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The influence of gasifier operating parameters on syngas composition of coal-fired power plant with CO_2 capture

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Abstract. This work investigated the influence of the operating parameters of the gasifier (pressure, temperature of the syngas at the outlet of the gasifier and the O_2/CO_2 ratio in the blast) on the composition of the syngas in relation to the Allam cycles and oxy-fuel IGCC. Thermodynamic modeling of the operation of Shell (Allam cycle) and MHI (oxy-fuel IGCC cycle) gasifiers by the entropy maximization method was carried out. For the Shell gasifier, a significant increase in methane concentration with an increase in pressure to 40 MPa has been revealed; it indicates the need to make changes to the syngas gas cleaning system. The optimal temperature at the outlet of the gasifier (1100°C) has been found for the MHI gasifier. At this temperature, there were high values of CO and H_2, and, hence, the heating value of syngas. For both gasifiers, the most theoretically reasonable ratio of O_2/CO_2 in blast was 0.3, at which CO reached almost maximum values and decreased its growth rate.

1. Introduction

The decarbonization of the economy, declared in the Paris Agreement, poses a number of fundamentally new tasks for the world community. Coal energy is one of the most problematic sectors of the economy in terms of greenhouse gas emissions into the atmosphere. This leads to the intensification of work on the creation of technologies with zero or near-zero CO_2 emissions into the atmosphere. Carbon capture and storage (CCS) energy cycles fall into three large groups at the site of carbon capture:

1) pre-combustion - capture of CO from syngas before its combustion in the combustion chamber of a gas turbine;

2) post-combustion - capture of CO_2 from the flue gases of a gas turbine;

3) oxyfuel - combustion of fuel in oxygen with the further capture of the products of its combustion, which are almost entirely CO_2.

The most promising, but at the same time, technically challenging is the oxyfuel technology, since it is the only one that allows reducing CO_2 emissions to zero. The same fact makes this technology attractive from the point of view of the production of high-purity commercial CO_2. Theoretically, any oxyfuel cycle running on natural gas can be converted to coal, but the Allam cycles [1] and the oxyfuel integrated coal gasification combined cycle (IGCC) [2] have been elaborated practically.

The Allam coal cycle is the gas turbine unit (Brighton cycle) with oxyfuel technology, operating on supercritical CO_2 ($P = 7.38$ MPa, $t = 31$°C). High parameters of the working fluid, the use of a recuperative heat exchanger and heat recovery of exhaust gases provide this cycle with an estimated efficiency of 37.7-40.6% [3]. However, in practice, this is hampered by several technical problems: an ultra-high pressure turbine (20-40 MPa); the presence of a syngas compressor; the use of cold gas cleaning; the need for drying fuel; operation of the gas path in a corrosive environment.

The IGCC oxy-fuel cycle is devoid of the above disadvantages with an efficiency of 40-42% [2]. All the main components of this scheme (gasifier, combustion chamber, gas purification, etc.) have already been tested on laboratory scale units. Nevertheless, several questions remain open at the industrial level: lowering the temperature of the syngas at the outlet of the gasifier; difficulty of its ignition; soot formation on sorbents, etc.

Many problems of the considered cycles are associated with the operating parameters of the gasifiers used. The Allam cycle assumes the use of a Shell gasifier, and the oxyfuel IGCC - MHI. Both gasifiers are in-line, oxygen-based, using CO_2 as a transport agent and an oxygen blast diluent. The main difference is the operating pressure in the gasifier. The Allam cycle gasifier should ideally operate at a pressure of 20-40 MPa. The oxyfuel IGCC cycle gasifier can also operate at the nominal pressure for MHI units (about 3 MPa), however, in the future, increasing the operating pressure can be considered as one of the ways to increase the efficiency of the cycle.

In addition, the gasifiers in these two cycles differ in the temperature at the outlet of the gasifier and the O_2/CO_2 ratio in the blast. The Shell gasifier has a fairly high outlet temperature (1400-1650°C) typical of traditional single-stage gasifiers. For the gasifier of the MHI type, this temperature is noticeably lower (1100-1200 ° C) due to its two-stage design.

The aim of this work is to investigate the influence of the main parameters of the gasifier operation on the composition of the resulting syngas: pressure, temperature, and O_2/CO_2 ratio in the blast. All three of these parameters must be selected individually for such promising and little-studied cycles as the cycle of Allam and oxyfuel IGCC. The study is carried out using the entropy maximization method.

2. Method of modeling

Zero-dimensional thermodynamic modeling of the equilibrium composition of the reaction products was carried out using the entropy maximization method (the extreme principle of the maximum entropy generation rate) [4]. A detailed description of the practical implementation of this method and its verification were presented in [5].

It follows from the laws of thermodynamics that in the state of equilibrium the entropy of an isolated system is maximum. Therefore, the problem of calculating the equilibrium composition can be reduced to finding the coordinates of the conditional maximum of entropy. The principle of maximum entropy is valid for any equilibrium system, regardless of the path along which the system reaches equilibrium (according to the second law of thermodynamics):

$$S = \sum_{i=1}^{k} S_i^{(p_i)} \cdot n_i + \sum_{l=1}^{L} S_l \cdot n_l = \sum_{i=1}^{k} (S_i^0 - R_0 \ln \frac{R_0 T n_i}{v}) \cdot n_i + \sum_{l=1}^{L} S_l^0 \cdot n_l,$$

where S is the entropy (J / (kg K)); S_i (p_i) is the entropy of the i-component of the gas phase (J / (mol · K)) at the partial pressure of its equilibrium state $p_i = R_0 T n_i / v$ (Pa); n_i is the content of the i-th gaseous component in the system (mol / kg); S_l is the entropy of the condensed phase l, which depends only on temperature; v is the specific volume of the system; Si_0 is the standard entropy of the i-th component of the gas phase at a temperature T and a pressure of 0.1 MPa; and R_0 is the universal gas constant (J / (mol · K)).

Determining the parameters of the equilibrium state consists in finding the values of all dependent variables, including the number of moles of the components and phases at which the value of S reaches its maximum. When finding an extremum, additional connections are imposed on the values of the unknown quantities, reflecting the conditions for the system existence: the constancy of the total internal energy, because the system is isolated by condition, the constancy of the mass of chemical elements for a closed system and the condition of general electroneutrality:

$$-U+\sum_{i=1}^{k+L} U_i \cdot n_i = 0; \quad b_j=\sum_{i=1}^{k+L} a_{ji}n_i,\ j=1,2,\dots m; \quad \sum_{i=1}^{k} a_{ei}n_i = 0,$$

where U is the internal energy (J / (kg K)); U_i is the internal energy of the i-th component (J / mol · K); a_{ji} are the stoichiometric coefficients; m is the number of chemical elements in the system; and b_j is the content of the j-th element in the system.

As a result, to find the composition and properties of an arbitrary composition corresponding to the state of maximum entropy of a conditionally isolated system, it is necessary to solve a nonlinear system of equations:

$$G_i - R_0 \ln\frac{R_0 T}{v} - R_0 \ln n_i + \sum_{j=1}^{m} a_{ji}\lambda_j + a_{ei}\lambda_e = 0,\ (i=1,2,\dots k);$$

$$\left(G_l + \sum_{j=1}^{m} a_{jl}\lambda_j\right)\cdot n_l = 0,\ (l=1,2,\dots L);$$

$$\sum_{i=1}^{k+L} a_{ji}n_i - b_j = 0,\ (j=1,2,\dots m);$$

$$\sum_{i=1}^{k} a_{ei}n_i = 0;$$

$$R_0 T\sum_{i=1}^{k} n_i - pv = 0; \quad \sum_{i=1}^{k+L} U_i n_i - U = 0,$$

where G_i is the Gibbs energy of the i-th component (J / (mol K)); and λ_j is the Lagrange multiplier of the j-th component.

This system is solved iteratively. Thermochemical and thermodynamic characteristics of individual substances are taken from domestic and foreign databases.

3. Results and discussion

One of the problems of the Allam coal cycle is: operation of a gas turbine unit with direct heating of the working fluid at ultra-high pressure (20-40 MPa), which has no practical application. The study is carried out to determine the theoretically possible composition of syngas in the Shell gasifier at two different pressures: 4 and 40 MPa (maximum for the Allam cycle). The initial mode is taken from [6]. The technical and elemental composition of coal is given in Table 1, and the operating parameters are in Table 2.

Table 1. Proximate and ultimate analysis.

Proximate	Shell (Illinois №6) [6]	MHI (Coal M) [7]
Moisture, %	11,12	4,2
Fixed carbon, %	44,18	56.2
Volatiles, %	34,99	30.9
Ash, %	9,7	8.7
Ultimate		
Carbon, %	63,75	76.3
Hydrogen, %	4,5	5.31
Nitrogen, %	1,25	1.54
Sulfur, %	2,51	0.46
Oxygen, %	6,88	7.31
Highest heating value, MJ/kg	27	30

Table 2. Operation parameters of gasifiers.

Parameters	Shell [6]	MHI [7]
Coal flow rate, kg/s	28.35	20
Stochiometric factor	0.42	0.42
Pressure, MPa	4	2.7
Gasifiers exit temperature, °C	1600	1100

The simulation results at a pressure of 4 MPa and 40 MPa are shown in Figure 1.

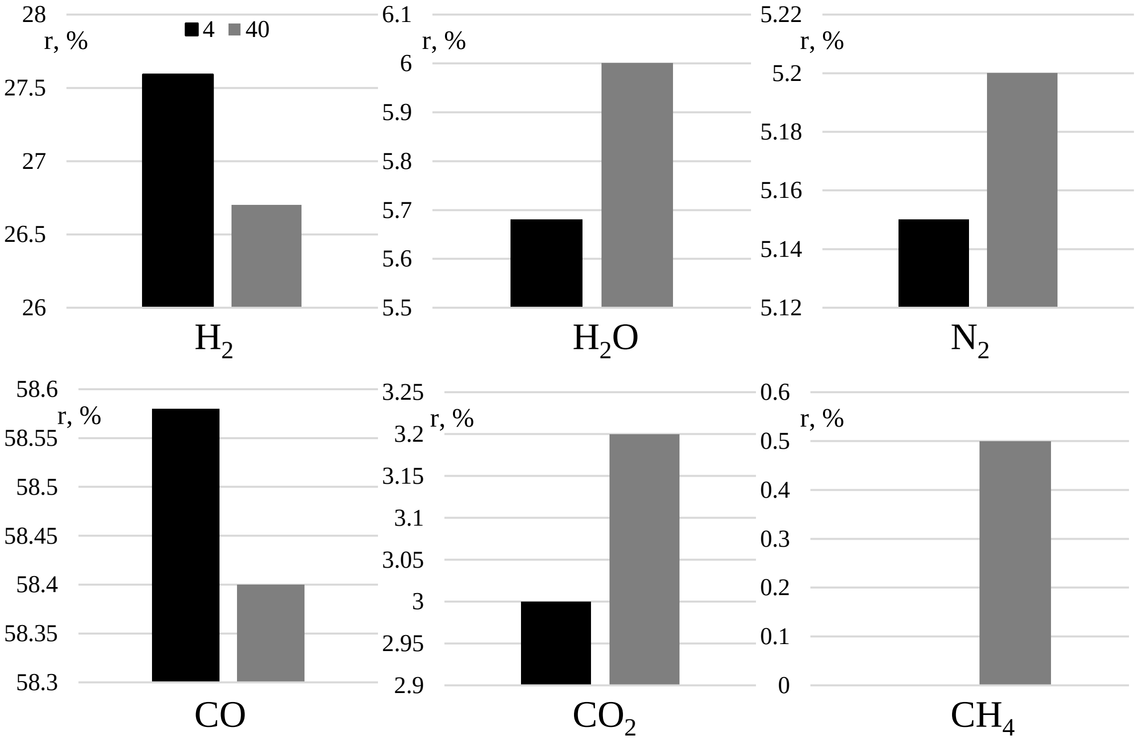

Figure 1. Volume fractions of gases at a pressure of 4 and 40 MPa in a Shell gasifier.

When the pressure in the Allam cycle reaches 40 MPa, the gas concentrations practically do not change. However, methane (CH4) appears in the system; it is a complex molecule that decomposes in smaller quantities with increasing pressure. The equilibrium is always underestimated by methane, but in real technology it is always higher. As the methane rises, there may be problems with tar condensation. This must be taken into account, since it is necessary to change the gas cleaning accordingly.

The MHI gasifier operating with IGCC oxy-fuel does not require an increase in operating pressure as this cycle is not designed for supercritical CO_2 operation. However, the MHI gasifier has another parameter for optimization - the outlet temperature. Unlike the Shell gasifier, the MHI one has a large height due to its two reaction stages. The higher the gasifier, the lower the outlet temperature, but the higher capital and operating costs. The dependence of the syngas composition on the outlet temperature will help determine the optimal gasifier height. The relationship between the height of the reactor and the outlet temperature cannot be obtained in the used zero-dimensional thermodynamic model; therefore, this issue will be considered in subsequent works using CFD modeling.

Figure 2 shows the results of calculating the composition of syngas depending on the temperature at the outlet of the MHI gasifier.

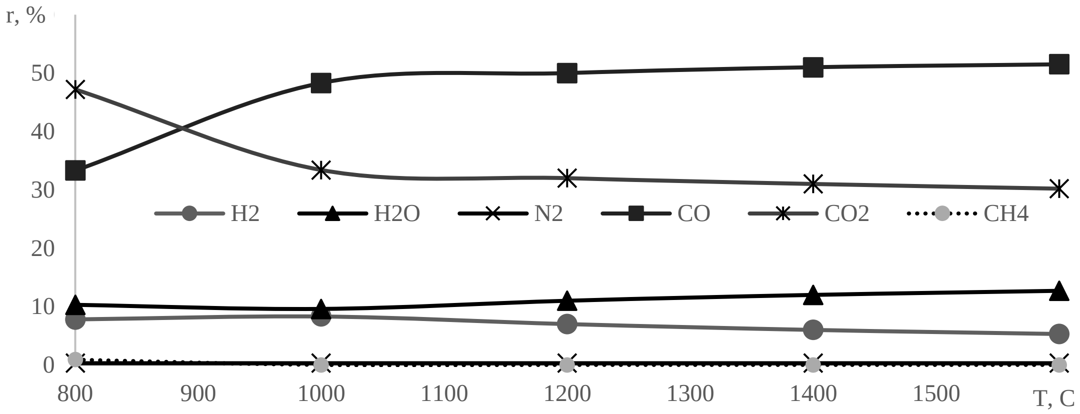

Figure 2. Influence of temperature at the gasifier outlet on the syngas composition.

Figure 2 shows that the rapid increase in the concentrations of the combustible components of syngas (H_2 and CO) stops after a temperature of 1100 ° C, which is optimal in this case. After this temperature, the CO content increases slightly, while the H_2 content decreases, due to the shift in the equilibrium of the water gas shift reaction.

The O_2 / CO_2 ratio is a new little-studied parameter that significantly affects the operating mode of gasifiers (Fig. 3). Modern cycles with CCS inevitably face the conversion of gasifiers to work with such an oxidizer. This leads to the need for a thorough study of the influence of this parameter on the main characteristics of the operation of gasifiers, primarily on the composition of the syngas.

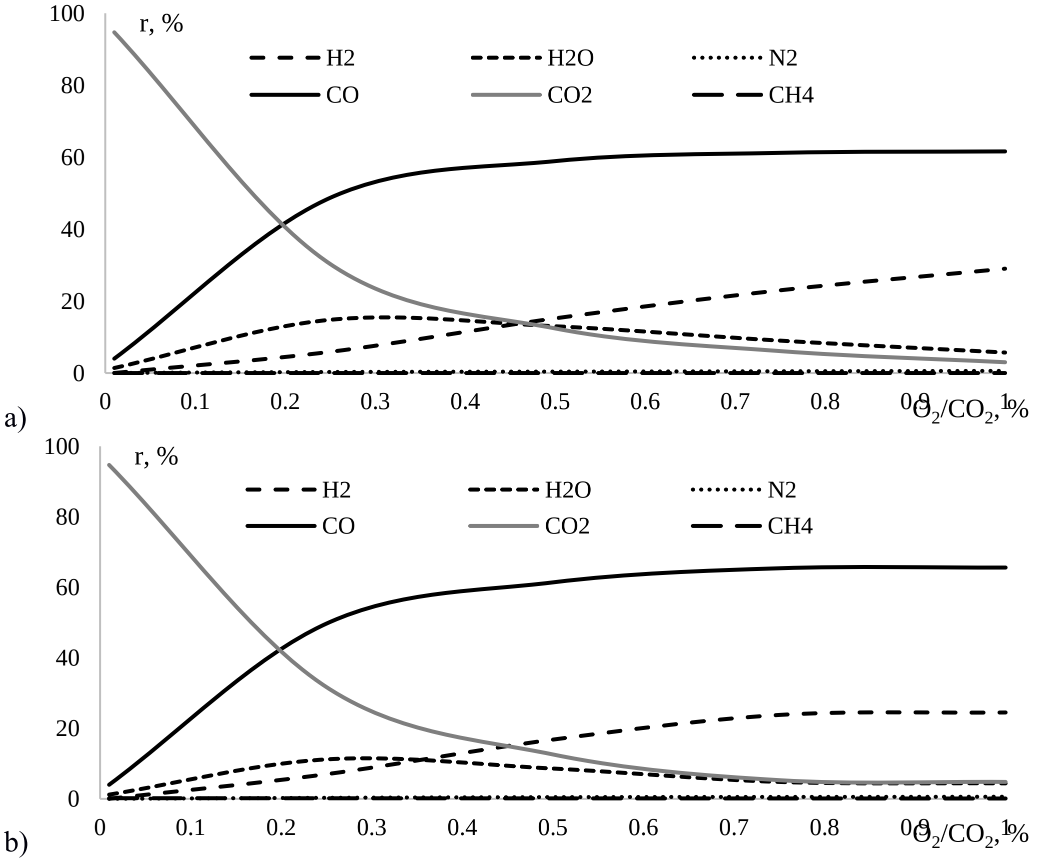

Figure 3. Influence of O_2/CO_2 ratio on syngas composition in Shell (a) and MHI (b) gasifiers.

The composition of the syngas from the O_2/CO_2 ratio in the blast in the Shell and MHI gasifiers changes only qualitatively. This is due to the fact that in these gasifiers, as in other in-line gasifiers, the composition of the syngas mainly determines the water gas shift reaction. The existing quantitative discrepancies are caused by different modes of operation and coal compositions. Nevertheless, in both gasifiers, the inflection of the lines is clearly pronounced at $O_2/CO_2 = 0.3$. With this ratio, CO stops growing rapidly, H_2O begins to decrease, which is also due to the nature of the water gas shear reaction.

4. Conclusion

The influence of the operating parameters of the gasifier (pressure, temperature of the syngas at the outlet of the gasifier and the O_2/CO_2 ratio in the blast) on the composition of the syngas in relation to the Allam cycles and oxy-fuel IGCC has been investigated. Thermodynamic modeling of the operation of Shell (Allam cycle) and MHI (oxy-fuel IGCC cycle) gasifiers by the entropy maximization method has been carried out.

1) For the Shell gasifier, a significant increase in methane concentration with an increase in pressure to 40 MPa has been revealed; it indicates the need to modify the syngas gas cleaning system.

2) The optimal temperature at the outlet of the gasifier (1100°C) has been found for the MHI gasifier. At this temperature, there were high values of CO and H_2, and, hence, the heating value of syngas.

3) For both gasifiers, the most theoretically rational O_2/CO_2 ratio in blast turns out to be 0.3; at that, CO reaches almost maximum values and decreases its growth rate.

Acknowledgments

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