Numerical Study Of Operating Parameters Of A Single-Stage Air-Steam Blown Gasification Process Of Pulverized Coal

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Abstract — Gasification of solid fuels is a way to improve technical and environmental efficiency of solid fuels in the energy sector. Typically, gasifiers for large power stations operate as entrained flow reactors: pulverized coal particles are carried by gasification agent and undergo conversion stages. The study examines a single-stage process of steam-air coal gasification considering preliminary high-temperature air heating. To this end, a mathematical model is used, which includes the equations of one-dimensional transport and chemical transformations of fuel and gas mixture. The calculations show the main characteristics of the gasification process and their dependence on control parameters: air heating temperature, stoichiometric ratio and steam consumption.

Index Terms — coal, gasification, high-temperature air, numerical modelling.

I. INTRODUCTION

Improvement in the technical and environmental efficiency of solid fuel in the energy sector is an important scientific and technical issue [1]. One of the ways to solve it may be a transition from a steam cycle to a more efficient integrated gasification combined cycle (IGCC) [2]. The capacity of IGCC plants in the world is constantly growing, mainly in chemical and petrochemical industries and, to a lesser extent, in coal-fired power generation [3, 4]. This is due to a number of problems, such as insufficient reliability and high capital costs.

Most of integrated coal gasification combined cycle

plants use entrained-flow gasifiers in which coal dust (or coal slurry) is gasified in pressurized gaseous medium [5–7]. Oxygen-steam mixture is usually used as a gasification agent, however, there are also reactors that use air-steam mixture. Air is less commonly used in IGCC because low oxygen concentration and low flame temperature make it difficult to achieve full conversion of fuel at low stoichiometric ratios.

The latter problem can be solved by heating the gasification agent to high temperatures, similar to the processes of HiTAC and MILD combustion [8–12]. In this case, the losses associated with heating the system to the ignition temperature are reduced, and the energy costs of the endothermic reaction of the formation of combustible gases are partially compensated. On the one hand, it is possible to reduce the auxiliary power supply due to the rejection of air separation; on the other hand, the load on the compressors increases significantly and, most importantly, the thermodynamic and kinetic parameters change (due to the need to heat inert nitrogen and the decrease in the reactant gases concentration in the reaction zone of the gasifier).

High-temperature heating can be carried out using plasma sources [13] or burning additional fuel (natural gas, coal) [14, 15]. Issues of the implementation of high-temperature heaters are discussed in [16–18]. High-temperature gasification agent can also be used to gasify coal in oxyfuel conditions for efficient sequestration of CO2 [19–21]. The kinetics of high-temperature conversion of coal and semicoke was studied in [22, 23]. Methods for high-temperature air gasification of biomass and waste are proposed in [24–26]. Mathematical models for high-temperature fixed-bed and entrained-flow gasifiers were proposed in [27–34]. Conversion of coal particles and coalwater droplets in a stream of heated gases was studied in [35–39]. Efficiency of high-temperature coal-fueled power plants was estimated at [40–42].

In previous studies [31, 32], air heating effect was studied for a two-stage gasifier. However, at a sufficiently high air temperature, a one-stage process could be used.

Corresponding author. E-mail: donskoy.chem@mail.ru http://dx.doi.org/10.25729/esr.2019.03.0007 Received August 26, 2019. Revised September 25, 2019. Accepted, December 5, 2019. Available online December 25, 2019. This is an open access article under a Creative Commons Attribution-NonCommercial 4.0 International License.

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In this paper, using numerical simulation, we investigate coal gasification in a one-stage entrained flow reactor with heated steam-air media. Stationary operation of the gasifier under different conditions are considered, and optimal parameters in the selected parameter range are evaluated.

II. MATHEMATICAL MODEL OF COAL GASIFICATION PROCESS

The model is based on the heat balance of coal particles and the gas film around them. The following assumptions are made about the course of the gasification process [43, 44]:

- 1. the drying rate is limited by external mass transfer of particle with gaseous medium;
- 2. the pyrolysis rate is proportional to the content of volatiles in the particle and depends on temperature according to the Arrhenius law;
- 3. the gasification rate is determined from the well-known equation of the diffusion-kinetic theory of carbon combustion.

The heat balance equation for a coal particle is written as follows:

$$c_{p}\frac{d\left(m_{p}T_{p}\right)}{d\tau} = \varepsilon\sigma S\left(T_{w}^{4}-T_{p}^{4}\right) + \alpha_{T}S\left(T_{g}-T_{p}\right) - \mathcal{Q}_{w} + \mathcal{Q}_{r}.$$

Here c_p is the specific heat of the fuel, J kg⁻¹ K⁻¹; m_p is



Drying rate is calculated by the formula:

$$\frac{dm_w}{dt} = K_w S \left(C_{H_2O}^{eq} - C_{H_2O} \right)$$

Here K_w is drying rate constant, m/s; C_{H2O} is the concentration of water vapor, kg m⁻³.

The coefficient of convective heat and mass transfer for a particle in a stream is calculated by the formula:

$$Nu = Sh = 2 + 0.16 Re_p^{2/3}$$

Here Nu is the Nusselt number; Sh is the Sherwood number; Re_n is the Reynolds number for the velocity of the carrier flow and current particle size.

The pyrolysis rate is described by the first-order kinetic equation:

$$\frac{dm_{V}}{d\tau} = -k_{V}^{0} \exp\left(-\frac{E_{V}}{RT}\right)m_{V}$$

Here m_V is the mass of volatiles in the particle, kg; k_V^0 - pre-exponential factor, s^{-1} ; E_V is the activation energy of the pyrolysis stage, J/mol; R is the universal gas constant,



Fig. 1. The dependence of cold gas efficiency (%) on ratio, initial air temperature and steam stoichiometric consumption.



Fig. 2. The dependence of fuel conversion degree on ratio, initial air temperature and steam stoichiometric consumption.

J mol⁻¹ K⁻¹. The volatiles in the model are represented by a mechanical mixture of chemical elements. After exiting the fuel particle, volatiles achieve their molecular forms according to the conditions of chemical equilibrium.

The reaction rate of the fuel with gaseous oxidizing agents is recorded as follows: $\frac{dm_c}{d\tau} = -k_{eff}SC_{ox}$

Here m_C is the mass of fuel, kg; k_{eff} is effective rate constant for heterogeneous reaction, m/s; S is a fuel surface area, m²; C_{ox} is the oxidizer concentration, kg m⁻³.

The effective rate constant is expressed in terms of the kinetic and mass transfer coefficients (assuming that the kinetic order of the reaction with respect to the oxidant is one) as follows [45]:

$$k_{eff} = \frac{k_C k_d}{k_C + k_d}$$

Here k_c is the kinetic rate constant for a heterogeneous reaction, m/s; k_d is the mass transfer coefficient of the particle with the flow, m/s.

The kinetic rate constant for a heterogeneous reaction depends on temperature exponentially:

$$k_C = k_C^0 \exp\left(-\frac{E_a}{RT}\right)$$

Here k_C^0 is the pre-exponential factor, m/s; E_a is activation energy, J/mol.

Overall change in particle mass is written as follows:

$$\frac{dm_{p}}{d\tau} = \frac{dm_{w}}{d\tau} + \frac{dm_{V}}{d\tau} + \frac{dm_{C}}{d\tau}$$

Chemical kinetics of reactions in the gas phase is not considered. It is assumed that substances entering the gas phase attain a state of equilibrium. Thus, chemical transformations are described using a thermodynamic model with macrokinetic constraints on the rate of heterogeneous transformations [46, 47]. This approach is applicable to high-temperature processes in which the rates of gas-phase processes are quite high compared to the rates of heterophase processes [48].

The model proposed is stationary and one-dimensional. Similar models were previously used in [49–51] to estimate characteristics of the gasification process.

III. INITIAL DATA AND RESULTS

A tube reactor with a fuel capacity of 100 t/h and working pressure of 30 atm is considered. The length of the reaction zone is 15 m; inner diameter is 3 m. The temperature of the fuel entering the reactor is 27°C; steam temperature is 323°C; air temperature varies from 100°C to 1000°C (with increments of 100 degrees). Steam consumption varies from 0 to 0.2 mol/mol of carbon, stoichiometric ratio varies from 0.1 to 0.7 (with increments of 0.05). Coal characteristics are: $W^r = 2\%$; $A^d = 15.38\%$; $V^{daf} = 29.42\%$; $C^{daf} = 85.45\%$; $H^{daf} = 4.86\%$; $N^{daf} = 2.0\%$; $S^{daf} = 0.67\%$.

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Stoichiometric ratio, α Fig. 4. The dependence of outlet gas temperature on stoichiometric ratio, initial air temperature and steam consumption.

Fig. 3. The dependence of maximum combustion temperature on stoichiometric ratio, initial air temperature and steam consumption.

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The following characteristics were selected as key indicators: cold gas efficiency, or *CGE*, (fraction of the solid fuel combustion heat converted to the combustion heat of produced gas), maximum and final gas temperature, degree of fuel conversion, and concentration of combustible components in the produced gas.

$$CGE = \frac{Q_g G_g^{out}}{Q_f G_f^{in}} 100\%$$

The calculation results are presented in Figs. 1–6. Fig. 1 shows the contours of cold gas efficiency of the gasification process for different temperatures and specific air flow rates. A well-known pattern is observed: with a change in stoichiometry, the efficiency of the process has an extremum at fixed air initial temperature, corresponding to a complete fuel conversion (see Fig. 2) [52, 53]. An increase in air temperature enhances efficiency only if there is a sufficient amount of steam. Steam consumption of 0.2 mol/mol (C) allows increasing the cold gas efficiency of gasification from 72% (without additional steam) to 84%. Additional steam allows reducing the temperature in the core of the torch and at the reactor outlet (Figs. 3, 4).

At low stoichiometric ratio and low temperatures, the cold gas efficiency drops sharply: oxidative pyrolysis occurs under unstable temperature conditions, and large underburn is observed (Fig. 2). An increase in the stoichiometric ratio over optimal values (0.3–0.4) leads to the oxidation

of combustible gaseous components, which also leads to a decrease in efficiency, and this dependence is almost the same at each steam consumption (Fig. 1). As seen in Fig. 5, the stoichiometric ratios corresponding to maximum concentration of CO are shifted toward the pyrolysis region, while the maximum of H_2 formation corresponds to the maximum of cold gas efficiency (Fig. 6).

The diagrams of the dependence of the outlet gas temperature on the gasification conditions (Fig. 4) make it possible to choose the gasification parameters considering requirements of produced gas cooling and purification systems [54, 55]. As already mentioned above, the increases in the initial temperature improves the efficiency of gasification. In this case, the optimal value of the stoichiometric ratio decreases, and also due to the decrease in the gas density, the average gas velocity changes. Therefore, at high gasification agent temperatures, the efficiency of the process begins to decline due to a decrease in particles residence time in the reactor. Therefore, the length of the reactor should be a variable parameter (for future research).

IV. CONCLUSION

A numerical study of the pulverized coal gasification process in entrained flow of heated air-steam mixture was performed. A grid of control parameters (initial air temperature, stoichiometric ratio, steam consumption) was



Fig. 6. The dependence of H_2 content in produced gas (% vol.) on stoichiometric ratio, initial air temperature and steam consumption.

Fig. 5. The dependence of CO content in produced gas (% vol.) on stoichiometric ratio, initial air temperature and steam consumption.



set, in which the dependences of the main characteristics of the gasification process were obtained (cold gas efficiency, temperature, gas composition). The calculations show the possibility of enhancing the cold gas efficiency up to 84% with a steam consumption of 0.2 mol/mol of carbon fuel when air is heated to the temperatures of about 800°C.

V. ACKNOWLEDGEMENTS

The study was performed with partial support of the Russian Foundation for Basic Research (project No. 16-08-00739) and Siberian Branch of the Russian Academy of Sciences (Fundamental Research Program, project III.17.1.2, AAAA-A17-117030310448-0, Melentiev Energy Systems Institute).

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