Thermodynamic Assessment of the Influence of Syngas Composition on Characteristics of Solid Oxide Fuel Cell

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***Abstract* — A mathematical model is proposed to calculate the characteristics of a high-temperature solid oxide fuel cell running on combustible gases obtained by thermochemical conversion of plant biomass. The calculations rely on the approximation of thermodynamic equilibrium for the reacting mixture and the polarization equations recommended in the literature. The proposed mathematical model is used to assess the influence of the produced gas composition (obtained under different conditions) on fuel cell performance. The study has identified the gasification conditions which allow producing syngas whose electrochemical conversion is the most efficient.**

***Index Terms*: mathematical model, fuel cell, high-temperature solid oxide, thermodynamic equilibrium, polarization equations, syngas.**

Introduction

Fuel cells combined with gasification unit can significantly increase the biomass-to-electricity conversion efficiency. In this case, however, gas needs to be cleaned not only from tar and solid particles, but also from sulfur and nitrogen compounds. For example, in [1], the calculated efficiency of a power plant with a fuel cell and an organic Rankine cycle using the exhaust gases achieved almost 55%. In [2], the integration of a Stirling engine and a fuel cell yielded the efficiency of about 40% (with the optimal gas distribution). With a fuel cell used without engines, the estimated efficiency of electricity production was 30% [3-6]. A three-day experiment on a fuel cell operating on syngas obtained by staged gasification of biofuels showed the cell efficiency of about 40% [7].

The assessment of the technical and economic efficiency requires that the dependence of the fuel cell characteristics on the operating conditions, including the fuel gas composition, be known. In the biomass gasification, the gas composition normally depends on the specific air flow rate, process temperature, and fuel moisture. The reactor operation is usually accompanied by natural fluctuations in the flow and temperature parameters (associated with the operation of compressors, granular bed motion, and porous fluid flow), which also affect the composition of the produced gas. In this regard, it is of interest to study the characteristics of the combined operation of a fuel cell and a gasifier.

I. Thermodynamic Model

The theoretical cell potential can be easily estimated through the Gibbs energy change in an electrochemical reaction. However, in real-world devices, the reaction is accompanied by Ohmic and polarization losses. Formulas for the calculation of these losses are proposed in [3, 8].

Consider the oxidation of generator gas that contains CO, H_2, CH_4, CO_2, H_2O, N_2 (the other components are assumed to be removed at the gas cleaning stage). The oxidizing agent is atmospheric oxygen. Then, with the known final composition of the products, the equilibrium cell potential can be calculated:

$$E^0 = -\frac{\Delta G}{nF},$$

where n is the number of electrons transferred in electrochemical reaction (defined as an average number of electrons per one molecule of fuel mixture), F is Faraday constant, ΔG is a Gibbs energy change resulting from the conversion of reagents into oxidation products. The value of ΔG is calculated using thermodynamic data [9].

The real cell potential can be determined using semi-empirical formulas [3, 8]:

$$E = E^0 - \chi(I).$$

Here χ is the sum of losses, I is the current density. Usually, the dependence of E on I has a long linear range due to ohmic resistance. When the potential difference is obtained, the useful power can be calculated by the simple formula:

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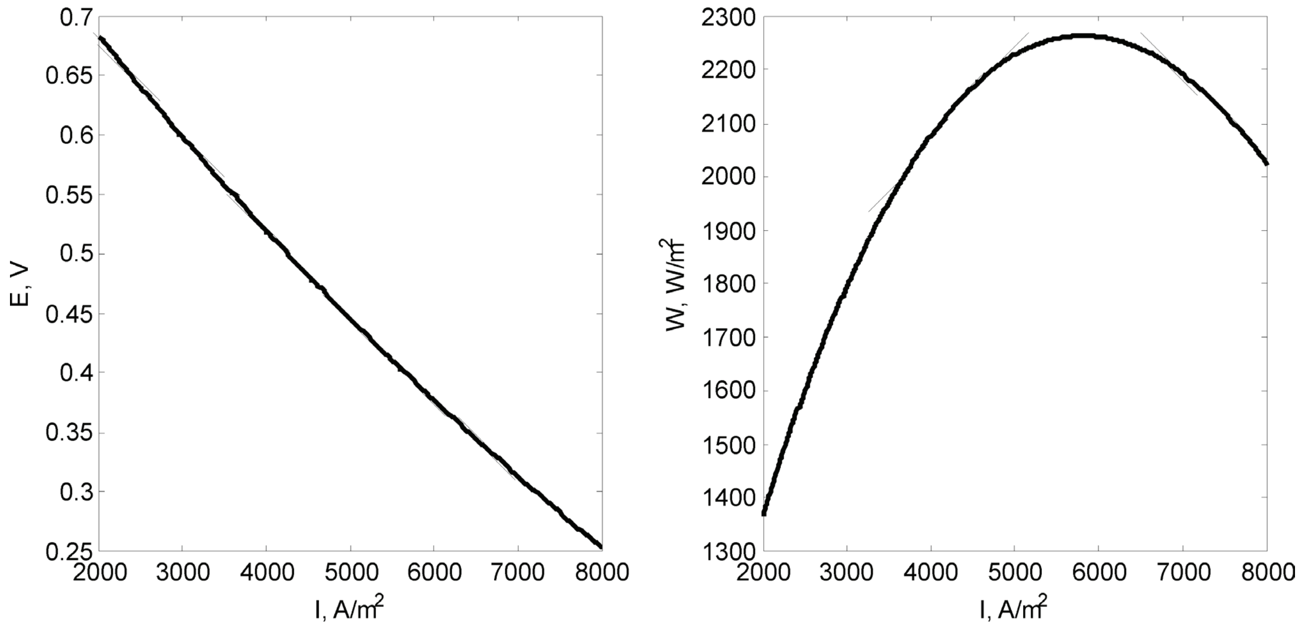

Fig. 1. The dependences of cell potential and power production of the fuel cell on the current density for the gas consisting of CO (20%), H_2 (20%), CO_2 (14%), H_2O (3%), N_2 (43%) (1073 K, 1 atm).

TABLE 1. Gas composition variants, %

No.	Reference	Conditions	CO	H_2	CH_4	CO_2	N_2
1	[12]	steam, entrained flow	40.0	20.0	10.0	30.0	0.0
2	[13]	air/steam, entrained flow	15.0	10.0	5.0	10.0	60.0
3	[14]	air/steam, quartz tube	14.7	12.6	2.0	14.2	56.5
4	[15]	oxygen, fluidized bed	27.5	30.0	5.0	27.5	10.0
5	[16]	steam, quartz tube	15.0	32.0	4.0	49.0	0.0
6	[17]	air, downdraft	20.0	15.0	2.0	10.0	53.0

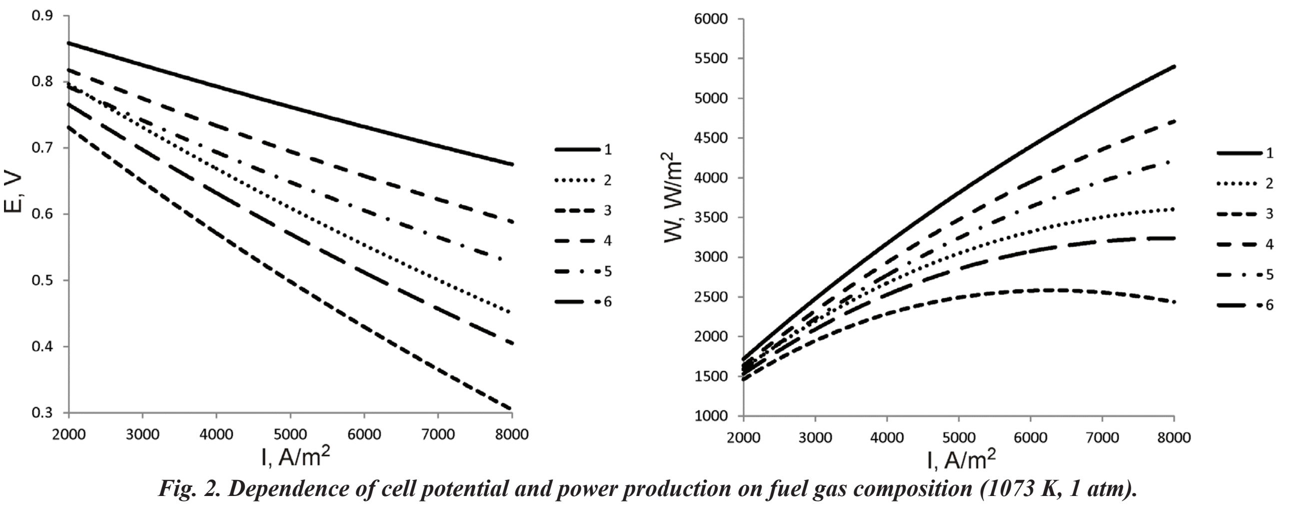

Fig. 2. Dependence of cell potential and power production on fuel gas composition (1073 K, 1 atm).

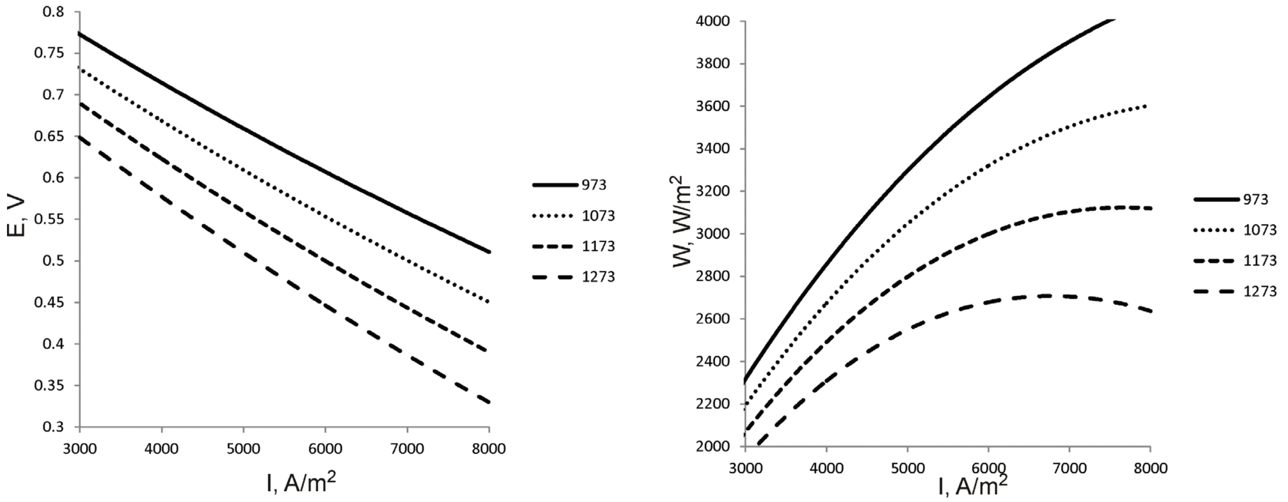

Fig. 3. Dependence of cell potential and power production on temperature for gas composition No. 2, Table 1, (1 atm).

$$W = IE.$$

Calculated dependences of cell potential and power production on current density are presented in Fig. 1.

II. Influence of Fuel Gas Composition

The study presented in [10] examined the solid oxide fuel cell (SOFC) characteristics for different variants of composition of biogas, which contained 50-60% vol. of hydrogen. For the purposes of the present research, several experimental variants of syngas composition were selected. The variants of gas composition are presented in Table 1.

Characteristics of the fuel cell operating on the gases given in Table 1 are shown in Fig. 2. Calculations were carried out for dry gases (pre-treatment is assumed to imply sufficiently deep cooling for water vapor to condense). The composition obtained during steam gasification showed the highest efficiency (in this case, the hydrogen content in the produced gas increases). The air added to the blast in all cases reduces the fuel cell performance, but stabilizes the gasification process and simplifies the gas purification (as pointed out in [11], allothermal gasification is usually accompanied by high tar yield). It can be assumed that there is an optimal air flow rate that allows maintaining the autothermal mode of biomass gasification with the least possible losses.

Additional calculations were carried out for the composition from [16] to evaluate the effect of temperature of the fuel cell on its characteristics. Figure 3 shows that an increase in temperature has a negative effect on the efficiency of the electrochemical conversion. This result may be interesting for thermal management of fuel cells [18]. Note that the model does not take into account the kinetics of oxidation reactions, and the fuel gas conversion is considered complete even at low temperatures, which is why the calculated patterns may show an incorrect dependence of the efficiency on current density in the low-temperature range.

III. Conclusion

The paper proposes a model of a fuel cell, which makes it possible to study the influence of the composition of syngas on its characteristics. Calculations indicate that the highest efficiency of electrochemical conversion is observed for the gas produced by steam gasification of biomass.

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