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Determination of Combustion Parameters of a PEM Fuel Cell at Various Combustion Conditions

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Abstract: This study evaluates the parameters that are associated with a combustion process of a Proton Exchange Membrane (PEM) fuel cell at various combustion conditions. Combustion parameters such as adiabatic flame temperature, air-fuel ratio, and fraction of water that condenses at 25°C and 1 atm, are considered in the analysis, which is performed at a theoretical air ratio ranging from 100 to 300% (from 0 to 200% excess air). Furthermore, exergy destruction associated with the combustion process was evaluated at each specified condition. The calculated results illustrated that the adiabatic flame temperature reached a maximum value of 2,526 K at 100% theoretical air and then reduced to 1,270 K at a theoretical air of 300%. Conversely, exergy destruction was evaluated to be 53,236 and 96,949 kJ kmol^{-1} at 100 and 300% of theoretical air, respectively.

Key words: PEM fuel cell, theoretical air, adiabatic flame temperature, entropy, exergy destruction, combustion

INTRODUCTION

It is widely acknowledged that the study of fuel combustion, by assuming a complete combustion process is considered to be important especially in design procedures of a system. Key combustion parameters such as adiabatic flame temperature, air-fuel ratio and fraction of water that condenses at standard conditions are extremely helpful in controlling both the temperature in the combustion chamber, and adjusting the excess air, which is used as a coolant[1].

Thermodynamically, there are two types of combustion processes namely complete and incomplete combustion processes. The complete combustion process occurs by assuming no heat loss to the surroundings and the temperature of the product reaches a maximum value referred to as the adiabatic flame temperature as depicted in Fig. 1a. On the other hand, the incomplete combustion process shown in Fig. 1b occurs at a theoretical air lower than 100% and the temperature of the product is determined to be less than the adiabatic flame temperature due to the presence of the heat loss to the surroundings. Generally, an increase in the adiabatic flame temperature of a system could lead to increase in the entropy from the reactants to the products. Exergy destruction or irreversibility, which is viewed as the amount of energy that could have been converted to work but was not, can be determined based on the entropy change between the reactants and the products in the chemical reaction. Therefore, the performance of a system can be greatly improved through minimization of exergy destruction during the process[1].

In recent years, hydrogen has been widely regarded to be the ideal fuel to run fuel cells in order to generate electric power. Utilization of fuel cells especially Proton Exchange Membrane (PEM) fuel cells for stationary power generation and transportation has gained a worldwide attention due to their attractive features such as being environmentally clean, low operating temperatures and achieve a quick response[2]. In addition, although PEM fuel cells are commonly thought that they attain high operating efficiencies since they were assumed to be not limited by the Carnot Cycle[3], they have the same second law limitations as heat engines[4,5].

In this study, combustion analysis of a PEM fuel cell will be performed at various theoretical air ratios assuming a complete combustion process. The analysis will be carried out to evaluate the adiabatic flame temperature, air-fuel ratio and fraction of water to condense at the standard condition. Furthermore, the current work will take into consideration exergy destruction associated with the combustion process at each combustion condition.

COMBUSTION PARAMETERS OF A PEM FUEL CELL

From the First Law of Thermodynamics, if the fuel is burned in an adiabatic combustion chamber of a fixed volume, so that the chemical energy is neither lost

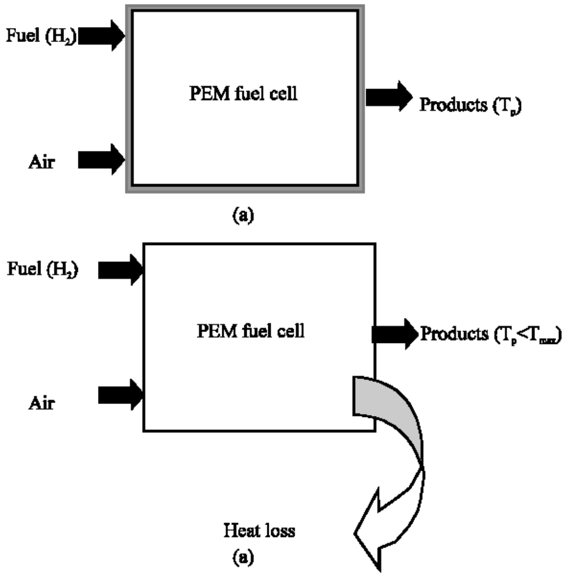

Fig. 1: PEM fuel cell at a) complete and b) incomplete combustion

through heat transfer nor to work, then the maximum temperature can be achieved. This temperature can be referred to as the adiabatic flame temperature. So, in order to drive the required equations associated with such process, we start with First Law relation of an open system by assuming negligible heat Q, work W, kinetic KE and potential energy PE:

$$\cancelto{0}{Q}-\cancelto{0}{W}=\Delta H=0 \tag{1}$$

Now, the change in enthalpyΔH can be expressed as the sum of the balanced enthalpy of the products equal sum of the balanced enthalpy of the reactants such that:

$$\begin{gathered}\Delta H=\sum_P H-\sum_R H=0\\ \sum_P H=\sum_R H\end{gathered} \tag{2}$$

In this study, a negligible heat loss during the combustion process in the PEM fuel cell is assumed. A balanced chemical equation for the combustion process is written in order to determine the enthalpy of the products as well as the reactants and to calculate the adiabatic flame temperature. Then, Eq. 2 can be re-expressed in terms of number of moles of each reactant and product involved in the balanced chemical reaction N_1[6]:

$$\sum_P N_i\left(\bar{h}_f^o+\bar{h}-\bar{h}_{298}^o\right)=\sum_R N_i\left(\bar{h}_f^o+\bar{h}-\bar{h}_{298}^o\right) \tag{3}$$

where $\bar{h}_f^o$, $\bar{h}$ and $\bar{h}_{298}^o$ are enthalpy of formation at standard condition, sensible enthalpy at the specified state and sensible enthalpy at the standard reference state of 25°C and 1 atm, respectively. By taking the above equation into account, the adiabatic flame temperature is calculated through performing trail and error analysis and by means of interpolation.

Determination of air-fuel ratio AF, which is defined as the ratio of the mass of air to the mass of fuel for a combustion process, can be done through the following relation[1]:

$$AF=\frac{m_{air}}{m_{H_2}}=\frac{N_{air}\,M_{air}}{N_{H_2}\,M_{H_2}} \tag{4}$$

where M is the molar mass of either air or hydrogen.

In the combustion process, the fraction of water that condenses as the products are cooled to 25°C and 1 atm N_w can be calculated through the following relation[1]:

$$\begin{gathered}\frac{N_v}{N_{prod,gas}}=\frac{P_v}{P_{prod}}\\ \frac{N_{prod,H_2O}-N_w}{N_{prod,total}-N_w}=\frac{P_v}{P_{prod}}\end{gathered} \tag{5}$$

where $N_{pprod,H2O}$, $N_{pprod\ total}$ are numbers of moles of water produced and total moles of the product gases produced from the chemical reaction, respectively. In addition, the vapor pressure P_v and the total pressure of the product P_{prod} at the above-specified condition are determined to be 3.169 and 101.325 kPa, respectively.

Now, from the Second Law of Thermodynamics, exergy destruction associated with a fuel cell having an adiabatic flame temperature X_{dest}, can be described in terms of entropy generation S_{gen}, assuming a negligible entropy change of the surrounding (S_{surr} = 0) and the temperature considered at the standard condition is set to be T_o= 298 K:

$$\begin{gathered}X_{dest}=T_o\,S_{gen}=T_o\left(S_{sys}+\cancelto{0}{S_{surr}}\right)\\ X_{dest}=T_o\,S_{sys}\end{gathered} \tag{6}$$

where, S_{sys} represents entropy change between the reactants at the standard condition (T= T_o = 298 K and P = P_o = 1 atm) and the products of the chemical reaction in the fuel cell, such that:

$$S_{sys} = \sum_P N_i s_i - \sum_R N_i s_i \tag{7}$$

where, N_i represents number of moles of each species in the combustion process. In addition, entropy of each species in the reactants and the products of the chemical reaction s_i, is described as a function of absolute entropy value $\bar{s}_i^o$, mole fraction y_i, universal gas constant R_u, total pressure of the gas P_m and the reference pressure P_o, such that:

$$s_i = \bar{s}_i^o - R_u \ln\left(\frac{y_i P_m}{P_o}\right) \tag{8}$$

where, the universal gas constant and the total pressure are set to equal R_u = 8.314 kJ kmol^{-1}.K and P_m = 1 atm, respectively.

The current analysis will be conducted on a PEM fuel cell at a complete combustion process and at various theoretical air ratios ranging from 100 to 300% (from 0 to 200% excess air) with properties of the reactant and the product gases are presented in Table 1.

Table 1: Properties of water, hydrogen, oxygen, nitrogen[1]

Substance	$\bar{h}_f^o$ (kJ kmol^{-1})	$\bar{h}_{298}^o$(kJ kmol^{-1})	$\bar{s}_{298}^o$(kJ kmol^{-1} K)
H_2O (v)	-241,820	9,904	188.7
H_2	0	8,468	130.6
O_2	0	8,682	205.0
N_2	0	8,669	191.5

Table 2: Complete combustion processes of a PEM fuel cell at various combustion conditions

Theoretical air (%)	Combustion process	(kJ kmol^{-1})
100	H_2+ 0.5(O_2+3.76 N_2)→H_2O + 1.88 N_2	268.022
150	H_2+ 0.75(O_2+3.76 N_2)→H_2O+0.25 O_2+2.82N_2	278.341
200	H_2+(O_2+3.76 N_2) →H_2O + 0.5 O_2 + 3.76 N_2	288.660
250	H_2+ 1.25(O_2+3.76 N_2)→H_2O + 0.75 O_2 + 4.7 N_2	298.980
300	H_2+ 1.5(O_2+3.76 N_2)→H_2O + O_2 + 5.64 N_2	309.299

Table 3: AF ratio, fraction of H_2O condensation at 25°C and 1 atm and adiabatic flame temperature of a PEM fuel cell at various combustion conditions

Theoretical air (%)	AF ratio	Fraction of H_2O condenses at 25°C and 1 atm, N_w (mol)	Adiabatic flame temperature (K)
100	34.5	0.94	2,526
150	51.8	0.90	1,975
200	69.0	0.86	1,647
250	86.3	0.82	1,427
300	103.5	0.79	1,270

Table 4: Entropy change and exergy destruction associated with the adiabatic flame temperature of a PEM fuel cell at various combustion conditions

Theoretical air (%)	Entropy of reactants $\sum_R N_i s_i$ (kJ kmol^{-1}K)	Entropy of products $\sum_P N_i s_i$ (kJ kmol^{-1} K)	Entropy change S_{sys} (kJ kmol^{-1}K)	Exergy destruction X_{dest} (kJ kmol^{-1})
100	603	782	179	53.236
150	840	1.070	230	67.550
200	1.080	1.340	260	78.988
250	1.312	1.610	298	88.602
300	1.549	1.874	325	96.949

RESULTS AND DISCUSSION

The complete combustion processes and their conserved enthalpy in the product gases at various theoretical air ratios are presented in Table 2. In order to cover a wide range of possibilities, the analysis was performed at selected theoretical air ratios ranging from 100 to 300%. The results show that enthalpy of the products H_P, increases as the theoretical air ratio is increased as a result of the presence of excess air in the chemical reaction. For instance, enthalpy of the products is increased by 15% as the theoretical air is raised from 100% (0% excess air) to 300% (200% excess air).

Generally, improvement in the fuel cell performance can be accomplished if the air stoichiometric ratio in the fuel cell is raised from 2 to 4. However, one should be extremely cautious in setting up the air stoichiometry to be greater than the recommended range between 2 to 4. This is mainly because at a high fuel cell operating temperature and air stoichiometry, the relative humidity at the exit air will be dropped causing a higher risk for the cells to dry-out and a sharp decrease in the fuel cell efficiency would occur[7].

In Table 3, AF ratio along with the fraction of water that condenses at 25°C and 1 atm and the adiabatic flame temperature of the fuel cell at various combustion conditions are presented. Clearly, AF ratio increases with an increase in the theoretical air ratio since more air would be added in the chemical reaction while the amount of fuel hydrogen is held constant. For instance, a 200% increase in the A/F ratio could occur as a result of increase in the theoretical air ratio from 100 to 300%. On the other hand, the fraction of water that condenses at 25°C and 1 atm has dropped as the theoretical air is raised. This is because the number of moles of the products increases with an increase in the theoretical air ratio, leading to a lower condensation of the fraction of H_2O vapor at the specified condition. These findings are consistent with the works of Lutz *et al.*,[5].

It is obvious that the adiabatic flame temperature reaches a maximum value of 2,526 K at a complete combustion process of 100% theoretical air, and it gradually decreases to 1,270 K with a gradual rise in the percentage of the theoretical air to 300%. This is due to the usage of excess air in the combustion process as a coolant. An important point that should be addressed here is that the obtained results are clearly consistent with the findings demonstrated by Cingle[1] and Dunbar and Lior[8].

In reality, the maximum temperature in the fuel cell is substantially lower than the adiabatic flame temperature since some heat will be rejected during the process and as a result of an incomplete combustion process, where the theoretical air would be less than 100%. However, it should be noted that in order to have a successful electrochemical process in the PEM fuel cell, a complete reaction should take place rather than an incomplete reaction with a release of heat[9]. Moreover, the second law of thermodynamics requires heat rejection from the fuel cell conversion process[4]. Therefore, it is essential to treat the fuel cell with an incomplete combustion process, which is eliminated in this study for the sake of simplicity.

The current work covered processes where oxygen is formed in air rather than utilizing oxygen as a pure gas. It is reported that the adiabatic flame temperature could be far greater in the case if oxygen is used instead of air since nitrogen, which occupies 79% of air, will not take any part in the combustion process, hence leaving the reaction to be at a higher adiabatic flame temperature[10]. Hydrogen could be another issue that needs to be carefully dealt with since the optimum routes to produce hydrogen fuel from conventional or derivative fuels at an economical rate are still questionable. For instance in the natural gas steam reformation process, the use of products emanating from partial oxidation of fuels under cool flame conditions could be done, but this has not yet been tested[11].

Generally, an increase in the adiabatic flame temperature caused by a low theoretical air would result in an increase in the entropy from the reactants to the products. Table 4 shows entropy change and exergy destruction associated with the adiabatic flame temperature of a PEM fuel cell at the previously specified combustion conditions. Although, the entropy of each species increases with increasing adiabatic flame temperature especially at lower theoretical air, the number of moles of each species is much lower than at higher theoretical air, resulting in lower entropy of each species of the reactants and the products. Thus, lower entropy change and exergy destruction would take place at lower theoretical air. For example, entropy change and exergy destruction are approximately 45% lower at a theoretical air of 100% than at 300% (200% excess air).

Thermodynamically, lower exergy destructions or irreversibilities must be acquired in order to obtain high exergetic efficiency during the conversion process. On the other hand, higher exergetic efficiency could be accomplished through a high theoretical air in the chemical reaction[6]. Therefore, optimum operating conditions should be set in order to maximize the exergetic efficiency of the fuel cell in terms of lower exergy destruction and higher theoretical air. Furthermore, it should be noted that the calculated exergy destruction in the current case would be equivalent to the reversible work since no actual work is going to occur.

CONCLUSION

In this study, determination of combustion parameters associated with the combustion process in a PEM fuel cell was conducted. The conclusions are summarized as follows:

- Enthalpy of the products increases with higher theoretical air ratio as a result of an increase in the excess air present in the chemical reaction.
- Air-fuel ratio increases with increasing the theoretical air ratio since more air will be added in the chemical reaction while keeping the amount of fuel hydrogen constant.
- The fraction of water that condenses at 25°C and 1 atm drops as the theoretical air is raised, since the number of moles of the products increases with increasing the theoretical air ratio, resulting in a lower fraction of H_2O vapor to condense at the standard condition.
- The adiabatic flame temperature reached a maximum value of 2,526 K at a complete combustion process of 100% theoretical air (0% excess air), and gradually decreased to 1,270 K as the percentage of theoretical air is gradually increased to 300%.
- Lower entropy change and exergy destruction would occur in a combustion process with a lower theoretical air rather than at higher theoretical air.

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