>2</sub> concentration in product gas (observed for about 60% of vapor on inlet) is probably connected with decrease in amount of oxygen in gasification agent. For higher concentrations of steam in oxidizer, amount of CO<sub>2</sub> in syngas increases, what may be explained by reduction of temperature in reactor which promotes formation of substrates in endothermic Boudouard reaction (5). Subsequent drop of CO<sub>2</sub> concentration in product is probably connected with significant decrease of CO amount in reacting system (from which carbon dioxide is formed).

Finally, systematic drop of CO in product gas is due to both decrease of oxygen amount in gasification agent and reduction of temperature in reactor.



**Fig. 11 – Influence of steam concentration in converting medium on composition and heating value of product gas.**



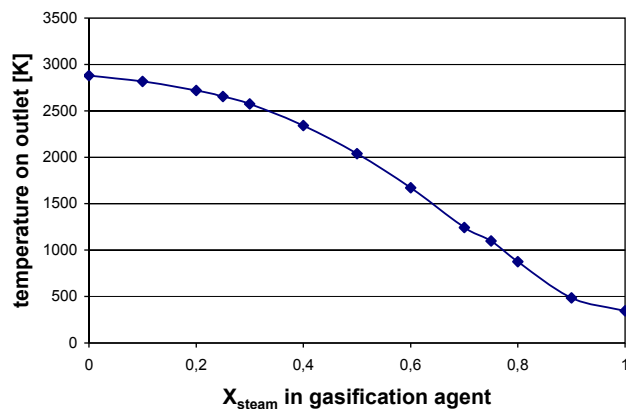


Fig. 12 – Influence of steam concentration in converting medium on temperature of product gas on outlet of reactor.

## 5. Conclusions

- CFD simulations permit to the complex analysis of UCG process. Models based on computational fluid dynamics enable not only for inclusion in calculations wide range of phenomena connected with gasification (like turbulence or flow through the porous medium, considered in presented paper), but also for investigation of various parameters in chosen time step of process or point of reactor (as in example of presented model – on outlet of reactor).
- At the beginning of simulations UCG process showed unstable character, with considerable changes of concentrations of syngas components (taking place in short period of time). Nevertheless, in subsequent phase, parameters of process balance about some determined values. This fact is very important, because indicates possibility for control of process.
- Kind of applied gasification agent has an effect not only on syngas composition but also on temperature of process. Too high concentrations of steam in oxidizer cause significant reduction of temperature in system, which leads to decrease of product gas parameters (composition and heating value).
- Oxygen is more intensive converting agent than steam. When the gasification is carried out in pure  $O_2$ , temperature in reactor may reach values approximately to 2800 K, while in case of process conducted in steam only temperature is very low – near to 300 K (which means that process was really turned off).
- Analysis and design of UCG reactor should include (if it is obviously possible) effect of temperature changes due to exothermic and endothermic reactions. Otherwise simulations may lead to obtain results which significantly differ from values observed in real (non-isothermal) reactors.

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