

Optimization of a Cyclonic Combustion Chamber for the Thermochemical Conversion of Alternative Fuels

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This work provides an insight into the influence of the design parameters, specifically the configuration of the outlet section, on the fluid dynamic field and residence times distribution of a cyclonic flow burner, designed to operate under Moderate or Intense Low oxygen Dilution (MILD) combustion conditions with alternative energy carriers. The investigated geometric parameters play a key role in determining the velocity pattern and mixing process of the reactant mixture, fluids residence time distribution and burned gas internal recirculation, by influencing the oxidation process efficiency and pollutant emissions. These latter characteristics are essential in the framework of the recent global energy transition toward renewable sources. Indeed, the intermittency of renewables sources requires the development of specific processes and technologies able to mitigate their inherent variability. Among them, chemical storage ensures large storage capacity for long period and with high efficiency, ensuring easy and safe transportation and storage. In this context, bio-derived alcohols and free carbon fuels such as ammonia and hydrogen have been identified as alternative energy carriers to efficiently storage the renewable energy. Nevertheless, the exploitation of these molecules poses some relevant challenges. The most considerable obstacles are related to the variable composition of the bio-derived products and the consequent lower heating value with respect to traditional hydrocarbon fuels. These aspects greatly limit the technologies capable of employing such energy carriers. Therefore, it is necessary to identify innovative thermochemical conversion technologies highly flexible with respect to the type and composition of the fuel, which ensure reduced pollutant emissions and the stability of the oxidation process for each required operational condition. In this respect, MILD combustion represents an efficient technology matching these issues. In this context, the obtained results allow to identify the appropriate design features of a cyclonic flow burner in order to ensure the complete conversion of the inlet charge and the effective process stabilization.

1. Introduction

The achievement of global energy requirements has to deal with numerous constraints that are continuously modifying the possible outlines behind the future energy market. A typical limitation for the employment of several renewable energy sources (RES) is their strong source-dependency. Thus, the need of very effective transmission systems and reasonable techniques for energy storage is mandatory in order to face with such energy security issue (Johansson, 2013). Among the several technologies, the chemical-based storage is highly competitive solution, offering the possibility of gathering large energy amounts for long time.

These arguments represent fundamental elements that boost toward the use of renewable or alternative energy carriers in chemical, transportation and power generation sectors (Hoque et al., 2019). Specifically, the employment of several alternative fuels requires the development of thermochemical conversion systems that simultaneously ensure flexibility, high efficiency and very low pollutant emissions, such as advanced combustion technologies (Nemitallah et al., 2018). Flexible backup power plants based on gas turbines (Richards et al., 2001), engines and stationary systems (Sabia et al., 2019) represent potential solutions to the inherent intermittency of renewables. In this context, a paradigm shift is needed in the development of advanced combustion systems, which have to be suitable for the complexity and variability of the energy mix.

In the scenario of innovative thermochemical conversion technologies, MILD combustion (Cavaliere and de Joannon, 2004) is usually reported as a key solution to ensure fuel flexibility (Ye et al., 2015) and high combustion efficiency with near-zero emissions (Tu et al., 2017).

Such oxidation process is practically realized through internal or external recirculation of burned gases into fresh reactants and it requires proper designs of the combustion chamber.

Specifically, the combustion chamber geometry is a fundamental aspect to establish a fluid-dynamic flow field that allows to attain MILD Combustion conditions. In this respect, a thorough control of several reactor and aerodynamic features is needed, such as the residence time, the strength of the internal recirculating flows, the turbulent mixing and the volumetric distribution of the reactants (Khidr et al., 2017). In fact, these aspects play an essential role in ensuring an efficient mixing between burned gases and fresh reactants, thus achieving a stable oxidation process in a diluted environment with low oxygen availability.

The architecture of the combustor geometry and its size are the main parameters that affect the extension and the position of the reactive region, the local recirculation rate, the temperature distribution inside the burner and the pollutant formation. Therefore, both the aerodynamic configuration and the geometry of the combustion chamber are critical parameters in determining the stabilization of a MILD oxidation regime (Xing et al., 2017).

A promising configuration to achieve simultaneously large recirculation zones and long residence times was proposed in previous literature works, specifically related to a cyclonic-flow chamber (Sorrentino et al., 2015). It showed very good performances in terms of load and fuel flexibility, pollutant reduction (Sorrentino et al., 2018) and alternative fuel utilization (Ariemma et al., 2021). However, some limitations related to the fluid-dynamic flow field and the residence time distribution have been identified and need to be addressed in order to increase the oxidation process efficiency. In this regard, simple modifications of the combustion chamber configuration can help in obtaining very effective improvements in both the aerodynamics and residence time distribution (Sharma et al., 2018).

In particular, previous studies by the same research group (Sorrentino et al., 2017) suggested that, by tailoring the flow field in proper ways through simple chamber configurations, it is possible to achieve the suitable residence time distribution (RTD) of fluid elements with beneficial effects on pollutant emissions.

Higher fraction of fluid having lower residence time can lead to overall high emission of carbon monoxide in the exhausts when burning hydrocarbons or high levels of nitrogen oxides for ammonia combustion (Van Der Lans et al., 1997). Therefore, a proper shape of the residence time curve can be tailored through fluid-dynamic pattern modifications to enhance the pollutant reduction (Arghode and Gupta, 2013).

On the other hand, the strength of the toroidal vortex structure for cyclonic combustors is strongly influenced by the inlet velocity of the reactant jets because it modifies the internal entrainment processes and the ternary mixing between fuel, oxidizer and burned products.

On the basis of this background, the present paper aims at providing possible simple modifications of the cyclonic chamber geometry to improve the combustion system performance. In particular, the non-reacting flow field of the cyclonic configuration is examined with a particular focus on the entrainment and recirculation generation in order to achieve a distributed combustion and enhance the environmental performance in terms of ultra-low emissions. The main flow characteristics inside the combustor, along with the turbulence generated and the mixing characteristics were analyzed for several modifications of the combustion chamber geometry.

In this context, different geometrical configurations of the combustion chamber were proposed here, with the twofold aim of realizing large recirculation regions and to obtain a tailored residence times distribution of the fluid elements. As reported above, previous literature studies on the cyclonic combustion chamber highlighted some critical aspects related to the fluid-dynamic patterns within the cyclonic chamber. The presence of dead volume regions or channeling phenomena lead to the decreasing of the reactants conversion efficiency. A possible solution to overcome such issues deals with simple modifications of the geometric configuration of the burner. The variation of some characteristic dimensions of the prismatic chamber can help in modifying the internal fluid-dynamic, to increase the intensity of the recirculation regions and reduce the dead volumes/channeling patterns inside the reactor.

The effect of geometry modifications on the reactor performance was evaluated on the basis of both the fluid-dynamic field and the fluid elements residence time obtained for each configuration. Numerical simulations for several configurations were carried out to obtain information about the aerodynamic features when geometric modifications are performed.

Such optimization process permits to achieve promising results for the identification of a proper configuration that is able to satisfy simultaneously the requirements of sustainability, efficiency and flexibility.

2. Numerical methodology

Numerical simulations by means of CFD were performed for several configurations of the cyclonic chamber on the basis of hexahedral grids. The numerical analysis considered the oxidant stream as the only one that generate the toroidal vortex inside the chamber, for the simplicity of non-reacting flow simulations. A commercial finite volume based tool, Ansys Fluent (Ansys Fluent, 2017) was used as the CFD solver. The simulations mainly involved the turbulence modeling of the cold flow. Several computational grids were obtained through the ANSYS meshing software Icem CFD software to achieve a three-dimensional (3D) geometry of the cyclonic chamber. A mesh independency study was carried out and finally an unstructured computational mesh, built with approximately five hundred thousand hexahedral elements (500 k), clustered near the inlets, was used with specific boundary conditions (BCs). Inlet velocity boundary conditions were used for main jets, whereas a pressure outlet was used for the exit of the chamber.

RANS equations were solved using the $k-\epsilon$ RNG turbulence model with the option "Swirl Dominated Flow" (used for flows with strong swirl and recirculation) (Shilapuram et al., 2011). Pressure-velocity coupling was solved using a SIMPLE resolution scheme, whereas for the momentum equation a second order upwind scheme was used. The residuals for the simulations were set to 10^{-5} for the continuity equation and 10^{-6} for all the velocity components.

Helium at 300 K was used as working fluid in order to reproduce high temperature conditions of reactive flows under MILD combustion conditions (i.e. similar properties of H_2O and CO_2 at 1400 K).

An inlet average velocity value of 38 m/s was set for the helium jets in accordance with the inlet stream velocities used in previous works under MILD reactive conditions. Such inlet velocity value ensures a Reynolds number at the inlet duct of about 2000. The average velocity inlet value is related to the nominal thermal power that is used under reactive conditions and of course it is also a function of the fuel that was used.

3. Results

In Figure 1 (a-b) the geometry of the standard cyclonic combustion chamber and the flow fields inside the reactor are reported for an average inlet flow velocity equal to 38 m/s. Such a configuration represents the reference case to compare the performances of the investigated modifications of the combustion chamber geometry.

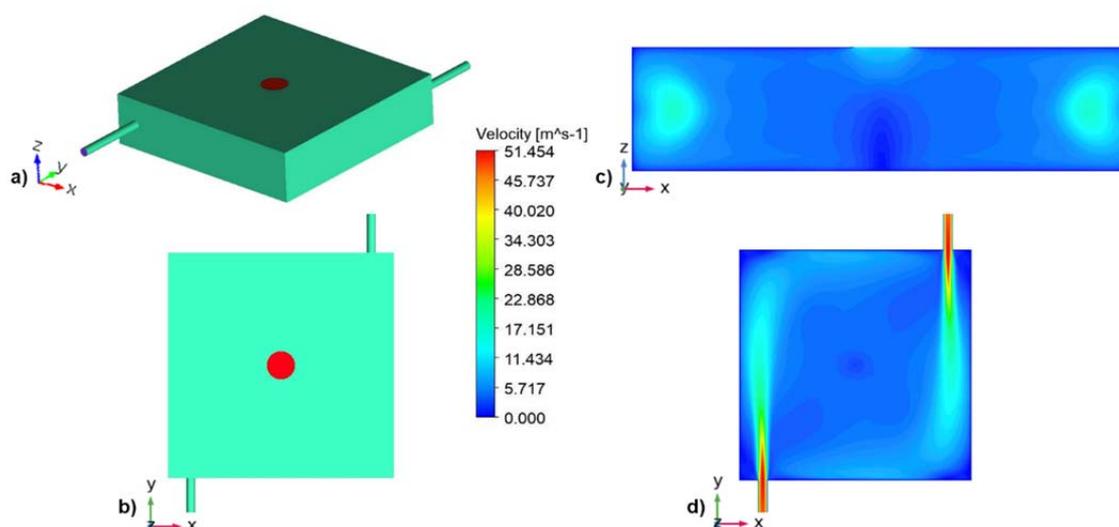


Figure 1. Geometry (a-b) and velocity field (c-d) of the "standard" cyclonic combustion chamber.

The reactor (Figure 1a-1b) consists in a prismatic chamber ($0.2 \times 0.2 \times 0.05 \text{ m}^3$) fed by means of two tubes (ID 0.008 m), which are placed in an anti-symmetrical configuration on the corners of two opposed walls of the combustion chamber. The exit (ID 0.025 m) is positioned in the center of the top face of the chamber. This injection configuration coupled with the outflow position allows to establish a centripetal cyclonic flow field inside the reactor. The cyclonic flow field of Figure 1 (c-d) is evaluated at two orthogonal mid-planes, parallels to the inlet section (plane xz) and the outlet one (plane xy) of the reactor, respectively. Both the velocity fields assessed at the xy and xz planes show decreasing velocities by moving toward the outlet section of the

reactor, where the influence of the inlet jet momentum is less pronounced. In particular, with reference to Figure 1d, the velocity contour at the xy plane shows a very uniform central region, with average velocity values in the order of 5 m/s. At the xz plane (Figure 1c) the velocity field shows very low velocity values close to the outlet section. In particular, in the lower part of Figure 1c it is possible to identify a central region characterized by close to zero velocities, which highlight the presence of a dead volume caused by the depression region close to the outlet section. Due to the establishment of this region, part of the fluid bypasses the central region of the reactor without completing the cyclonic motion. This behaviour entails a reduction of the mean residence time for the fuel conversion inside the reactor with a resulting decrease of the combustion efficiency.

In order to prevent such critical features related to the flow bypass toward the outlet section and dead volumes, thus increasing the active residence time of the fluid elements inside the reactor, the effectiveness of several improvements was investigated. In particular, a modification of the top section of the combustion chamber was considered. In this context, the standard configuration of the reactor was modified with a truncated cone protrusion. The cone was originated from the center of the top face of the chamber, aligned with the outflow, and projecting toward the inward of the reactor.

In order to evaluate the effectiveness of the conical protrusion at the outlet section of the combustion chamber, several fluid-dynamic simulations were performed by varying the protrusion length, namely 0.02, 0.025 and 0.03 m. Numerical analyses were carried out to identify the optimal condition in terms of flow field patterns and residence time distribution (RTD) inside the combustion chamber, in order to ensure the complete conversion of a wide palette of fuels in the cyclonic combustor.

In Figure 2 are reported the combustion chamber configurations, iso-surfaces at $v=6$ m/s and the velocity field on the xz plane for the three different protrusion lengths here investigated. The iso-surface at $v=6$ m/s is identified as characteristic of the peripheral region of the combustion chamber.

The iso-surfaces show slight differences for the three configurations here investigated whereas the velocity field on the xz plane is characterized by a marked influence of the conical protrusion. In fact, the addition of a truncated cone protrusion reduces the width of the region at lower velocity values, close to the outlet section of the reactor, with respect to the standard combustion chamber configuration (Figure 1c), as confirmed by the velocity contour reported on the xz plane of Figure 2 and thus influencing also the pressure field nearby the exit. In particular, qualitatively this reduction seems to be characterized by a non-monotonic trend with the length of the truncated cone protrusion, being more marked for protrusion lengths equal to 0.02 m and 0.025 m.

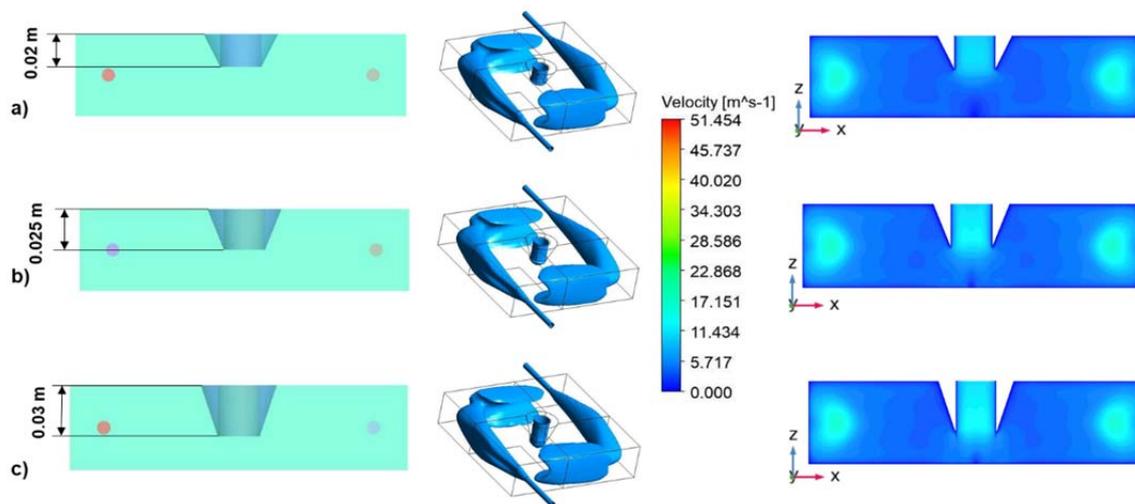


Figure 2. Combustion chamber configuration, iso-surfaces at $v=6$ m/s and velocity field on the xz plane for three different protrusion lengths: a) 0.02 m; b) 0.025 m; c) 0.03 m.

In order to quantify the effectiveness of the investigated solutions to optimize the cyclonic combustion chamber configuration with respect to the fluid-dynamic, normalized residence time distributions (E_θ) were computed for the three investigated cases and they were compared with the reference case of Figure 1.

The normalized residence time distribution E_θ is defined in agreement to the equation 1 (Levenspiel, 1999):

$$E_\theta = \tau \cdot E_t \quad (1)$$

with $\theta = t/\tau$, τ is the mean residence time inside the reactor and E_t is the residence time distribution.

The purpose of using this normalized distribution function is that the flow performance inside reactors with slightly different sizes can be directly compared. In fact, the protrusion of a truncated cone of different height slightly reduces the combustion chamber volume with respect to the standard configuration one. In addition, to better highlight the differences and improvements with respect to the standard chamber geometry, the percentage difference between the E_θ of the modified configurations and the E_θ of the standard combustion chamber ($E_\theta^{standard}$) was analyzed in agreement to the equation 2:

$$\Delta E_\theta \% = (E_\theta - E_\theta^{standard}) \cdot 100 \quad (2)$$

In Figure 3 are reported the normalized residence time distributions (E_θ) and ΔE_θ % for the examined cases.

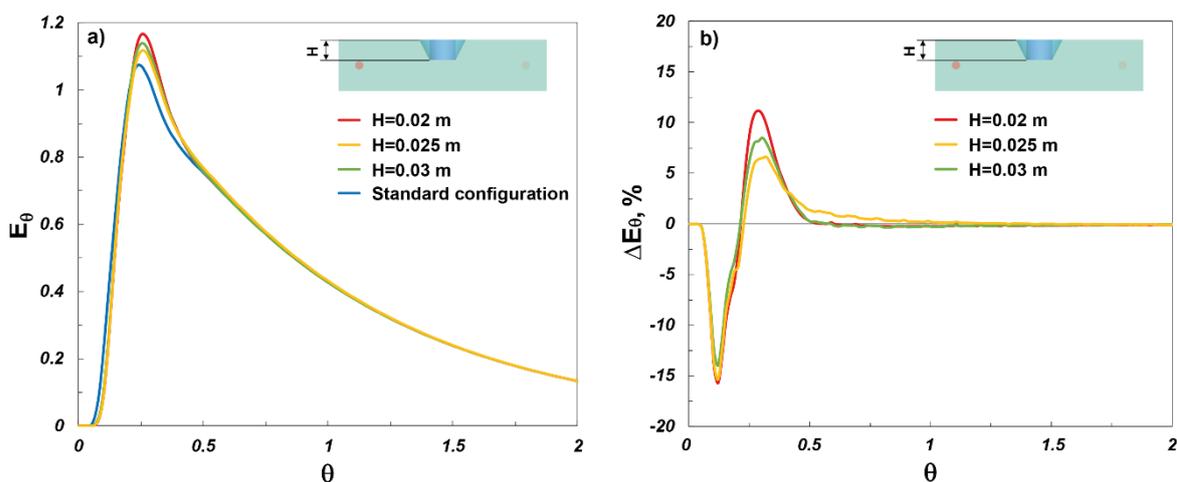


Figure 3. Normalized residence time distributions (E_θ) and ΔE_θ % for investigated chamber configurations.

With reference to Figure 3a, all the E_θ show profiles characterized by an initial lag time of about 0.08 mimicking a PFR-like behavior, then they reach a maximum for θ of about 0.26 and finally they exhibit a typical exponential decay of a CSTR-like profile. In particular, the global behaviour of the analyzed combustion chamber under non-reacting conditions can be represented as a series of PFR-CSTR with a bypass and a dead volume. In particular, with respect to the E_θ of the standard combustion chamber configuration (blue line), E_θ profiles related to configurations with the truncated cone protrusion are characterized by a higher initial lag time and a higher maximum value, which entail an increase of fluid fractions that leave the reactor with normalized residence times higher than 0.26. This behaviour represents a fundamental aspect related to the need of ensure the complete conversion of a wide palette of fuels. In particular, the increase in the maximum of normalized residence time distribution with respect to the standard configuration is not linear with the protrusion length of the truncated cone, showing a more marked increase for $H=0.02$ m than the cases with higher protrusion lengths. With reference to Figure 3b, the analysis of the percentage differences (ΔE_θ %) with respect to the normalized residence time distribution of the standard configuration highlights that for the three investigated configurations is detected a negative percentage gain in the initial part of the curve (up to $\theta=0.26$), whereas a positive gain for longer times is detected. In particular, the negative gain, which entails a higher initial lag time with respect to the standard reactor configuration, shows no significant differences for the three configurations with different length of the truncated cone protrusion. On the other hand, although all the three configurations are characterized by an increase of the fluid-dynamic performances of the combustion chamber with respect to the standard configuration, only one with a protrusion length $H=0.02$ m reaches a positive gain of about 11%, confirming the better performances identified in the Figure 3a.

The reported results clearly show the effectiveness of the investigated combustion chamber configurations with respect to the standard one, in terms of fluid-dynamic and thus residence times inside the reactor. In particular, the configuration with a truncated cone protrusion length equal to 0.02 m, on the top face of the combustion chamber, shows the better performances.

4. Conclusions

The present study provides an insight into technological issues related to the utilization of cyclonic flows for the thermochemical conversion of wide palette of fuels. In particular, the combustion chamber optimization is an important step to overcome several drawbacks related to the system efficiency. In the present work such

optimal design procedure was carried out by investigating the influence of geometric parameters of the cyclonic combustion chamber, operating under MILD combustion conditions. In particular, the effectiveness of a truncated cone protrusion with several lengths, namely 0.02 m, 0.025 m and 0.03 m was numerically investigated by analyzing the fluid-dynamic field and the normalized residence times distributions for three different geometric configurations. The investigated configurations play a key role in determining the complete conversion of reactants fed to the reactor and the burned gases internal recirculation, influencing the oxidation process stability and pollutant emissions.

The results that have been obtained in the present work allow to identify the beneficial effect of all the three examined configuration on the reduction of fluid-dynamics issue related to the presence of dead volumes and/or bypass caused by a depression region close to the outlet section. These affect the standard reactor design entailing channeling phenomena close to the central region of the combustion chamber. In particular, the design configuration with a truncated cone protrusion length equal to 0.02 m was identified as the best solution to ensure an effective percentage increase of the residence time inside the reactor, thus allowing both the complete conversion of the inlet charge with reduced pollutant emissions and the oxidation process stability.

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