Variation of residence time in non-premixed turbulent bluff-body ethylene flames as a function of burner diameter

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Abstract
The knowledge of the residence time distribution (RTD) in practical combustion applications, such as gas turbines, is of crucial importance as it has been correlated to soot formation and emission indices. However, the measurement of RTD is challenging in reacting environments. Computational Fluid Dynamics (CFD), on the other hand, offers an easier tool with which to estimate RTD in complex reacting flows. The effect of the bluff-body diameter on the residence time distribution within the recirculation zone, in a turbulent non-premixed ethylene flame stabilized on a bluff-body burner, has been numerically investigated. Models of 2-D axisymmetric bluff-body burners, with three bluff-bodies of different diameter (38, 50, and 64 mm), but identical in other dimensions, have been used in this work. Stochastic tracking model was employed to estimate the particle residence time distribution in the recirculation region. The CFD model was validated using the well-known turbulent bluff-body diffusion flame-HM1 before it was applied to predict similar flames with pure ethylene as fuel. The calculations predict that increasing the bluff-body diameter results in an increase in the recirculation zone length by a factor of two, and a considerably longer residence time in the recirculation zone while keeping jet and co-flow Reynolds numbers the same.

Introduction
The combustion of hydrocarbon fuels in boilers, furnaces and engines is often accompanied by soot formation. While soot is hazardous for human health due to its carcinogenic effects, its presence within the flame envelope can benefit combustion efficiency by increasing the radiative heat transfer [1]. One of the key controlling parameters that can affect soot formation, growth and oxidation is the residence time of soot and its precursors within the flame. The amount of soot which is formed during the combustion process depends on the residence time [2]. Although the global residence time estimation suggested by Turns and Myhr [2] is useful as an indication of the characteristic strain rate in a flame, the distribution of the particle RT is required since the flame span over an extended range of the local strain. So, to gain a deep understanding of the distribution of the particles in different zones of a flame, both experimental and computational investigations are required.

Measuring the distribution of the particles in a specified zone of a reacting environment is quite complex. A few attempts have been made by researchers to evaluate the RTD in different non-reacting/reacting systems. The concept of RTD was first introduced by Danckwerts [3] which discussed two types of flow-plug flow and well-stirred flow that exist. The RTD concept was then developed to predict the burn-out of a pulverized coal combustion [4]. Pedersen et al [5] determined the RTD in a swirled pulverized coal flame by tracing fluids and inert particles and developed an ideal chemical reactor capable to simulate the RTD.

The RTD measurement in reacting flows is challenging due to the high temperature reacting environment. To reduce such complexity, some researchers investigated the RTD in non-reacting flows [6-9]. In these works, the RTDs have been evaluated by the measurement of the concentration of a tracer that can be solid or gaseous, employing a technique like Laser-Induced Fluorescence (LIF) or gas analysis methods. For instance, Cheng et al. [6] measured the residence time using a time-resolved planar laser-induced fluorescence (PLIF) combined with Particle Image Velocimetry (PIV) technique to evaluate the fuel concentration response to a sudden cut-off in the injection of the fuel stream. They used this system for the residence time measurement in a single-phase isothermal flow, although this technique can also be adapted to a reacting environment.

In another work, the radioactive gaseous tracers [7], was used as particle tracers. This trace, although costly, was preferable to the injection of solid particles [8] particularly in the environment containing solid particles such as sooting flames. A new in-situ method was applied to measure the cumulative distribution function and the residence time distribution of both non-reacting and reacting flows by Bürkle et al. [9], and a simple chemical reactor network model was proposed to fit cumulative density function. This study, despite its significance, was limited to a lab-scale oxy-fuel combustor. Despite the investigations above, to the authors’ best knowledge no measurement or calculations of the RTD in a turbulent axisymmetric bluff-body flame have been reported previously. Bluff-body stabilized flames have been under investigation for decades due to their broad application in many combustion systems such as ramjets and afterburners. Furthermore, such flames in laboratory scales have been investigating since they mainly emulate some of the combustion phenomenon encountered in other systems in a controlled environment. Considering all the complexities and challenges in the measurement of RTD in a turbulent sooting flame with the presence of recirculating flows, the aim of this paper is to conduct a Computational Fluid Dynamics (CFD) study to investigate the effect of bluff-body diameter on the residence time distribution of the inert particles within the recirculation zone, and to investigate the recirculation zone characteristics of the mean flow field for each burner dimension.

Methods
A 2-D axisymmetric model was generated in ANSYS FLUENT 19. The bluff-body burner with the central jet diameter of 4.6 mm, and the bluff-body diameter of 50 mm which was centred in a co-flow air coming from a wind tunnel with the exit cross-section of 150×150 mm^2 was considered. The model was extended for 1D_{in} upstream to ensure a fully-developed flow at the inlet. In order to minimize the effect of the surrounding environment on the flame, the model was extended to 10D_{in} downstream of the domain, and 5D_{in} in the radial direction. The 2D geometry and the boundary conditions are shown in Figure 1.
Mesh structure plays an important role in obtaining high-accuracy and cost-efficient numerical results. A mesh sensitivity study was performed to find out the dependency of the results on the mesh resolution. A structured quadrilateral cell shape grid was generated with high resolution near the jet, bluff-body and the co-flow inlets. A comparison of the radial temperature distribution at a specific axial distance for 220,000, 470,000, and 770,000 cells revealed that increasing the number of mesh to 770,000 does not change the results by more than 2% in comparison to the 440,000 case. So, 440,000 mesh was selected for modelling the bluff-body flames.

The steady incompressible Reynolds-averaged Navier–Stokes (RANS) equations were used for the turbulent bluff-body flame, and the conservation equations of mass, momentum, and energy were numerically solved. The standard $k-\varepsilon$ model was selected owing to its well-known capability of predicting recirculating flows. Dally et al. [10] suggested a modification for the standard $k-\varepsilon$ turbulence model in order for the model not to over-predict the decay rate of a round jet. So, the modified $C_1$ coefficient has been modified to 1.6. The steady flamelet model coupled with a DRM-22 reduced Kinetic mechanism (22 species and 104 reactions) were used for the combustion model. The DRM-22 has been shown to give a reasonable prediction of a bluff-body flame with less computational costs in comparison to other mechanisms [11]. The SIMPLE pressure-velocity coupling with standard pressure scheme was used. All equations were discretised using a second order upwind scheme. The convergence criteria were set to $10^{-6}$ for all equations. The residence time of the particles was estimated by calculating the trajectory of the particles in a Lagrangian frame. This method was recently employed by Chinnici et al. [12] to calculate the particle residence time and trajectories in a solar vortex particle reactor. The trajectory of the particles is computed based on the integration of the particle force balance equation. Turbulent dispersion of the particles was calculated using the stochastic tracking model. Inert particles with diameter of 1mm were injected to the domain from the air and fuel inlet boundaries and measured at the exit plane from the recirculation zone where the axial velocity components are positive. Since in turbulent flows, the species transport is mainly dominated by turbulent diffusion rather than molecular diffusion, it is possible to track these inert particles [5].

In the first step of the numerical study, the predicted flame properties such as axial and radial velocity components, temperature and the mixture fraction were validated against the existing experimental data from the well-known Sydney/Sandia bluff-body HM1 flame [10]. A 50:50 mixture (by volume) of CH$_4$ and H$_2$ was issued at a velocity of 118 m/s with surrounding co-flow air at 40 m/s is used for model validation. Having compared the radial distribution velocity, temperature, and the mixture fraction at different axial locations in the recirculation zone, the neck zone and the jet-like region (from $x/D_{bb}=0.26$ until a downstream distance of $x/D_{bb}=2.4$), a very good agreement was observer between the calculations and the experiment. A sample comparison of the experimental and the CFD results at $x=13$ mm ($x/D_{bb}=0.26$) from the burner tip, plus the temperature contour can be seen in Figure 2. The axial and radial distance are normalised by the bluff-body diometer ($D_{bb}$).

![Figure 1. 2D drawing of the computational domain and related boundary conditions](image)

The results and discussion

Shown in Figure 3 are the calculated streamlines from the recirculation zone of three flames each with a different bluff-body diameter burner. Also indicated in the figure is the length of the recirculation zone, defined by the furthest point with zero axial velocity. It is observed that, as expected, increasing the bluff-body diameter resulted in increasing the length of the recirculation zone. This increase is attributed to the level of mixing and interaction between the jet and the co-flow and is found to be governed by the momentum flux ratio and the diameter of the bluff-body burner [10]. Since this ratio of both jet and the co-flow was kept the same for all three burners, the length is only controlled by the change in the bluff-body diameter. Here we can see that increasing the diameter from 38 mm to 50 and 64 mm, resulted in an increase in the recirculation zone length by almost 40% and 85%, respectively (from 50.7 mm to 70.25 and 93.4 mm). Hence, we expect that this increase in the length of the recirculation zone will increase the residence time of the particles in this zone, and consequently will affect soot formation in this region. The residence time distribution for the three burners has been compared in Figure 4. The different distributions indicate that less than 10% of the particles, that is introduced, does not enter the circulating zone.

![Figure 2. Comparison of the radial velocities, mixture fraction and the temperature profiles of CFD results with the experimental data for a bluff-body HM1 flame [10]](image)
and escape out to the neck zone. The distribution of the rest of the particles can be observed in this figure. The mean residence time of the particles is almost doubled when the diameter increases from 38 mm to 64 mm. Since there is an overlap of the timescales of turbulent mixing and the soot formation in turbulent flames, which is in the order of few millisecond-10 milliseconds, it is inferred that this residence time of the particles can affect soot formation in the recirculation zone.

Figure 3. Computed flow field for three bluff-body burners: 38 mm (Top), 50 mm (middle), and 64 mm (bottom)

The calculated mixture fraction distribution within the recirculation zone, RZ, for all three bluff-body burners and at three axial locations is shown in Figure 5. It can be observed that the mixture fraction and location of the reaction zone are almost identical on the outer part of the RZ irrespective of bluff-body diameter. Also noticeable, is that increasing the bluff-body diameter induces a larger amount of the fuel into the inner part of the RZ creating richer mixtures that are favourable for soot formation.

Figure 4. Calculated mean residence time of the particle inside the recirculation zone, and the length of the zone (Top), Residence Time Distribution (RTD) of the particles in the recirculation zone (bottom)

Based on the chemical reactor theory, flow in the recirculation zone can be interpreted as a continuously stirred tank reactor (CSTR) flow. The RTD function in a CSTR flow model can be obtained from the following equation. This function quantitatively describes how much time fluid particles spend in a reactor. Details on chemical reactor theory can be found in [13].

$$E(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right)$$  

(1)

where $E(t)$ is the RTD function, $t$ is time, and $\tau$ is the mean residence time.

The cumulative RTD function $F(t)$ describes the fraction of the particles that leave the reactor at less than time $t$. The CSTR model enables us to represent the flow pattern in a simplified form based on an ideal chemical reactor. The comparison of the cumulative function of the particles leaving the recirculation zone obtained from the CFD, and the RTD function based on a CSTR is shown for all three bluff-body burners in Figure 6. It is clear that except for the low residence time particles, which are likely to be associated with jet, the analytical model captures the residence time distribution reasonably well.
the RZ can be quantified with a factor of two which can considerably influence the soot residence time.

A computational model of an ethylene turbulent flame stabilized on bluff-body burners with different bluff-body diameters has been conducted in order to increase understanding of the effect of bluff-body dimension on the recirculation zone characteristics and to predict the distribution of the residence time of inert particles within the recirculation zones of those flames. Results show that increasing the bluff-body diameter from 38 mm, to 50 mm, and 64 mm can almost double the recirculation zone length. This increase in the size and length of the recirculation zone can also lead to increase the residence time of the particles inside the recirculation zone by a factor of two which can considerably influence the soot formation in this region. It can be observed that the mixture fraction and the reaction zone in the recirculation region are not significantly influenced by increasing the bluff-body diameter. The flow pattern in the recirculation zone of a bluff-body flame is shown to be interpreted as a simplified CSTR chemical reactor model. It is also shown that the RTD of the particles in the RZ can be quantified with CSTR model.

Conclusions

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References