INFLUENCE OF THE HYDROGEN GAS CONTENTS OF A GASEOUS FUEL ON COMBUSTION CHARACTERISTICS

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Abstract. Carbon dioxide emissions represent the main environmental issue characteristic to combustion processes. Therefore, any effort in this direction is justified by the benefits that result. The paper puts forward a CO₂ abatement technique involving the enrichment in hydrogen gas of a gaseous fuel (natural gas). The original combustion calculus algorithm developed by the authors takes into account dissociation and its output consists of the flue gases temperature and composition in terms of mole fractions and volumes as well. Analysis of output data obtained for different fuel compositions in terms of H₂ percentage shows that low CO₂ flue gases result and thus the main hypothesis is confirmed. Other consequences are also considered and highlighted, confirming that fuel enrichment in H₂ can represent a promising candidate for CO₂ emissions abatement.

Keywords: combustion, carbon dioxide emissions, gaseous fuel, hydrogen gas enrichment.

1. INTRODUCTION

Carbon dioxide emissions resulted from industrial combustion processes, especially from power plant boilers, represent a very important environmental issue in the context of the climate change triggered by increased greenhouse gases emissions. A good understanding of the combustion mechanisms and consequently of CO₂ generation allows designing various techniques of CO₂ emissions abatement. By following this path, a number of ideas have arisen among which CO₂ sequestration proved to be one of the most promising.

By this technique, the carbon dioxide gas generated in combustion processes is separated from flue gases, purified and subsequently sequestered in special locations (Russo et al., 2013). The resulting flue gases are carbon dioxide-free and thus they no longer harm the environment. Three leading capture methods are presently in view (Acharya et al., 2005): post-combustion scrubbing, gasification with pre-combustion carbonization, and oxycombustion. Post-combustion scrubbing removes CO₂ by means of a sorbent (i.e., MEA – methylethylamine) that regenerates by releasing the gas (Radgen et al., 2006), (Russo et al., 2013). Gasification with pre-combustion de-carbonization involves gasification of coal into syngas that is subsequently converted into a H₂-CO₂ mixture from which carbon dioxide is separated, resulting only hydrogen (Acharya et al., 2005). Oxycombustion involves fuel combustion with pure O₂ produced by an air separation unit (ASU). This way, the flue gases will only contain water vapor (that can be condensed) and CO₂ that can be easily captured after condensation (Figueroa et al., 2008; Metz et al., 2005).

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A less radical CO$_2$ abatement technique might be to burn a gaseous fuel (i.e., natural gas) enriched with hydrogen gas produced from renewable sources. The idea behind this solution is to reduce CO$_2$ emissions and at the same time to take advantage of the heating values of the hydrocarbons composing the gaseous fuel, which are significantly higher than the heating value of hydrogen.

In this paper we study the impact of an increasing hydrogen gas content of a gaseous fuel on the adiabatic flame temperature and on the flue gases composition in terms of CO2 and CO contents.

2. MATHEMATICAL MODEL OF THE COMBUSTION PROCESS

2.1. Combustion calculus

We consider a gaseous fuel the composition of which is: 86.5% CH$_4$, 7.9% C$_2$H$_6$, 2.2% C$_3$H$_8$, 0.3% C$_4$H$_{10}$, 0.5% CO$_2$, and 2.6% N$_2$. By considering the mole fractions of the components expressed in m$^3$ component/m$^3$ fuel and symbolized in brackets – e.g. for CH$_4$: [ch4], we have written the stoichiometric combustion equations, which allowed us to determine the minimum volume of oxygen gas necessary for the complete combustion of the unit volume of fuel:

$$V_{O_2}^{\text{min}} = 2(\text{ch4}) + 3.5(\text{c2h6}) + 5(\text{c3h8}) + 6.5(\text{c4h10}) .$$  (2)

By assuming that the combustion air is dry and that the excess air $\lambda = 1$, the combustion air volume is:

$$V_{\text{air}}^{\text{min}} = \frac{V_{O_2}^{\text{min}}}{0.21} = 4.76V_{O_2}^{\text{min}} .$$  (3)

Figure 1 shows the schematic of the combustion chamber with the fuel and air inflows and with the flue gases outflows. The material balance of the combustion chamber is presented in Table 1.

2.2. Dissociation

Due to the high temperatures that develop during combustion, some of the resulting species dissociate in more simple molecules and these chemical reactions remove heat from the flue gases, the result being a decrease of the adiabatic flame temperature. We have developed an original model that provides the final flue gases temperature (after dissociation) along with the composition of the combustion effluents.

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**Fig. 1. Schematic of the combustion chamber.**

**Table 1**

<table>
<thead>
<tr>
<th>Material balance of the combustion chamber</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>IN</strong></td>
</tr>
<tr>
<td>REACTANTS</td>
</tr>
<tr>
<td>Fuel: (ch4)+(c2h6)+(c3h8)+(c4h10)</td>
</tr>
<tr>
<td>Minimum volume of oxygen: $V_{O_2}^{\text{min}} = 2(\text{ch4}) + 3.5(\text{c2h6}) + 5(\text{c3h8}) + 6.5(\text{c4h10})$</td>
</tr>
<tr>
<td><strong>DO NOT PARTICIPATE IN COMBUSTION REACTIONS</strong></td>
</tr>
<tr>
<td>$V_{N_2}^{\text{in}} = V_{N_2}^{\text{min}} + (n2)$</td>
</tr>
</tbody>
</table>
Table 2 displays the dissociation reactions and their outcome. The reactions have been divided into primary (dissociations of combustion effluents) and secondary ones (some of the products of primary reactions dissociate themselves or react with other products).

**Dissociation reactions synopsis**

<table>
<thead>
<tr>
<th>REACTION</th>
<th>VOLUMES OF REACTANTS</th>
<th>RESULTING VOLUMES AFTER DISSOCIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>As final products</td>
</tr>
<tr>
<td>A. PRIMARY REACTIONS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. CO₂ dissociation</td>
<td>2CO₂ ↔ 2CO + O₂</td>
<td>y₁ [m³CO₂/m³ fuel]</td>
</tr>
<tr>
<td>2. H₂O dissociation</td>
<td>2H₂O ↔ 2H₂ + O₂</td>
<td>y₁ [m³H₂O/m³ fuel]</td>
</tr>
<tr>
<td>3. N₂ dissociation</td>
<td>N₂ ↔ 2N</td>
<td>y₁ [m³N₂/m³ fuel]</td>
</tr>
<tr>
<td>4. O₂ dissociation</td>
<td>O₂ ↔ 2O</td>
<td>y₁ [m³O₂/m³ fuel]</td>
</tr>
<tr>
<td>5. Combination of O₂ and N₂</td>
<td>O₂ + 2N₂ ↔ 2NO</td>
<td>y₁ [m³NO/m³ fuel]</td>
</tr>
<tr>
<td>6. H₂ dissociation</td>
<td>H₂ ↔ 2H</td>
<td>y₁ [m³H₂/m³ fuel]</td>
</tr>
</tbody>
</table>

In order to obtain the dissociated fractions, one must determine the equilibrium constant $K$ for each of the dissociation reactions. We have used the general equation:

$$K = \frac{z_C^{y_C} \cdot z_D^{y_D}}{z_A^{y_A} \cdot z_B^{y_B}}. \quad (4)$$

where $z_A$, $z_B$, $z_C$ and $z_D$ are the equilibrium mole fractions of reactants and products of a generic equation $v_A \cdot A + v_B \cdot B \leftrightarrow v_C \cdot C + v_D \cdot D$. We have supposed a temperature dependence of the equilibrium constants described by the law:

$$\log K = -\frac{1}{T} \cdot x_1 + (\log T) \cdot x_2 + T \cdot x_3 + T^2 \cdot x_4 + T^3 \cdot x_5. \quad (5)$$

where the coefficients $x_1 \ldots x_5$ can be determined as the solution of a set of five linear equations of the type (5) for a temperature range comprising five known values of the equilibrium constants corresponding to equally-distributed temperatures in the range. As long as these coefficients have been determined, one can calculate the value of the equilibrium constant for any temperature in the considered range. With this value, the dissociated fractions can be determined by using the specific
forms of Eq. (5) written for each of the dissociation reactions.

2.2. Flue Gases Temperature after Dissociation

The flue gases temperature can be determined from the heat balance equation written for the combustion chamber. We have considered that the air-fuel mixture is preheated at a temperature of 590 K ($T_{PH} = 590$ K). The heat balance equation results as follows (Horbaniuc et al., 2010):

$$H_f + H_a = H_{ig} \left( T_{ig}, V_i (T_{ig}) \right). \quad (6)$$

where: $H_f$ – fuel enthalpy at the preheat temperature $T_{PH}$; $H_a$ – combustion air enthalpy at the preheat temperature $T_{PH}$; $H_{ig}$ – flue gases enthalpy at the temperature $T_{ig}$ after dissociation, as a function of this unknown temperature and of the temperature-dependent flue gases composition; $V_i$ – volumes of flue gases components as they result after dissociation

The enthalpies that intervene in Eq. (6) can be written as follows:

- The fuel enthalpy:

$$H_f = (cH4) \left[ \left( h_f^0 \right)_{C,H_4} \frac{T_{PH}}{T_0} + \int c_{p,C,H_4} dT \right] +$$

$$+ (c2H6) \left[ \left( h_f^0 \right)_{C_2H_6} \frac{T_{PH}}{T_0} + \int c_{p,C_2H_6} dT \right] +$$

$$+ (c3H8) \left[ \left( h_f^0 \right)_{C_3H_8} \frac{T_{PH}}{T_0} + \int c_{p,C_3H_8} dT \right] +$$

$$+ (c4H10) \left[ \left( h_f^0 \right)_{C_4H_{10}} \frac{T_{PH}}{T_0} + \int c_{p,C_4H_{10}} dT \right] +$$

$$+ (co2) \left[ \left( h_f^0 \right)_{CO_2} \frac{T_{PH}}{T_0} + \int c_{p,CO_2} dT \right] +$$

$$+ (n2) \int c_{p,N_2} dT \left[ \frac{J}{m^3 \text{fuel}} \right] \quad (7)$$

- The combustion air enthalpy:

$$H_a = V_a \left[ x_{O_2} \int c_{p,O_2} dT + x_{N_2} \int c_{p,N_2} dT +$$

$$+ x_{H_2O} \left( h_f^0 \right)_{H_2O} \frac{T_{PH}}{T_0} + \int c_{p,H_2O} dT \right] \left[ \frac{J}{m^3 \text{fuel}} \right] \quad (8)$$

- Flue gases enthalpy:

$$H_{ig} = V_{CO_2} \left[ \left( h_f^0 \right)_{CO_2} \frac{T_{ig}}{T_0} + \int c_{p,CO_2} dT \right] +$$

$$+ V_{CO} \left[ \left( h_f^0 \right)_{CO} \frac{T_{ig}}{T_0} + \int c_{p,CO} dT \right] +$$

$$+ V_{H_2O} \left[ \left( h_f^0 \right)_{H_2O} \frac{T_{ig}}{T_0} + \int c_{p,H_2O} dT \right] +$$

$$+ V_{OH} \left[ \left( h_f^0 \right)_{OH} \frac{T_{ig}}{T_0} + \int c_{p,OH} dT \right] +$$

$$+ V_{O} \left[ \left( h_f^0 \right)_{O} \frac{T_{ig}}{T_0} + \int c_{p,O} dT \right] +$$

$$+ V_{H} \left[ \left( h_f^0 \right)_{H} \frac{T_{ig}}{T_0} + \int c_{p,H} dT \right] +$$

$$+ V_{N} \left[ \left( h_f^0 \right)_{N} \frac{T_{ig}}{T_0} + \int c_{p,N} dT \right] +$$

$$+ V_{NO} \left[ \left( h_f^0 \right)_{NO} \frac{T_{ig}}{T_0} + \int c_{p,NO} dT \right] +$$

$$+ V_{N_2} \left[ \left( h_f^0 \right)_{N_2} \frac{T_{ig}}{T_0} + \int c_{p,N_2} dT \right] +$$

$$+ V_{O_2} \int c_{p,O_2} dT +$$

$$+ V_{H_2} \int c_{p,H_2} dT \left[ \frac{J}{m^3 \text{fuel}} \right] \quad (9)$$

In the above equations, $\left( h_f^0 \right)_{i}$ accounts for the enthalpy of formation of component $i$. The heat capacities have been considered as temperature-dependent and corresponding polynomials from literature have been used (Sonntag&Van Wylen, 1982). For the heat capacities of O, H, and N, we took the constant value 0.9273 kJ/m$^3$K.

In order to solve Eq. (6) which is a transcendental one, we have chosen to use the Newton-Raphson technique which is very effective, but it involves the laborious procedure of obtaining the derivative of the function. Once this step is accomplished, the algorithm is rather simple and easy to transpose into computer code.

3. RESULTS AND DISCUSSION

In order to obtain the required numerical results, we have developed a software that calculates the flue gases temperature and the flue gases composition for different hydrogen gas contents in the natural gas fuel. By entering the
value of the hydrogen gas percentage, this software generates output screens. Four screenshots are displayed in Fig. 2 for 0% H₂, 50% H₂, 90% H₂, and 100% H₂ respectively.

Fig. 3 shows the dependence of the flue gases temperature after dissociation versus the percentage of hydrogen gas in fuel. The plot exhibits an increase of the temperature as the H₂ percentage increases: at 0% H₂, $T_{fg} = 2362.824$ K, whereas at 100% H₂, its value is $T_{fg} = 2520.443$ K.

In Fig. 4 we have represented the variation of the carbon dioxide mole fraction in flue gases.
versus the H₂ percentage. The range stretches from 0 at 100% H₂ to 0.0814 at 0% H₂. One can notice that the higher the hydrogen gas contents in the fuel, the lower the CO₂ mole fraction is in the flue gases. Obviously, with 100% H₂ there are no CO₂ emissions but this is a limit situation; the aim is to reduce carbon dioxide emissions by adding up hydrogen gas to the natural gas fuel and not by totally replacing it by another fuel.

Fig. 5 displays the plot CO contents in flue gases versus the H₂ percentage in fuel. The graph shows that as the H₂ percentage increases, so does the carbon monoxide mole fraction. This seemingly unexpected outcome can be explained by the fact that the higher the temperature, the more intense is the CO₂ dissociation the result of which is the formation of CO. As shown by Fig. 3, there is a relation between the H₂ percentage and the flue gases temperature in that a higher percentage leads to a higher temperature and thus to a higher CO mole fraction.

In Fig. 6 we have plotted the flue gases volume versus the H₂ percentage of the fuel. The graph shows that the dependence is linear, the increase in H₂ contents of the fuel determining a linear decrease of the flue gases volume. In terms of CO₂ emissions, this result, corroborated with the decrease of the CO₂ mole fraction that accompanies the increase of the hydrogen gas contents of the fuel, evidences a double beneficial effect: as the H₂ percentage increases, both the CO₂ mole fraction and the flue gases volume decrease, which means that by adding up hydrogen gas to the fuel, CO₂ emissions decrease in two ways: by reducing the carbon dioxide mole fraction in flue gases and simultaneously by decreasing the flue gases volume.
4. CONCLUSIONS

By injecting hydrogen gas in a gaseous fuel in a controlled proportion in the range 10 ... 90%, the flue gases temperature increases and thus the performance of the combustion section of a boiler or of a gas turbine may improve, provided that the parts that enter into contact with the flue gases can withstand higher temperatures. The carbon dioxide emissions decrease with the increase of hydrogen percentage and the flue gases volume diminishes concurrently, thus leading to an overall CO₂ abatement. Further investigation will consider using oxycombustion instead of atmospheric air combustion in order to assess the combined influence of the oxidant and of hydrogen gas on combustion characteristics.

REFERENCES