Analysis of combustion stability and efficiency of a meso-scale combustor by means of Continuously Stirred Tank Reactor model

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1. Introduction

Miniaturization of electronics and mechanical systems has triggered the need for the development of small-scale power generation and propulsion systems. The higher energy density of hydrocarbon fuels as compared to currently available top rechargeable chemical batteries (respectively 45 MJ/kg vs. ~0.6 MJ/kg) [1] has readily focused the attention towards combustion based systems. Moreover the cube square law suggested that micro-propulsion and micro-power generation systems based on combustion could outperform macro-scale propulsion devices and chemical batteries. Nevertheless combustion in meso and micro combustor could be hindered by the high surface to volume ratio (heat losses and wall quenching issues) and by the quite short residence time (poor chemical conversion), thus a proper management and understanding of the thermo-chemical issues connected to size reduction are mandatory in order to realize operational and efficient meso-combustors [1-6].

The present work originated from an on-going research activity carried out by some of the authors on a meso-scale whirl combustor of about 254 mm³ in volume and burning H₂, CH₄ or C₃H₈ [7-11]. Their experimental results evidenced that under isothermal condition the meso-combustor has an internal flow field characterized by an asymmetric vortex structure, a high turbulent region near the reactants injection zone and a quite quiescent region at its center [10]. By means of the shadowgraph technique a similar flow structure has been also observed under combustion conditions [11]. These results supported the possibility to numerically investigate the meso-scale combustor by representing it as a Continuously Stirred Tank Reactor (CSTR). The CSTR approach is very attractive because compared to other complex approach (i.e. CFD simulation) it allows to quickly evaluate basic combustor performances at different operating conditions and to use detailed kinetical scheme for hydrocarbon oxidation.

To this aim, the stability (blow-off) limits and the chemical efficiencies of a meso scale whirl combustor burning hydrocarbon fuels have been numerically investigated by a Continuously Stirred Tank Reactor model coupled with a detailed kinetic scheme. Analyses of the relevant numerical results and a comparison with the relevant experimental data have been also reported.

2. Meso-scale combustor

The simulated meso-scale combustor is shown in Fig. 1, the cylindrical combustion chamber is 6 mm in diameter and 9 mm height and it has a volume of about 254 mm³. Tangential air injection allowed generating a whirl flow, while to improve mixing the gaseous fuel was injected in the radial direction at 90° respected to the air flow. Further detail about this meso-combustor, the experimental set-up, and the main experimental outcomes can be found in [9-11]. Just as an example the experimental blow-off limits for propane/air combustion are reported here, Fig. 2.
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Figure 1: Photo (left) and sketch (right) of the meso-scale combustor.

Figure 2: Blow-off limits of the meso-scale combustor feed with propane and air [11].

3. Continuously Stirred Tank Reactor

The meso-scale whirl combustor has been modeled as a single spherical non-adiabatic CSTR of \( d = 7.8622 \) mm in diameter and about \( 254 \) mm\(^3\) in volume. It has been experimentally observed that due to thermal losses a minimum flow rate exists below which flame extinguished independently from \( \phi \) [9-11]. Being an adiabatic CSTR unable to reproduce such result, see Fig. 3, the heat losses have to be taken into account. Heat losses have been computed as \( \dot{Q} = U S (T - T_e) \) where \( U \) is the overall heat transfer coefficient, \( S \) the surface area of the CSTR, \( T_e \) the external temperature and \( T \) the reactor temperature. The product \( U S \) has been fixed in such a way that the closure of the numerical and experimental blow-off curve occurred at the same minimum mass flow rate.

Being interested in analyzing both efficiency and blow-off limits a transient (dynamic) CSTR simulation is required. A description of the dynamic and non-adiabatic CSTR can be found in [12-13] and in the present work it has been solved by using the software DSMOKE developed at Politecnico di Milano [14]. A detailed kinetic scheme (tot0407) developed by Ranzi et al. [15] has been used for hydrocarbon oxidation. This scheme is composed of 8011 reactions and 310 species.

Numerical simulation were performed by imposing a fixed inlet flow rate of air and fuel, the inlet gas temperature was set to 300 K while the initial pressure of the CSTR was set to 101325 Pa. To ignite the fuel/air mixture, the initial gas temperature inside the CSTR was set to 1800 K. To allow the system to reach a steady state condition the simulation last 0.1 s of physical time. The stable operating region of the meso-combustor was identified by selecting the solution for which the final reactor temperature was well above the inlet gas temperature, see Fig. 4. Thus a stability (blow-off) boundary can be defined in terms of equivalence ratio, \( \phi \), and total mass flow rate, \( \dot{m} \).
The chemical efficiency, $\eta_{ch}$, was defined as the fraction of the hydrocarbon fuel converted to CO$_2$. Its value was estimated from the computed mole of CO$_2$ in the exhaust, $\dot{n}_{CO_2}^{\text{out}}$, divided by the input moles of fuels, $\dot{n}_{CH_n}^{\text{in}}$, multiplied by number of C atoms, $x$, contained in the fuel molecule:

$$\eta_{ch} = \frac{\dot{n}_{CO_2}^{\text{out}}}{x \cdot \dot{n}_{CH_n}^{\text{in}}} \tag{1}$$

Figure 3: Numerical blow-off limits for adiabatic CSTR (black line), CH$_4$/air combustion. Experimental data: o.

Figure 4: Time evolution of CSTR temperature at several equivalence ratio and fixed total flow mass rate.

4. Results and discussion

A preliminary numerical analysis of combustor performances has been carried out by imposing a value of the overall heat transfer coefficient equal to $U=122$ W/m$^2$K. Two different hydrocarbon fuels have been analyzed (methane and propane). The blow off curves and the chemical combustion efficiency are shown in Fig. 5. The blow-off curves evidenced that compared to methane/air mixture the propane/air mixture allows the CSTR to operate in a wider range of mass flow rates and equivalence ratios, Fig. 5. This result is due to the faster oxidation kinetic of propane as compared to that of methane. On the same figure it can be observed that for both fuels the highest chemical efficiencies occurred for lean fuel/air mixtures and small mass flow rates. This behavior can be explained by the fact that at low mass flow rates the longer residence time allows more fuel to be converted into CO$_2$, while under lean mixture less CO is produced. For a
too lean mixture, the chemical efficiency drops down because the low gas temperature significantly reduces the rate of CO oxidation [16].

**Figure 5:** Numerical blow-off limit (black line) and chemical efficiency (colored map) of the CSTR when burning methane/air mixture (left) and propane/air mixture (right), for both cases $U=122 \text{ W/m}^2\text{K}$.

Figs. 6 show as a function of the total mass flow rates the experimental (black circles) and numerical (colored lines) blow-off limits. The reference value of the heat transfer coefficient $U$ was set to $61 \text{ W/m}^2\text{K}$ for the propane/air case and to $45 \text{ W/m}^2\text{K}$ for the methane/air case; correspondingly the value of $US$ resulted to be $1.18\times10^{-2} \text{ W/K}$ and $8.74\times10^{-3} \text{ W/K}$. These values allowed the closure of the numerical blow-off curve to occur at the same mass flow rate observed in the experiments. Anyway for methane/air combustion the numerical minimum flow rate limit resulted to be located at approximately stoichiometric condition, i.e. $\phi=1$, while the experimental value was displaced towards the lean side ($\phi\sim0.7$), Fig. 6(left). At total mass flow rate above $1.0\times10^{-4}\text{ kg/s}$ the numerical lean blow-off limit resulted to be approximately constant and in agreement with the experimental data. On the other side the numerical upper blow-off limit was always located on the rich side and at higher $\phi$ than those experimentally observed. Moreover the numerical rich limit stayed approximately constant while the experimental data clearly showed a decreasing trend (i.e. a displacement towards stoichiometric/lean conditions), Fig. 6 (left).

Respect to results for the methane/air case, those for propane/air were in a better agreement with the experimental data, Fig. 6 (right) vs. Fig. 6 (left). First of all the closure of numerical and experimental blow off curves occurred at about the same value of $\phi$, and secondly at flow rates below $1.0\times10^{-4}\text{ kg/s}$ the two blow-off curves resulted very close to each other, Fig. 6 (right). Anyway even in this case, the decreasing trend of the experimental upper limit cannot be reproduced by the numerical one.

To verify the influences of heat losses on blow off limits, the heat loss coefficient $U$ was increased from $U=45 \text{ W/m}^2\text{K}$ up to $U=122 \text{ W/m}^2\text{K}$ for methane/air, and from $U=61 \text{ W/m}^2\text{K}$ up to $U=151 \text{ W/m}^2\text{K}$ for propane/air. Results evidenced that by increasing heat losses the closure of blow-off curve shifted at higher mass flow rates, at the same time the rich and lean limits shrank towards stoichiometric values, Figs. 6. Both fuels showed, above some mass flow rate, an approximately constant numerical rich blow-off limits, see Figs. 6. These results support the conclusion that heat losses alone could not be responsible for the mismatch between the trends observed for the numerical and the experimental blow-off limits. The mismatch can likely be due to a change in the flow field structure that shrinks the size of the region where fuel oxidation takes place, and which cannot be taken into account in the present model.
Combustion efficiency, $\eta_{ch}$, evaluated at $\phi=0.9$ and according to Eq. (1) are shown for methane in Fig. 7(left) and for propane in Fig. 7(right). The values of $\eta_{ch}$ range from $\sim 0.9$ down to $\sim 0.7$. Once again propane showed a better agreement with the experimental results than methane, nevertheless for both fuels the mismatch between numerical and experimental results significantly increased as mass flow rate increased. It should be highlighted that by using the hypothesis of the CSTR it is quite difficult to reproduce the complicated behavior shown in Figs. 6-7. Likely a more elaborated model like a multi-zone reactor that allows for presence of both reacting and quenched zones could allows to improve the results.

Figure 6: Numerical (lines+symbols) and experimental (○) blow-off limits when burning methane/air mixture (left) and propane/air mixture (right). Blue line: $U=45\text{ W/m}^2\text{K}$ (methane/air), $U=61\text{ W/m}^2\text{K}$ (propane/air). Green line: $U=61\text{ W/m}^2\text{K}$ (methane/air), $U=122\text{ W/m}^2\text{K}$ (propane/air). Red line: $U=122\text{ W/m}^2\text{K}$ (methane/air), $U=151\text{ W/m}^2\text{K}$ (propane/air).

Figure 7: Numerical and experimental chemical efficiencies at $\phi=0.9$. Methane/air (left) propane/air (right). ∗: $U=45\text{ W/m}^2\text{K}$ (methane/air), $U=61\text{ W/m}^2\text{K}$ (propane/air). ▽: $U=61\text{ W/m}^2\text{K}$ (methane/air), $U=122\text{ W/m}^2\text{K}$ (propane/air). ○: $U=122\text{ W/m}^2\text{K}$ (methane/air), $U=151\text{ W/m}^2\text{K}$ (propane/air). Experimental values: ●, ●
5. Conclusion

The blow off limits and the chemical efficiency of a meso scale whirl combustor burning propane or methane at ambient pressure have been numerically investigated by a Continuously Stirred Tank Reactor model coupled with a detailed kinetic scheme. A quite good agreement was evidenced between the numerical lean blow-off limits and the experimental data, on the other side the numerical results fail to reproduce the decreasing trend of the rich blow-off limit. Numerical and experimental combustion efficiencies were in quite good agreement in the low mass flow rate range, for the propane/air test case they both showed a decreasing trend with flow rate. A better agreement between numerical and experimental results was systematically observed for propane/air combustion than for methane/air combustion.

These results evidenced that, even with some restraints, the approach based on a single non-adiabatic CSTR could help in estimating the performances of the meso-scale whirl combustor and in understanding its behavior. A more elaborated model like a multi-zone reactor that allows for the presence of both reacting and quenched zones is likely needed to improve the results.

7. References