Modelling of coal dust gasification in a cyclone furnace under oxy-fuel combustion conditions

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Abstract

This study presents the concept of a cyclone furnace for coal dust gasification under conditions of oxy-fuel combustion. A two-chamber design of the cyclone furnace allows for division of the process of heating, drying and devolatilization of fuel from processes of gasification and combustion of carbon residue. The choice of process parameters helps control fuel gasification. Addition of the driving gas to the chamber PC1 with specific composition (O\textsubscript{2}, CO\textsubscript{2}) ensures the control of temperature and composition of the combustible gases obtained through gasification. These gases can be used as a fuel for power boilers and, consequently, allow for utilization of the oxy-fuel combustion technology in new or present power boilers.

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Keywords: cyclone furnace; coal gasification; oxy-fuel combustion; numerical modelling of coal dust gasification

Nomenclature

| Symbol | Definition     |
|--------|----------------|
| VM     | volatile matter|
| FC     | fixed carbon   |
| A      | ash            |
| M      | moisture       |

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1. Introduction

The challenges that have to be faced by contemporary energy sector that utilizes solid fuels, with particular focus on fossil fuels (black coal and brow coal), are not reduced only to limitation of CO₂ emissions, but also have to concern the problem of flexibility of production entities since growing share of renewable sources causes "suppression" of coal energy sources from the National Energy System in the subapical area. This work within the National Energy System involves the necessity of changing load in blocks over a substantial range, often much below current technical minimum (40% of MCR). These difficult problems also include new solutions connected with further limitations in permissible levels of emissions of standardized components of fuels to the atmosphere and management of coal-combustion by-products. In this situation it is necessary to search and develop new technologies of fossil fuel combustion which are capable of meeting these challenges. One of such methods is the use of a cyclone furnace, developed in the Energy Engineering Department within the Strategic Programme [1,2]. Wider description of this concept was presented in studies [3,4,5,6,7,8,9,10,11,12,13], whereas the physical model is kept in the Energy Engineering Department. Numerical modelling and the investigations carried out in the laboratory stand fully supported the assumptions for achievement of the controlled process of coal dust combustion/gasification under condition of oxy-fuel combustion. This paper analyses opportunities for coal dust gasification in such conditions.

Gasification, followed by combustion in the oxygen environment allows for application of this type of combustion chamber in CCS technology. Furthermore, through incorporation of such pre-combustion chamber into current facilities e.g. pulverized-fuel boilers, it is possible to elongate their life and adjust to new emission standards and operational requirements (improvement in block flexibility, vitrification of coal combustion by-products).

2. Cyclone furnace

Cyclone furnaces are power-generating devices where fuel combustion or gasification processes occur in a strong eddy flow of gas. With effective mixing and a relatively small combustion chamber in cyclone furnaces, it is also possible to ensure combustion of fuels with low calorific values, containing a lot of ash and humidity. Through a relative heat load in the combustion chamber it is possible to implement the process of gasification e.g. fragmented hard coal and black coal. After purification, gas obtained during gasification can be used as a substrate for various industrial purposes or for combustion in chambers of power boilers. Depending on the potential use, it is possible to design the process so that gas with desired composition can be obtained. Therefore, gasification process in the atmosphere of air, oxygen or water steam can be performed in a cyclone furnace. This study presents the results of computations for one of these variants i.e. coal dust gasification in the oxygen atmosphere.

For the purposes of the gasification process, we developed a concept of a cyclone furnace discussed below (Fig. 1). It is composed of two chambers: upper chamber (PC2) and lower chamber (PC1). The chamber PC2 is cylinder-shaped. Its upper part contains tangentially designed channels used for pneumatic supply of fragmented fuel. The upper part also features a plunger used to limit transport of fine coal dust grains outside the chamber PC2. The lower
chamber PC1 is comprised of several steps with reduced diameters. Each step features tangential nozzles that allow for supply of the "driving" gas with the specific composition (O2, CO2) to the chamber PC1. Both chambers (PC1 and PC2) are connected with a channel where an internal plunger allows for separation of the flow of flue gas from the chamber PC1 to PC2 and the fuel flow (carbon residue) from the chamber PC2 to PC1 (Fig. 1).

The discussed design of a cyclone furnace containing two chambers allows for:

- heating, drying and gasification of fuel in the chamber PC2;
- coal gasification process in the atmosphere of recirculated flue gas (CO2 and O2) or (CO2 and O2, and H2O) in order to maximize production of CO and H2, as well as combustion of certain part of carbon residue in order to generate the necessary amount of heat for maintaining and control over endothermic reactions.

3. Modelling of the process of coal gasification in a cyclone furnace

The results of numerical calculations for the process of coal dust gasification are a selected part of a vast experimental examinations and numerical calculations, necessary for determination of the final geometry of a cyclone furnace and optimal aerodynamic parameters with respect to fuel flow (eddy flow) [2,3,4,5,7,10,12]. Geometry and the grid used for computation of the cyclone furnace was developed in the Gambit software (Fig. 1). ANSYS FLUENT 14 software was used for calculations of the flow of coal dust and gasification process. The numerical model of the process allows for computation of coal dust gasification in the atmosphere of O2, CO2 through flue gas recirculation.

The lower part of the cyclone furnace (the chamber PC1) (Fig. 1) features nozzles that allow for implementation of the driving medium with oxidant (O2, CO2), whereas the upper part of the chamber PC2 contains inlets for coal dust through which the dust is supplied to a cyclone furnace pneumatically, using CO2. The lower part of the PC1 chamber is equipped in a burner that allows for stabilization of carbon residue gasification and combustion through burning of methane or recirculated combustible gases that were formed in the fuel gasification process.

Calculations of gas and fuel flow were performed using the turbulence model of Reynolds Stress, which was also used for calculations performed during the design of pre-combustion chamber geometry [2,4,5,6,12]. This model can be successfully used for strong eddy flow. Modelling of flow of coal grains was based on the Discrete Phase Model, whereas coal dust combustion was performed using Species Transport model, which allows for modelling chemical reactions both in the solid phase and gaseous phase [14,15,16,17]. Calculations used a radiation model termed Discrete Ordinate (DO).

Calculations of the combustion process and gasification of coal dust with replacement diameter of 500 μm were carried out for the fuel with physicochemical parameters as presented in Table 1. For simplification purposes, it was adopted that the fuel does not contain sulphur. Reaction rate constants were derived from the studies [14,15]. The model of the process takes into consideration opportunities for supplying water steam to perform coal gasification [18,19].

| Technical analysis [-] | Elemental analysis [-] |
|------------------------|------------------------|
| VM                     | 0.45                   |
| FC                     | 0.45                   |
| A                      | 0.05                   |
| M                      | 0.05                   |
| C                      | 0.85                   |
| H                      | 0.1                    |
| O                      | 0.04                   |
| N                      | 0.01                   |

Calculations for combustion and gasification of coal dust were described with seven reactions:

\[ x_1 \text{VM} + x_2 \text{O}_2 = y_1 \text{CO} + y_2 \text{H}_2\text{O} + y_3 \text{N}_2 \] (1)

where \( x_1, x_2, y_1, y_2, y_3 \) are stoichiometric coefficients

\[ \text{CO} + 0.5 \text{O}_2 = \text{CO}_2 \] (2)
\[ \text{C}(c) + 0.5 \text{O}_2 = \text{CO} \] (3)
\[ \text{C}(c) + \text{CO}_2 = 2 \text{CO} \] (4)
\[ C(s) + H_2O = CO + H_2 \quad (5) \]
\[ H_2 + 0.5 O_2 = H_2O \quad (6) \]
\[ CH_4 + 1.5 O_2 = CO + 2H_2O \quad (7) \]

Model of fuel devolatilization from the FLUENT software uses the internal procedure (1) to predict generation of specific amounts of CO, H_2O, N_2, from total amount of VM, with these compounds involved in further reactions depending on conditions (atmosphere composition, temperature etc.).

Conditions of coal dust gasification process analysed through numerical modelling were as follows: flow of coal dust with mean grain size of 500 μm in the amount of 1·10^{-3} kg/s introduced tangentially with two inlets located at the opposite sides of the chamber. Following a helical line, the fuel moves downwards as it is heated, dried and devolatilized through the effect of hot flue gas that flows in the furnace axis and contact with hot walls of the chamber PC2. Fuel gasification occurs through partial combustion of fixed carbon (FC) in the chamber PC1 [2,7,10,12]. A set of "driving" nozzles supplies "driving" gas tangentially to the chamber PC1 at the speed of 3 m/s, temperature of 600 K and with molar fractions O_2/CO_2 varied for individual variants from 10% O_2 and 90% CO_2 to 60% O_2 and 40% CO_2.

The lower part of the chamber PC1 features a burner nozzle from which a mixture with molar fraction O_2/CH_4 of 80/20% is discharged at the rate of 10 m/s and temperature of 350 K. This burner was expected to initialize the process and stabilize the process if necessary (depending on the variant - combustion/gasification) in the area of the chamber PC1 and to supply oxygen for the process. The numerical model also takes into consideration the heat transfer through furnace walls to its surroundings. Calculation of heat loss took into consideration actual thickness of individual components of the laboratory furnace [4,7,10] with coefficients of heat penetration and conduction for the materials used. It was assumed that air temperature around the furnace is 300 K.

4. Analysis of coal dust gasification process

Analysis of the effect of oxygen concentration in the "driving" gas on coal dust gasification in a cyclone furnace can be carried out based on mean values of selected process parameters in two representative cross-sections. Figs. 2a and 2b illustrate geometry of a cyclone furnace with location of control planes. The first control plane is denoted as CP1 (Fig. 2a), located at the inlet to the plunger that separates the chambers PC1 and PC2. The second plane, denoted as CP2, is located inside the plunger which was installed in the upper chamber PC2 (see Fig. 2b), at the outlet from the pre-combustion chamber.

The effect of oxygen concentration in the driving gas on mean values of fuel concentration in the cross-sections of PC1 and PC2 are presented in Fig. 3a. A maximum of fuel concentration is observed for the concentration of O_2 in the range of from 30 to 40%. This is connected with the fact that the increase in oxygen concentration leads to an insignificant increase in the value of the vertical component of the velocity V_z (Fig. 7c), which to a certain degree causes an increase in transport of the finest grains of the devolatilized fuel.
However, further increase in O₂ concentration leads to a noticeable increase in temperature (see Fig. 4a), which, with simultaneous increase in O₂ concentration in the upper part of the chamber, contributes to the increase in the rate of fuel grain (fly ash) burning. This is reflected by the relationship presented in Fig. 3b (black line). In the case of O₂ concentrations of over 40%, a noticeable decline in fly ash concentration can be observed in the plane CP1. Furthermore, analysis of the concentration values in the plane CP1 does not reveal substantial changes with the increase in the O₂ concentration in the driving gas. This results mainly from the fact that the upper chamber PC2 where the flow of fuel and gas also forms a strong eddy allows to a certain degree for separation of the finest grains of the transported fuel.

Distributions of mean combustion rates for gasified fuel are presented in Fig. 3b. The diagrams show that the increase in oxygen concentration affects the speed of fuel combustion in both cross-sections analysed. This is, on the one hand, connected with the increase in the component Vₓ (Fig. 7c), which causes an increase in fuel transport, and, on the other hand, with the effect of temperature (Fig. 4a), which substantially modifies the speed of the process of fuel combustion.

Distributions of temperature in both cross-sections with respect to oxygen concentration in the driving gas are presented in Fig. 4a. The expected increase in O₂ concentration leads to the increase in temperature in both cross-sections CP1 and CP2.

Distribution of mean percentage molar fractions of O₂ in the planes CP1 and CP2 with respect to oxygen concentration are presented in Fig. 4b. Oxygen content in gases that leave the chamber PC2 is equal to zero for the plane CP2. In the plane CP1, oxygen content in gases that leave the chamber PC2 is also close to zero to the concentration of around 40% in the driving gas, followed by an increase for higher O₂ concentrations.

Figures 5a and 5b compare mean values of molar fractions for CO₂ and CO, respectively. The changes in CO₂ (Fig. 5a) show that the increase in O₂ concentration in the range from 10 to 30% substantially reduces concentration of this component of flue gas. On the one hand, this is caused by its declining (with the increase in O₂ content) flow
supplied to the chamber PC1. The corresponding changes in CO₂ concentration are indicated by a green line (Fig. 5a). However, the difference between these two profiles is so important that its explanation requires taking into consideration the effect of Boudouard’s endothermic reaction (4). The increasing contribution of the effect of this reaction is also reflected by an increase in temperature illustrated in Fig. 4a. Eventually, this observation is supported by a noticeable increase in CO (Fig. 5b), which, for ca. 40÷50% of O₂ content in the “driving” gas, reaches its maximum value. The increase in O₂ in the driving gas over 50% causes an increase in CO₂ concentration with simultaneous decline in CO concentration. Insignificant differences in CO₂ and CO concentrations are observed between the control planes CP1 and CP2, which result mainly from the fact that fuel is transported to the chamber PC2 pneumatically in CO₂ stream and from the process of fuel devolatilization that occurs in the chamber PC2, forming a new component of volatile matter (VM). The figures above lead to the conclusion that there is an optimal O₂ concentration in a driving gas which allows for maximization of the CO formed during coal gasification for the analysed process conditions. The use of a pneumatic method to introduce fuel to the chamber PC2 can cause an insignificant reduction in CO contribution at the inlet with cyclone furnace (CP2).

**Fig. 5.** (a) Changes in mean molar fractions of CO₂ in the planes CP1 and CP2 with respect to oxygen concentration; (b) Effect of oxygen concentration in the driving gas on mean values of molar fractions of CO in the planes CP1 and CP2 with respect to oxygen concentration.

Figs. 6a and 6b present mean values of percentage contributions of H₂O and H₂ in the analysed planes CP1 and CP2. Presence of H₂O results from combustion of methane in a burner mounted in the lower part of the chamber PC1. With low O₂ concentrations in the driving gas, relatively high concentrations of H₂O and H₂ are observed in gas that leaves the analysed cross-sections. This is primarily connected with low temperature in the upper part of the chamber PC1 which controls the reaction of synthesis of the water gas (reaction (5)). As an effect of elevated O₂ concentration in the driving gas of over 20% (Fig. 4a) leads to a noticeable decline in H₂O concentration (Fig. 6a) and, consequently, to an increase in H₂ (Fig. 6b).

**Fig. 6.** (a) Changes in mean molar fractions of H₂O in the planes CP1 and CP2 with respect to oxygen concentration; (b) Changes in mean molar fractions of H₂ in the planes CP1 and CP2 with respect to oxygen concentration.

Figure 7a presents diagrams for mean percentage concentrations of the volatile matter VM in selected control cross-sections CP1 and CP2 with the change in oxygen concentration. Noticeable changes are the consequence of the
increase in temperature, which causes that the process of fuel grain devolatilization occurs largely in the chamber PC2.

The results, illustrated in Fig. 7b, represent an interesting starting point for the analysis of nitrogen oxides formed in the process analysed in the study. Analysis of the diagrams reveals that the increase in \(O_2\) content in the driving gas causes an increase in \(N_2\) concentration, especially in the cross-section CP2. The order of magnitude for contribution of this factor should be emphasized. Furthermore, nitrogen in the numerical model is not calculated (solved) but it only closes the system of equation for conservation of mass of all the components. Therefore, the values presented in the diagram 7b contain a certain computational error. Adoption of nitrogen as a component that closes the equations of continuity seems to be justified since it allows for obtaining accurate solutions for concentrations of these gaseous components, which are significant due to the problem of fuel gasification analysed in the study.

Changes in mean values of the vertical component \(V_z\) for gases in selected cross-sections are compared in Figure 7c. It is noticeable that, with the increase in \(O_2\) concentration in the flue gas, the component of this velocity increases in both analysed control planes. However, the gradient of velocity changes in the CP1 plane is noticeably higher than in the CP2 plane, which is the consequence of specific increases in temperature (Fig. 4a).

![Fig. 7.](image)

**5. Conclusions**

The results of modelling of coal dust gasification in a cyclone furnace discussed in this study lead to the following conclusions:

- Aerodynamics of the design of the cyclone pre-combustion chamber presented in the study ensures a stable process of fuel gasification over a broad range of concentrations of the “driving” gas supplied to the lower furnace chamber;
- Geometric configuration of lower part of the combustion chamber and distribution of fuelling nozzles at individual levels helps control the time when fuel grains (fly ash) remain in the range suitable for obtaining a high level of reaction (gasification);
- A parameter that determines fuel grain combustion and gasification processes is concentration of oxygen supplied through a system of driving nozzles. Changing the values of this concentration leads to maximization of CO content in the gas that leaves the cyclone pre-combustion chamber;
- For the process conditions adopted in the study and the operation of the burner in the lower part, optimal oxygen concentration in the driving gas is around 40%. In these conditions it is possible to obtain the CO concentration at the outlet from the chamber PC2 at the level of 80.5%;
- The profile of reactions of fuel gasification allows for control of temperature inside the chamber PC1 of the cyclone pre-combustion chamber, even for relatively high oxygen contents in the driving gas;
- Changing oxygen concentration allows for control of the location of fuel devolatilization, combustion and gasification.
- A methane burner used in the chamber PC1 ensures generation of hydrogen;
- Gaseous products of the gasification process leaving the cyclone pre-combustion chamber are characterized by a low content of combustible fractions through strong gas eddies present in the chamber PC2.
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