Numerical investigation of fuel flexibility in a small-scale flameless combustor

P Rijo and P J Coelho

1IDMEC, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal

Abstract. Numerical simulation of a laboratory flameless combustor was performed to investigate the flexibility to burn alternative fuels to natural gas. The studied fuels are biogas, syngas and a mixture of ammonia and methane. The inlet temperatures of air and fuel, the equivalence ratio and the geometrical characteristics of the combustor were maintained constant. The results show that flameless combustion is observed in the biogas and in the NH$_3$/CH$_4$ mixture, while the syngas burns according to the conventional non-premixed combustion mode. According to the predictions, the biogas emits 1.1 ppm of NO$_x$ and 229 ppm of CO, syngas produces 7.8 ppm of NO$_x$ and 35 ppm of CO and the NH$_3$/CH$_4$ mixture emits about 3900 ppm of NO$_x$ and 608 ppm of CO. The high NO$_x$ and CO emissions in the NH$_3$/CH$_4$ mixture show that the combustor needs to be optimized to burn a nitrogen-containing fuel.

1. Introduction

Flameless combustion, also known by moderate or intense low-oxygen dilution (MILD) combustion, high temperature air combustion (HiTAC) and colorless distributed combustion (CDC), is a promising technology that allows to increase the thermal efficiency along with a reduction of pollutant emissions, namely NO$_x$, and fuel consumption [1]. This combustion mode is characterized by a relatively uniform distribution of temperature and oxygen concentration in the combustion chamber, which is promoted by a good internal recirculation of the hot flue gases that allows the heating and dilution of reactants prior to combustion [1].

The flameless combustion of methane was studied numerically and experimentally by Rebola et al. [2,3], who used a burner that consists of a central port for fuel injection surrounded by an annular port for air injection. The authors verified that it is possible to obtain flameless combustion for various equivalence ratios and air inlet temperatures. They concluded that NO$_x$ emissions are always low regardless of the tested operating conditions, while the CO and unburned hydrocarbons emissions and the combustion efficiency are affected by the equivalence ratio and the air inlet temperature [2,3].

Hosseini et al. [4,5] studied experimentally and numerically the biogas flameless combustion in a burner similar to that of Rebola et al. [2,3], but in this case the air injection was done through several ports distributed radially instead of through an annular section. Hosseini et al. [4,5] concluded that this combustion mode is achieved for an O$_2$ concentration below 15% and a furnace temperature above 1000 K. In this case, the NO$_x$ emission is lower in comparison with the natural gas flameless combustion, while the CO emission is higher due to a high CO$_2$ concentration in the fuel, which tends to act as an oxidizing agent at higher temperatures [4,5].

Huang et al. [6] studied the syngas flameless combustion in a burner similar to that of Rebola et al. [2,3]. They concluded that the flameless combustion mode is promoted by an increase of the fuel jet...
velocity, which causes an increase of the homogeneity of the mixture of reactants and flue gas. However, the authors found that the increase of the fuel jet velocity decreases the residence time of the flue gases, which promotes an increase of CO emissions, despite the drastic reduction in NO\textsubscript{x} emission, when compared to emissions of the syngas diffusion flame [6].

Sorrentino et al. [7] investigated the flameless combustion of pure ammonia in a cyclonic combustor and concluded that the NO\textsubscript{x} emission increases with the increase of the air inlet temperature and with the excess air coefficient. In the case of rich-fuel conditions, the H\textsubscript{2} and NH\textsubscript{3} emissions exceed 1000 ppm, despite the low NO\textsubscript{x} emission [7].

The aim of this work is to study the flexibility of a small-scale flameless combustor to burn several fuels while maintaining the operating conditions, the geometric characteristics of the burner and the combustion chamber.

2. Numerical Modelling
The furnace investigated in this study is similar to the one used by Rebola et al. [2,3]. The burner consists of a central gas gun and a combustion air supply in a conventional double concentric configuration. The dimensions of the combustion chamber and of the burner are available in [3]. The simulations were carried out using a two-dimensional axisymmetric and unstructured mesh composed by quadrilateral elements. The computational domain is represented in figure 1 and the mesh is composed by about 79 000 elements.

![Figure 1 – Computational domain of the combustor.](image)

The governing equations for continuity, momentum, energy and species mass fractions are solved in the simulation process. The realizable k-\(\varepsilon\) turbulence model is used, which requires the solution of two additional transport equations, one for the turbulent kinetic energy (k) and the other one for the dissipation rate of turbulent kinetic energy (\(\varepsilon\)). These two transport equations are mathematically deduced in order to respect the constraint of positive normal Reynolds stresses. When the standard k-\(\varepsilon\) model is used, this constraint is sometimes violated, yielding non-physical results when the computational domain has stationary and rotating fluid zones [8]. Combustion is modelled using the Eddy Dissipation Concept (EDC). Rebola et al. [3] compared several combustion models in the simulation of a flameless combustor and found that the EDC performed the best, allowing complex kinetic mechanisms to be used. The discrete ordinates model is used to simulate radiative heat transfer and the radiative properties of the participating medium are calculated using the weighted-sum-of-grey-gases model, which expresses the emissivity as a function of the temperature and molar fractions of water vapor and carbon dioxide (CO\textsubscript{2}).

The convergence criteria of the solution procedure for all the simulations carried out were based on the sum of the residuals for each equation and on the monitoring of a set of variables at predefined points. Convergence was achieved when the sum of the residuals was less than 10\(^{-4}\) for mass and species transport equations, 5\(\times\)10\(^{-6}\) for radiation and 10\(^{-6}\) for the other equations, and the axial velocity, temperature and molar fractions of CO\textsubscript{2} and CO at three different positions in the combustion chamber did not change by more than 0.5% between successive iterations.
Table 1. Test conditions

| Fuel      | Composition in molar fraction | Air inlet velocity (m/s) | Fuel inlet velocity (m/s) |
|-----------|------------------------------|--------------------------|---------------------------|
| CH₄       | 100% CH₄                     | 102.1                    | 24.4                      |
| Biogas    | 60%CH₄+40%CO₂                | 101.0                    | 39.74                     |
| Syngas    | 48%CO+38%H₂+14%N₂            | 79.93                    | 89.85                     |
| NH₃/CH₄  | 80%NH₃+20%CH₄               | 97.89                    | 46.22                     |

*For all conditions: fuel thermal input = 10 kW, fuel inlet temperature = 293 K, air inlet temperature = 773 K, wall temperature = 1173 K, equivalence ratio = 0.5.

Table 1 summarizes the test conditions used in this work. Methane combustion was experimentally and numerically investigated by Rebola et al. [2,3]. The air inlet and fuel inlet velocities were prescribed for the other fuels in such a way that the thermal input and the equivalence ratio remain unchanged.

3. Results and discussion

All simulations were carried out using the commercial code *Ansys Fluent* 18. Grid independence was checked by performing the calculations using meshes with different number of control volumes. Figure 2 shows the predicted axial temperature profiles for the different fuels used in this work. Based on the available data, it can be seen that the temperature profiles for the biogas and the NH₃/CH₄ mixture are similar to the methane temperature profile. In the case of syngas, there is a sudden increase of temperature by about 950 K over a distance of 50 mm, followed by a gradual decrease in temperature. This sudden increase in temperature causes an increase in the consumption rate of O₂ and CO.

Based on the O₂ molar fraction shown in figure 3, it can be seen that the increase of air jet velocity leads to an increase of the diffusion of O₂ to the centerline and the maximum O₂ molar fraction occurs upstream of x = 100 mm. In the combustion of syngas, the inlet air velocity is lower than the inlet fuel velocity, the diffusion of O₂ to the centerline is slower and the maximum O₂ molar fraction occurs downstream of x = 100 mm. Furthermore, it can be observed in figure 3 that the O₂ molar fraction profiles have a similar behavior, except for syngas. In the latter case, there is a faster O₂ consumption followed by a stabilization downstream of x = 300 mm. At this location, the O₂ molar fraction profile for the NH₃/CH₄ mixture departs from those of CH₄ and biogas, suggesting a slower combustion process.

The CO molar fraction profiles are presented in figure 4 and indicate the location of the reaction zone through the beginning of consumption/oxidation of this species. The consumption of CO for
biogas and methane start between the points \( x = 330 \) mm and \( x = 350 \) mm, while for the NH\(_3\)/CH\(_4\) it starts at \( x = 450 \) mm, i.e. near the exit of the combustor. This suggests that the combustion chamber is too short to burn this fuel under the studied operating conditions. In syngas, the first 110 mm of the combustion chamber corresponds to the dilution of CO in the surrounding environment and after this point occurs an increase of CO consumption.

Flameless combustion is characterized by smooth gradients of temperature and species concentrations. Based on the results shown in figures 2, 3 and 4, as well as on the temperature and species concentration fields (not shown here), it is concluded that syngas is not burning in this combustion mode. Table 2 summarizes the flue gas composition at the combustor outlet for each fuel. It can be seen that the NO\(_x\) emission is less than 10 ppm for the first three fuels, although the syngas burns according to conventional non-premixed combustion. The combustion of the NH\(_3\) leads to high CO and NO\(_x\) emissions due to the fact that the reaction zone is close to the combustor outlet, which shows that this combustor is not optimized for ammonia combustion.

4. Conclusions
From the results obtained, it can be concluded that the flameless combustion mode is achieved in the biogas and in the NH\(_3\)/CH\(_4\) mixture for the same operating conditions, while the syngas burns in the conventional non-premixed combustion mode. This combustor can work in two different combustion modes with low CO and NO\(_x\) emissions for ammonia free fuels. However, it needs to be optimized for the NH\(_3\) flameless combustion through the use of a larger combustion chamber or through external flue gas recirculation. The reduction of CO emission for all fuels can be obtained by increasing the residence time of the flue gas, e.g., by increasing the internal flue gases recirculation rate.

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