Increased heat transfer to sustain flameless combustion under elevated pressure conditions – a numerical study

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ABSTRACT
Sustaining flameless combustion under elevated pressure conditions remains a challenge that hinders its application in gas turbines. Previous attempts succeeded to sustain flameless operation up to 5 atm. In the present work, reaction rate is decreased by increasing heat transfer through combustor walls so that the reaction zone is kept distributed. Pressure is elevated from 1 to 15 atm. and its effect on reaction zone location and spread, and emissions is investigated. Two-dimensional computations are performed using ANSYS fluent package. Under adiabatic combustor wall conditions, increasing the pressure results in a more concentrated reaction zone, and a departure from flameless mode at 3 atm. The calculated Damköhler number is noticed to increase from 0.2 to 1.9. NOx emissions increases from 10 to 78 ppm. Nearly 90 % of the predicted NOx are generated via the thermal route. Under isothermal combustor wall conditions, increased heat transfer is noticed to limit the increase in heat of reaction and temperature with pressure. The calculated Damköhler number is noticed to increase from 0.12 to 0.85. This is nearly half the values encountered under adiabatic conditions, which demonstrate a distributed reaction under all pressures investigated. Finally, NOx emissions are found below 5 ppm for all pressures investigated.

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1. Introduction
Flameless or MILD combustion is a recent combustion technology that is based on mixing a considerable amount of recirculated product gases with fresh reactants before combustion takes place (Khidr, Eldrainy, & El-Kassaby, 2017; Wünning & Wünning, 1997; Zhang, Mi, Li, Wang, & Dally, 2015). To sustain combustion at these vitiated conditions, combustion air is preheated either before entering the combustor or through mixing with hot product gases inside the combustor. The resulted distributed reaction zone has led to many advantages for this type of combustion. The axial temperature profile appears to be more flat with no temperature peaks or hot spots. This in turn has led to single digit emission levels, low noise and high combustion stability (Cavaliere & de Joannon, 2004; Tsuji et al., 2002). Motivated by these features and the success of flameless combustion application in industrial furnace systems, research efforts have been conducted to extend its application to gas turbines (Flammme, 2004, 2005; Nemitallah, Rashwan, Mansir, Abdelhafez, & Habib, 2018; Perpignan, Talboom, Levy, & Rao, 2018). However, gas turbine combustors are intrinsically different from industrial furnaces as they operate under high-pressure levels typically in the range of 5–50 bars. It is well understood that increasing pressure leads to a subsequent reduction of the laminar flame speed as it slows down species molecular diffusion ($S_L \sim p^{-1/2}$) (Goswami et al., 2013; Zahedi & Yousefi, 2014). However, it also induces smaller turbulent scales, which in turn results in higher flame front wrinkling. A subsequent increase in the flame surface area is resulted which offsets the reduction in the laminar flame speed (Cohé, Halter, Chauveau, Gökalp, & Gülder, 2007). Consequently, pressure has a minimal effect on the turbulent flame speed of methane-air mixtures at least theoretically (Griebel, Siewert, & Jansohn, 2007). However, increasing the pressure is noticed to cause abortion from flameless combustion as previously reported in several works (Khalil & Gupta, 2015; Kruse, Kerschgens, Berger, Varea, & Pitsch, 2015; Lammel et al., 2010; Lückerath, Meier, & Aigner, 2008; Zornek, Monz, & Aigner, 2015). Increasing pressure, while maintaining constant inlet mass flowrate, reduces the reaction zone size due to the reduction in flow velocity (Khalil & Gupta, 2015). Consequently, heat release becomes more concentrated with pressure leading to a higher and more localized temperature zone. Due to the elevated temperature, the production of high carbonaceous compounds
are promoted leading to an increased flame luminosity (De Joannon, Saponaro, & Cavaliere, 2000). Limited number of studies were reported to address this problem of pressure according to authors’ knowledge (Khalil & Gupta, 2015; Lückerrath et al., 2008). In these studies, focus is given to enlarge the reaction zone size, despite the elevated pressures, through reducing the reaction rate or increasing reactants flow velocity. Reducing the reaction rate is achieved by increasing the amount of recirculated exhaust gases (Shareh, Silcox, & Eddings, 2018), while increasing reactants flow velocity is achieved by increasing the inlet momentum (Khalil, Eldrainy, Saqr, & Abdelghaffar, 2018). Previous approaches only succeeded to sustain flameless operation under slightly elevated pressures (up to 5 atm.). The primary reason for this limited pressure range is believed to be the significant effect of pressure on mixing between incoming reactants and recirculated products inside the combustor. In the present work, authors propose a different approach to sustain flameless operation under more elevated pressure conditions (above 5 atm.). This approach is based on decreasing the reaction rate by increasing heat transfer through combustor walls to keep the reaction zone distributed under more elevated pressure levels. It is believed that this approach could be able to extend flameless operation pressure limit beyond 5 atm. as it is independent from mixing. Therefore, the objective of this paper is to investigate the combined effect of pressure and increased heat transfer on flameless combustion. Computational fluid dynamics, CFD, is being employed in the current investigation and validation with experimental data is provided whenever possible. Recently, CFD has become a very powerful tool in tackling various engineering challenges (Akbarian et al., 2018; Faizollahzadeh Ardabili et al., 2018; Ghalandari, Mirzadeh Koohshahi, Mohamadian, Shamshirband, & Chau, 2019; Mou, He, Zhao, & Chau, 2017; Ramezanizadeh, Alhuyi Nazari, Ahmadi, & Chau, 2019).

2. Numerical setup

In this section, the geometry used for the present analysis is first presented. The details of the turbulence and combustion models along with the discretization theme and the solver type are then followed. After that, the generated mesh and imposed boundary conditions are then demonstrated. Finally, geometrical and operational aspects of the investigated cases are summarized.

2.1. Combustor geometry and computational domain

Figure 1(a) shows the geometry of the combustor employed in the present study. The combustor was originally constructed and employed by Rebola, Coelho, and Costa (2013; Rebola, Costa, & Coelho, 2013). Fresh reactants are introduced inside the combustor through one central fuel jet of 4 mm diameter, surrounded by a central air jet of 15 mm diameter in a concentric configuration. It is placed at the top of a cylindrical quartz combustion chamber, which has an inner diameter of 150 mm and a length of 300 mm. Combustor walls are preheated to 1173 K using an electric heating system. The combustor ends at the bottom with a 35° slopped nozzle of 50 mm length. Methane is employed as a fuel. All details about the experimental setup can be found in (Rebola, Costa, et al., 2013). As the combustor is axisymmetric, only a 2D axisymmetric section is employed for the present numerical work to save the computational time (Figure 1(b)).

2.2. Numerical model

The following steady state Reynolds averaged Navier-Stokes set of equations (RANS), are used in the present computations (short notation used) (Fluent, 2016):

\[
\frac{\partial}{\partial x_i} (\rho u_i) = 0. \quad (1)
\]

\[
\frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right] \\
+ \frac{\partial}{\partial x_j} \left( - \rho \bar{u_i} ' \bar{u_j} ' \right). \quad (2)
\]

Where \( \rho \) is the density of the fluid, \( t \) is the time, \( u_i \) is the mean component of velocity in the direction \( x_i \), \( p \) is the pressure, \( \mu \) is the dynamic viscosity, and \( u_i ' \) is a fluctuating component of velocity. Repeated indices indicate summation from one to two. Due to averaging, additional six terms \( - \rho \bar{u_i} ' \bar{u_j} ' \) appear which represent the contribution of turbulence to the mean flow. They are considered additional stresses resulted due to turbulence and named after Reynolds as ‘Reynolds turbulent stresses’.

Turbulence is modeled using the realizable \( k - \epsilon \) model (RKE) of Shih, Liou, Shabbir, Yang, and Zhu (1995). The transport equations for both \( k \) and \( \epsilon \) are shown below (short notation form):

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho k u_j) = \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_t}{\sigma_k}) \frac{\partial k}{\partial x_j} \right] \\
+ G_k + G_y - \rho \epsilon - Y_M + S_k \quad (3)
\]
\[
\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_j}(\rho \epsilon u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\epsilon}} \right) \frac{\partial \epsilon}{\partial x_j} \right] \\
+ \rho C_1 \epsilon - \rho C_2 \frac{\epsilon^2}{k + \sqrt{\nu \epsilon}} + C_1 \epsilon \frac{\nu}{k} C_3 \epsilon C_b + \epsilon
\]  \tag{4}

Where

\[C_1 = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right], \quad \eta = \frac{k}{\epsilon}, \quad S = \sqrt{2S_y S_{ij}}\]

In these equations, \(G_k\) represents the generation of turbulence kinetic energy due to the mean velocity gradients. \(G_b\) is the generation of turbulence kinetic energy due to buoyancy. \(Y_M\) represents the contribution of the fluctuating dilatation in compressible flows in the overall dissipation rate. \(C_2\) and \(C_1\) are constants. \(\sigma_k\) and \(\sigma_f\) are the turbulent Prandtl numbers for \(k\) and \(\epsilon\) respectively. \(S_k\) and \(S_\epsilon\) are any other defined source terms.

RKE demonstrates higher performance compared with other two equation models in strained and swirling flows (Khalil, Saqr, Eldrainy, & Abdelghaffar, 2018). In addition, it is the standard turbulence model often used in most of flameless combustion past numerical studies (Duwig, Stankovic, Fuchs, Li, & Gutmark, 2007; Hosseini, Bagheri, & Wahid, 2014; Khidr et al., 2017; Rebola, Coelho, et al., 2013). This is mainly because of its demonstrated accurate predictions of flameless combustion characteristics under various conditions (Rebola, Coelho, et al., 2013).

The modeled energy equation is as follows:

\[
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_j} \left[ \left( k_{th,\text{eff}} \frac{\partial T}{\partial x_j} + u_i \left( \tau_{ij,\text{eff}} \right) \right) \right] + S_h \tag{5}
\]

Where \(E\) is the total energy, \(k_{th,\text{eff}}\) is the effective thermal conductivity, and \(\left( \tau_{ij,\text{eff}} \right)\) is the effective stress tensor (in case of viscous heating which is not included in the present case). The effective thermal conductivity is modeled from:

\[
k_{th,\text{eff}} = k_{th} + \frac{C_p \mu_t}{Pr_t} \tag{6}
\]

where \(k_{th}\), in this case, is the thermal conductivity.

Near wall flow parameters are estimated using standard wall function with a coarse near wall grid; \(y^+ = 40–60\).

The non-flamelet eddy dissipation concept (EDC) of Magnussen (1989) is used for combustion modeling. The eddy-dissipation-concept (EDC) model is an extension of the eddy-dissipation model to include detailed chemical mechanisms in turbulent flows. It assumes that reaction occurs in small turbulent structures, called the fine
scales. The length fraction of the fine scales is modeled as Fluent (2016):

\[ \xi^* = C_\xi \left( \frac{\nu \epsilon}{k^2} \right)^{1/4} \]  

(7)

where \( \xi^* \) denotes fine-scale quantities and

\[ C_\xi = \text{volume fraction constant} = 2.1377 \]

\[ \nu = \text{kinematic viscosity} \]

The volume fraction of the fine scales is calculated as \( \xi^* \).

Species are assumed to react in the fine structures over a time scale (Fluent, 2016):

\[ \tau^* = C_\tau \left( \frac{\nu}{\epsilon} \right)^{1/2} \]  

(8)

where \( C_\tau \) is a time scale constant equal to 0.4082.

The source term in the conservation equation for the mean species \( i \), is modeled as (Fluent, 2016):

\[ R_i = \frac{\rho \xi^{*2}}{\tau^* |1 - \xi^{*3}|} (Y_i^* - Y_i) \]  

(9)

EDC is believed to be able to deal with both slow and fast chemistry regions that can coexist in flameless combustors (Locci, 2015). Moreover, it can deal with a wide range of both high and low Damköhler numbers (Hosseini et al., 2014; Hosseini & Abdul Wahid, 2015). For these reasons, it has been the standard combustion model often used for flameless combustion studies (Duwig et al., 2007; Hosseini et al., 2014; Khidir et al., 2017; Rebola, Coelho, et al., 2013).

A reduced version of GRI-MECH 1.2 with 22 species and 104 reactions (DRM-22) is used for chemical kinetics (Kazakov & Frenklach, 1994). However, this kinetic mechanism is further refined in the present work to improve CO predictions as will be explained in the validation section. The in-situ adaptive tabulation method (ISAT) is used to reduce the computational cost of the detailed chemistry calculations (Pope, 1997). Radiation heat transfer is taken into account using the Discrete Ordinates (DO) radiation model theory (Raithby & Chui, 1990). The weighted-sum-of-grey gases (WSGG) model is used to estimate all mixture radiative properties based on local mass fractions and temperatures inside the domain. The finite volume approach with the second order upwind scheme is employed for the spatial discretization of pressure, momentum and species transport equations. Pressure based solver is employed along with the Pressure Implicit with Splitting of Operator (PISO) algorithm for the solution of the pressure corrected continuity equation. A desktop computer with an Intel core i7 processor, and 16 GB RAM is employed for all computations along with ANSYS-Fluent 17 commercial package. Regarding boundary conditions, inlet mass flow is applied at combustor inlets. Pressure outlet is applied at the combustor exit. No-slip condition with either zero heat flux or isothermal boundary is applied at combustor walls according to the investigated case. Finally, axis condition is applied at the combustor centerline.

It should be noted that a critical parameter in flameless combustion which will be used throughout the present work is the recirculation ratio, \( K \). It is defined as the ratio between the mass of the recirculated product gases to the inlet mass of reactants. As we move axially along the combustor center line, this parameter is zero at the inlet, and starts to increase due to the added recirculated mass to the main inlet stream mass. After reaching its maximum, it then starts to decrease due to the detached mass from the inlet stream mass until it becomes zero again at the combustor exit. The recirculated mass is being determined by subtracting (in a separate excel sheet) the inlet mass from the total mass passing through a certain combustor radial section. The inlet air mass flowrate is given from the experimental conditions of Rebola et al. (Rebola, Coelho, et al., 2013; Rebola, Costa, et al., 2013). The total mass passing through a certain combustor section is computed numerically at each combustor section. Therefore, inlet recirculation ratio is not defined as a boundary condition and it has a zero value.

2.3. Grid independent test

Figure 2 shows the mesh generated for the present computational domain. As mentioned before, a 2D axisymmetric section is used for our numerical computations due to geometric symmetry. Three grid resolutions were tested for a grid independence solution; a coarse grid of 56700 cells, a moderate grid of 130000 cells, and a fine grid of 300000 Cells. All grids are refined where high turbulence, mixing, and high temperature gradient are expected. The operating case used for the study was reported in [53, 54] and is presented in Table 1 under constant wall temperature of 1173 K. Figure 3 demonstrates both predicted the axial velocity and mean temperature profiles along the combustor centerline for the three grids employed. Other parameters were also tested but not shown for brevity. Predicted axial profiles of velocity, temperature, and CH4, CO2, O2, and CO mole fractions (not included), were almost identical for the three grids. Maximum discretization error is 3.76% and is recorded for the temperature predictions between the first two grids. Finally, Table 1 demonstrates the grid densities and combustion parameters peak values for different grid resolutions employed. It can be concluded that
the coarse grid (56700 cells) can be used for the present analysis.

2.4. Solution convergence

A converged solution is reached when all computational residuals become less than $10^{-6}$. Moreover, to increase confidence in the solution adopted, velocity and temperature are monitored at several points inside the domain. The solution is considered to be converged when they reach steady state values. Figure 4 shows the development of the static temperature profile with number of iterations at four different axial locations ($x/L = 0.06, 0.3, 0.42, \text{ and } 0.54$). These axial locations are all located at the combustor centerline ($y = 0$). It can be noted from the figure that temperature profiles reach a steady state solution with number of iterations less than 5000 at all locations. Velocity profiles show a similar behavior, however, they were not included due to limited space.

2.5. Investigated cases

In the present paper, the combustor operating pressure is increased incrementally from atmospheric to 15 atm. to cover the typical operating range of gas turbine combustors. Equivalence ratio is maintained constant at 0.5

| Table 1. Grid densities and combustion parameters peak values for different grid resolutions. |
|---------------------------------------------------------------|
| No. of combustor cells in y direction | G1 = 56636 cells | G2 = 129434 cells | G3 = 295804 cells |
|--------------------------------------|-----------------|-----------------|-----------------|
| No. of fuel nozzle cells in y direction | 150 | 300 | 600 |
| No. of air nozzle cells in y direction | 10 | 15 | 23 |
| Peak temperature [K] | 1515 | 1460 | 1431 |
| Peak O$_2$ conc. (%) | 17.79 | 17.77 | 17.75 |
| Peak CO$_2$ conc. (%) | 5.055 | 5.05 | 5.049 |
| Peak CO conc. (%) | 0.195 | 0.193 | 0.191 |
Figure 4. Development of mean temperature profiles with number of iterations at various combustor axial locations, $y = 0, x/L = 0.06, 0.3, 0.42,$ and $0.54$.

Table 2. Geometrical parameters and operating conditions for investigated cases.

| Parameter                  | Value                  |
|----------------------------|------------------------|
| Thermal load [kW]          | 10 kW                  |
| Fuel                       | Methane                |
| Air jet diameter, $d_a$ [mm]| 15                     |
| Fuel jet diameter, $d_f$ [mm]| 4                     |
| Inlet air velocity, $V_{air\_inlet}$ [m/s] | 102.1                 |
| Inlet air mass flow rate, $m_{air\_inlet}$ [kg/s] | $6.9 \times 10^{-3}$ |
| Inlet fuel velocity, $V_{fuel\_inlet}$ [m/s] | 24.4                   |
| Inlet fuel mass flow rate, $m_{fuel\_inlet}$ [kg/s] | $0.2 \times 10^{-3}$ |
| Inlet recirculation ratio, $K$ | 0                     |
| Excess Air Ratio, $\lambda$ | 2                     |
| Inlet air temperature, $T_{air\_inlet}$ [K] | 773                    |
| Inlet fuel temperature, $T_{fuel\_inlet}$ [K] | 293                    |
| $Re_{Dh}$, at air inlet   | 14000                  |
| Operating pressure, $P_{op}$ [atm.] | 1, 3, 5, 10, 15        |

3. Results and discussion

In this section, validation of the numerical model is first conducted to gain confidence in the results obtained. The isothermal case under atmospheric pressure conditions is used for the validation. Predicted results are compared with the experimental measurements of Rebola, Costa, et al. (2013). Following the validation, the effect of pressure on mixing and recirculation, reaction zone location and spread, combustion global features, and emissions is investigated under adiabatic wall conditions. Finally, the combined effect of pressure and heat transfer on the previous parameters is studied.

3.1. Validation of the numerical model

The performance of the DRM22 reduced mechanism is first assessed and is briefed in the following lines. The mean temperature, $O_2$, and $CO_2$ predictions are found to agree well with the experimental data while CO is considerably over predicted. Primary CO production and consumption reactions in flameless combustion were identified in the work of Liu et al. (2017). Accordingly, four main reactions are selected for the tuning of their kinetic parameters. Following the approach of Tu, Yang, and Liu (2017), the reaction rate constant, $k$, can be tuned only through modifying the pre-exponential factor, $A$, to match the experimental conditions of Rebola et al. (Rebola, Coelho, et al., 2013; Rebola, Costa, et al., 2013). The effect of increasing the pressure on flameless combustion characteristics is investigated under two conditions of combustor walls. First, it is investigated under adiabatic wall condition where no heat transfer across the walls is included (referred to as ‘the adiabatic case’). Then, it is investigated under constant wall temperature of 1173 K where wall heat transfer is included (referred to as ‘the isothermal case’). Table 2 lists the geometrical aspects and operating conditions for both cases.
Table 3. CO primary reactions in flameless combustion with their original and modified pre-exponential factors.

| Reaction number (in DRM) | Reaction | Behavior | Original pre-exponential factor, $k$ | Modified pre-exponential factor, $k_{mod}$ |
|--------------------------|----------|----------|-------------------------------------|-------------------------------------------|
| R8                       | O + CO($+M$) $\leftrightarrow$ > CO$_2$($+M$) | Production | 6.02E+11                             | 6.02E+10                                  |
| R59                      | OH + CO $\leftrightarrow$ > H + CO$_2$ | Consumption | 4.76E+07                             | 4.76E+08                                  |
| R71                      | HO$_2$+CO $\leftrightarrow$ > OH + CO$_2$ | Production | 1.50E+14                             | 1.50E+13                                  |
| R100                     | HCO + O$_2$ $\leftrightarrow$ > HO$_2$ + CO | Production | 1.34E+12                             | 1.34E+11                                  |

Figure 5. Predicted radial profiles of CO concentrations for the different DRM22 modification scenarios, measurements are taken from Rebola, Costa, et al. (2013).

which reflects the number of collisions from the correct orientation. Consequently, as CO is over predicted, the pre-exponential factor is increased by order of magnitude for consumption reactions and decreased by order of magnitude for production reactions. The effect of each individual reaction modification on CO predictions is then studied. Table 3 summarizes the reactions selected with their original and modified pre-exponential factors.

Figure 5 shows the predicted CO radial profiles at three different axial combustor locations ($x/L = 0.3, 0.42$ and $0.54$) for the different DRM22 modification scenarios. Only the modification of R59 is noticed to improve the CO predictions. Increasing the pre-exponential factor of R59 by order of magnitude results in an increase of the CO consumption rate to a value that closely matches the actual case. Moreover, this improvement is noticed to be consistent at different combustor axial locations. Modifying other reactions does not lead to any predictions improvement. This can be attributed to the different role played by these reactions (production or consumption) at different combustor regions. Consequently, the DRM22 mechanism with modified R59 will be used for the present analysis. It should be noted that the present validation is conducted only under atmospheric pressure conditions. Experimental data under elevated pressure conditions are not available. However, the DRM22 mechanism is already validated in (Kazakov & Frenklach, 1994) under elevated pressure conditions for both ignition delay time and laminar flame speed. The tested pressure range is (0.1–10 atm.) while the tested equivalence ratio range is (0.2–2). Deviations from GRI-MECH 1.2 are below 2% for most cases.

It Figure 6 demonstrates the predicted and experimental radial profiles of mean temperature and O$_2$, CO$_2$ and CO concentrations at five combustor axial locations ($x/L = 0.06, 0.18, 0.3, 0.42, 0.54$) using the present numerical theme with the modified DRM22 mechanism. Generally, the numerical predictions are in fairly good agreement with the experimental measurements despite some discrepancies between the CO predictions and the experiments. These discrepancies in CO predictions are still noted despite the previous tuning of the reduced chemical reaction mechanism. The main reason for this might be the limited ability of the current chemical reaction mechanism to predict all CO consumption and production routes in flameless combustion. It is noteworthy to say that the DRM22 reduced mechanism is derived from the GRI-MECH 1.2 which was primarily developed for conventional combustion. Thus, it is important to consider the future development of new mechanisms for this purpose. In general, the present numerical model is able to regenerate the main flameless combustion characteristics of the present isothermal case with accepted accuracy. Temperature profiles are noticed to be nearly uniform except for the near burner region where mixing takes place. In this region, the development from a steep temperature increase at $x/L = 0.06$ to more gradual temperature increase at $x/L = 0.18$ is attributed to the effect of the central jet expansion. Temperature in the product gases region downstream the combustor is noticed to be slightly higher than the temperature in the recirculation zone upstream the combustor. This is apparently because of the heat transfer across the combustor walls which cools down the recirculated product.
gases before they are mixed with the incoming reactants. Overall, maximum temperature does not exceed 1480 K anywhere in the combustor. This moderate temperature increase along with the nearly uniform temperature profiles, can be attributed to the distributed reaction zone typical of the flameless operation. O₂ and CO₂ show complementary profiles while the latter appear to qualitatively follow the temperature trends. Maximum CO mole fraction is found below 0.3% which reflects the low emissions operation of the present combustor.

The ability of the present numerical model to capture the main differences between the flameless and conventional modes of combustion was assessed (not included in the present paper for brevity). This assessment was performed through studying the effect of increasing the air jet diameter, \( d_a \), from 15 to 30 mm. Increasing \( d_a \) to twice its value was noticed to cause abortion from the flameless mode due to the considerable reduction in the recirculation ratio, \( K = \frac{m_{\text{rec}}}{(m_{\text{air}} + m_{\text{fuel}})} \). Recirculation ratio is defined as the ratio between the recirculated product gases mass flowrate, \( m_{\text{rec}} \), and the inlet fresh reactants mass flowrate, \( (m_{\text{air}} + m_{\text{fuel}}) \) [1]. The model successfully generated the global combustion characteristics for both modes.
3.2. Effect of pressure – the adiabatic case

The effect of pressure on the characteristics of the mean flow field is first investigated. Increasing the pressure inside the combustor results in a proportional decrease in reactants density. Since the air and fuel inlet mass flowrates are kept constant, the increased density will lead to a subsequent decrease in both air and fuel inlet velocities. To further demonstrate the effect of pressure on flow turbulence and mixing, predicted contours of turbulent intensity at combustor symmetry plane are shown in Figure 7. Relatively high turbulence intensity is noticed to occupy most of the combustor volume under atmospheric pressure conditions. It reaches its peak at the shear layer between the inlet high velocity air jet and the surrounding medium. However, increasing the pressure suppresses the turbulence inside the combustor as noticed from Figure 7. This reduced turbulence intensity with increasing pressure can be attributed to the decreased inlet velocity. Figure 8 shows the variation of the recirculation ratio with pressure. Despite the considerable effect of pressure on turbulence intensity, increasing the pressure results in a slight decrease in recirculation ratio. This slight decrease of recirculation ratio with increasing the pressure can be explained using the following relation (Han & Mungal, 2001):

\[ K = \frac{m_{\text{rec}}}{m_{\text{air}}} = 0.32 \frac{x}{d_{\text{air}}(\rho_{\text{air}}/\rho_{\text{rec}})^{1/2}} - 1 \]  

(10)

Increasing the pressure results in a similar increase in both air and recirculated exhaust gas densities, hence,
it has minimal effect on the ratio $\frac{\rho_{\text{air}}}{\rho_{\text{rec}}}$. However, the slight increase in combustion products temperature with increasing the pressure (as will be shown) results in a slight decrease in the recirculated exhaust gases density, $\rho_{\text{rec}}$. Decreasing $\rho_{\text{rec}}$ results in an increase of the term $(\frac{\rho_{\text{air}}}{\rho_{\text{rec}}})^{1/2}$, however, it will be a slight increase due to the term’s power. Consequently, the recirculation ratio will be slightly decreased as noted in Figure 8. This slight decrease in recirculation ratio with pressure can be attributed to both the slight and hardly noticed increase in recirculated gases temperature and the square power of the term $(\frac{\rho_{\text{air}}}{\rho_{\text{rec}}})^{1/2}$. Despite the slight effect of pressure on recirculation ratio, its substantial effect on turbulence intensity is expected to affect the reaction zone characteristics, hence, the flameless combustion.

Figure 9 shows the effect of pressure on the predicted contours of OH mole fraction at the combustor symmetry plane. OH radicals are widely known for its high reactivity, hence, short living. Consequently, visualization of OH radicals is a frequent approach that is used to study the reaction zone structure. Under atmospheric pressure conditions, Figure 9 shows a widely distributed reaction zone with relatively high OH intensity. Although it occupies most of the combustor volume, its highest intensity is at the middle of the combustor ($x/L = 0.44$) close to the combustor centerline. This is the location where fuel and air are believed to be mixed with considerable amount of recirculated exhaust gases and preheated enough for the combustion to be initiated. The resulting distributed reaction zone structure appears to comply well with the high turbulence intensity noticed under the same conditions. It also represents one of the flameless combustion mode intrinsic characteristics. Under elevated pressures, reaction zone becomes more concentrated specifically at the combustor centerline. Reaction zone size is determined by both laminar flame speed and flow velocity. Increasing the pressure is found to reduce the laminar flame speed and subsequently the reaction rate as will be demonstrated at the last section of this paper. Consequently, the noticed reduction of the reaction zone size can be attributed to the decrease in laminar flame speed (reaction rate), flow velocity and turbulence intensity. OH intensity is also noticed to decrease with the increase in pressure. This decrease in OH intensity can be attributed to the recombination of OH radicals to form $\text{O}_2\text{H}_2$ compounds under elevated pressure conditions (Kazakov & Frenklach, 1994).

Figure 10 shows the effect of pressure on the predicted contours of mean temperature at the combustor symmetry plane. Under atmospheric pressure conditions, a gradual increase of temperature is noticed along the combustor center line. This gradual increase in temperature can be attributed to the widely distributed reaction zone previously noticed under the same conditions. No temperature peaks or definite flame front are apparent which further confirms the flameless mode of operation under these conditions. Increasing the pressure results in the appearance of a relatively high temperature zone.
at the middle of the combustor \((x/L = 0.4)\). This high temperature zone can be attributed to the more concentrated reaction zone previously noticed in Figure 9 under elevated pressures. It can be explained as follows: the reaction zone becomes more concentrated with pressure, consequently, heat of reaction increases as it becomes more localized leading eventually to the noticed elevated temperature spot. Moreover, the peak temperature increases with pressure leading to the noticed higher temperature gradient. To further support this conclusion, the effect of pressure on the predicted axial profile of heat of reaction along the combustor centerline is shown in Figure 11. It can be noticed from the figure that with increasing the pressure, the heat of reaction becomes higher and more concentrated. Moreover, it is shifted toward the combustor inlet as a result of the decreased flow velocity. The plotted profiles are noticed to confirm the previous results.

To further explain the previous results, Figure 12 shows the predicted axial profiles of mean temperature, and \(\text{CH}_4\), \(\text{CO}_2\) and \(\text{CO}\) concentrations for the adiabatic case. Looking at the mean temperature axial profiles, temperature is noticed to first increase from ambient temperature (fuel inlet temperature) until it reaches 773 K (the air jet inlet temperature) at \(x/L = 0.2\). In this region, fuel is preheated apparently due to the mixing
with the high temperature air jet. After that, temperature is noticed to increase at a higher rate from \(x/L = 0.2\) to \(0.3\) apparently due to the mixing with the hot recirculated exhaust gases. The following bifurcation in temperature increase rate noticed at \(x/L = 0.3\) reveals the difference between the flameless combustion under atmospheric pressure and the conventional combustion under elevated pressures. Under atmospheric pressure, temperature continues to increase with nearly the same rate till \(x/L = 0.45\) followed by a nearly uniform temperature profile till the combustor exit. However, under elevated pressures, temperature tends to increase at a higher rate with a peak noticed at \(x/L = 0.4\). This can be attributed to the more concentrated reaction zone (Figure 9) and more localization of heat of reaction (Figure 12). Moreover, this temperature peak is noticed to move upstream with increasing the pressure due to decreased axial velocity. These results comply with predicted mean temperature contours shown in Figure 10. It should be noted that product gases temperature does not show a noticeable increase with pressure as seen in Figure 12. This means that the recirculated gases density will not change considerably due to temperature, which explains the slight decrease in recirculation ratio noted in Figure 8. The predicted \(\text{CH}_4\) mole fraction axial profiles reflects the previous results. A gradual decrease of \(\text{CH}_4\) mole fraction from 1 at \(x/L = 0\) to 0.055 at \(x/L = 0.3\) is noticed. Apparently, this decrease is the result of the fuel jet mixing with air and recirculated exhaust gases. After that, reaction starts at \(x/L = 0.3\) and extends to \(x/L = 0.8\). Within the reaction zone, \(\text{CH}_4\) mole fraction is decreased at different rates under different pressures. This can be attributed to the increased methane consumption rate resulted by the more concentrated reaction zone and elevated temperature. \(\text{CO}_2\) mole fraction axial profiles appear to follow the temperature profiles in the reaction zone \((x/L = 0.3–0.8)\) as expected. Moreover, an increase in \(\text{CO}_2\) mole fraction is noticed from \(x/L = 0.2\) to \(x/L = 0.3\) apparently because of the mixing between air, fuel and the hot recirculated exhaust gases as previously mentioned. \(\text{CO}\) mole fraction axial profiles usually represents the location and size of the reaction zone. It can be noticed from these profiles that the reaction zone under atmospheric pressure is relatively wide compared with elevated pressure conditions. It extends from \(x/L = 0.3\) to \(0.9\) with its peak at \(x/L = 0.45\). Increasing the pressure results in a more concentrated \(\text{CO}\) profile, which demonstrates a more concentrated reaction zone. Moreover, it is noticed to shift the reaction zone in the upstream direction as noticed from the locations of the \(\text{CO}\) mole fraction peak. Finally, increasing the pressure results in reducing the \(\text{CO}\) emissions due to the increased residence time, the elevated temperature, and the encouragement of \(\text{CO}\) transformation to \(\text{CH}_2\text{O}\) as per the reaction \(\text{H}_2+\text{CO}(+\text{M}) \rightarrow \text{CH}_2\text{O}(+\text{M})\) (Kazakov & Frenklach, 1994).
Finally, Figure 13 shows the predicted NOx for the present combustor under adiabatic conditions and elevated pressures. Thermal, prompt and N2O intermediate NOx were evaluated. As noticed, NOx emissions increases with pressure, which can be attributed to the increase in both residence time and temperature. The majority of the predicted NOx are generated via the thermal route (nearly 90%) while the N2O intermediate and prompt NOx constitute less than 10%. Similar trends were noticed in the work of Khalil et al. (Khalil & Gupta, 2015).

### 3.3. Effect of pressure – the isothermal case

In the isothermal case, the combustor wall temperature is kept constant at 1173 K for all pressures investigated. To demonstrate the effect of pressure on flow turbulence and mixing under isothermal conditions, predicted contours of turbulent intensity at combustor symmetry plane are shown in Figure 14. As noticed in the adiabatic case, relatively high turbulence intensity which occupies most of the combustor volume is noticed under atmospheric pressure conditions. It reaches its peak at the shear layer between the inlet high velocity air jet and the surrounding medium. Similar to the adiabatic case, increasing the pressure appears to suppress this turbulence due to the decreased inlet velocity. Figure 15 shows the variation of the recirculation ratio with pressure. Despite the considerable effect of pressure on turbulence intensity, increasing the pressure appears to have a slight effect on recirculation ratio. Increasing the pressure from 1 to 5 atm. results in a slight increase in recirculation ratio. However, further increase in pressure from 5 to 15 atm. shows no effect on recirculation ratio. As explained in the previous section, the recirculation ratio is affected by temperature rather than pressure. Consequently, this slight variation of recirculation ratio with pressure can be explained to follow the slight variation of the combustion temperature with pressure (as will be shown).

Figure 16 shows the effect of pressure on the predicted contours of OH mole fraction at the combustor symmetry plane. Similar to the adiabatic case, a considerable decrease in OH intensity with increasing the pressure is noticed which can be attributed to the recombination of OH radicals to form O2H2 compounds (Kazakov & Frenklach, 1994). Moreover, the reaction zone size is noticed to decrease with increasing the pressure, which is expected due to the reduced laminar flame speed (as will be shown later) and flow velocity. However, in contrary to the adiabatic case, the reaction zone structure noticed at the atmospheric pressure appears to maintain its distributed shape under elevated pressure conditions. No high OH gradient is noticed with increasing pressure in the present case (Figure 16) in contrary to the adiabatic case (Figure 9). This difference in behavior can be explained as follows. In the adiabatic case, increasing the pressure results in a more concentrated reaction zone, which subsequently leads to an increase in heat of reaction and temperature. However, in the present isothermal case, heat transfer is believed to play a role in limiting the increase in heat of reaction and temperature resulting from increasing the pressure.

Figure 17 shows the effect of pressure on the predicted contours of mean temperature at the combustor symmetry plane. A gradual increase of temperature is noticed along the combustor centerline and in the recirculation zone for all pressure conditions. No temperature peaks appear with increasing the pressure in contrary to the adiabatic case (see Figure 10). Temperature gradient is noticed to be relatively low at atmospheric pressure but increases with increasing the pressure. This can be attributed to the increased tendency of the reaction zone to be concentrated with pressure as noticed in Figure 15 for all pressure conditions. The low gradient temperature contours conforms well to the distributed reaction zone noticed in Figure 16. These results confirm the flameless mode of operation under elevated pressure conditions for the present case. As mentioned before, in the present isothermal case, heat transfer limits the increase in heat of reaction and temperature resulting from increasing the pressure. Consequently, the variation of combustion temperature with pressure is relatively small compared with the adiabatic case (Figure 10), and the reaction remains distributed (Figure 16) rather than concentrated (Figure 9). To maintain the distributed combustion and low gradient temperature profile while increasing the pressure, heat transfer is noticed to increase. To further support these conclusions the effect of pressure on the predicted axial profile of heat of reaction along the combustor center line is shown in Figure 18. Compared with the adiabatic case (Figure 11), heat of reaction is
noticed to decrease considerably in the present isothermal case. This can be attributed to the effect of heat transfer either directly through drawing the excess heat of reaction or indirectly through maintaining distributed reaction zone. Looking at the trend of the heat of reaction with pressure, it is noticed to decrease with pressure from 1 atm. to 5 atm. This might be attributed to the considerable increase in radiative heat transfer across the walls. However, at pressures from 5 to 15 atm. an increase in the heat of reaction is noticed. The increase in heat of reaction due to the more concentrated reaction zone is higher than the heat loss due to radiation.

Figure 19 shows the predicted axial profiles of mean temperature, and CH$_4$, CO$_2$ and CO concentrations for the isothermal case. Looking at the mean temperature axial profiles, temperature is noticed to first increase from ambient temperature (fuel inlet temperature) until it reaches 773 K (the air jet inlet temperature) at x/L = 0.2. In this region, fuel is preheated apparently due to the mixing with the high temperature air jet. After that, temperature is noticed to increase at a higher rate from x/L = 0.2–0.3 apparently due to the mixing with the hot recirculated exhaust gases. The following bifurcation in temperature increase rate noticed at x/L = 0.3 is believed to result from the different levels of heat transfer at various pressures. However, temperature maintains the same flameless profile under elevated pressures with no apparent temperature peaks noticed thanks to the included effect of heat transfer. These results comply with the...
predicted mean temperature contours shown in Figure 17 and confirm the flameless combustion onset under high pressure conditions for the present case. Finally maximum temperature is noticed to decrease slightly with increasing the pressure from 1 to 5 atm. due to the dominant effect of increasing heat transfer. Further increase in pressure has no apparent effect on temperature, which may be attributed to the equal but opposite effects of pressure and heat transfer increase on temperature. This variation of temperature with pressure explains the previously noticed trend of recirculation ratio (Figure 15). The predicted CH₄ mole fraction axial profiles reflects the previous results. A gradual decrease of CH₄ mole fraction from 1 at x/L = 0 to 0.055 at x/L = 0.3 is
noticed. Apparently, this decrease is the result of the fuel jet mixing with air and recirculated exhaust gases. After that, reaction starts at $x/L = 0.3$ and extends to $x/L = 0.8$. Within the reaction zone, CH$_4$ mole fraction is noticed to decrease at different rates, which may be attributed to an oscillating reaction zone location with pressure. As pressure increases from 1 to 5 atm, methane consumption rate is noticed to decrease due to a slight shift of the reaction zone location in the downstream direction. Further increase in pressure from 5 to 15 atm results in a sharper methane consumption rate due to a slight shift of the reaction zone location in the opposite direction. CO$_2$ mole fraction axial profiles also show this oscillating behavior in the reaction zone location with pressure in the same distance range ($x/L = 0.3–0.8$) as expected. The oscillating reaction zone location is apparent and further confirmed from the locations of the CO mole fraction peak. Finally, increasing the pressure from 1 to 5 atm results in reducing the CO emissions due to the increased residence time, and the encouragement of CO transformation to CH$_2$O as per the reaction $\text{H}_2 + \text{CO} (+\text{M}) \rightleftharpoons \text{CH}_2\text{O} (+\text{M})$ (Kazakov & Frenklach, 1994). However, with further increase in the pressure from 5 to 15 atm, an unexpected increase of CO
Finally, Figure 20 shows the predicted NOx for the present combustor under isothermal conditions and elevated pressures. As noticed, NOx emissions decreases with pressure, which is opposite to the typical trend noticed in the adiabatic case (Figure 13). This unusual trend can be attributed to the more dominant effect of the increased heat transfer and the subsequent decrease in temperature with increasing the pressure. The majority of the predicted NOx are generated via the thermal route (nearly 90%) while the N2O intermediate and prompt NOx constitute less than 10%. Single digit NOx is noticed in the isothermal case compared with the two digit NOx demonstrated in the adiabatic case, which is apparently contributed to the absence of temperature peaks in the former case.

3.4. Identification of combustion regime

Figure 21 shows Borghi diagram for different combustion regimes (Abdel-Gayed, Bradley, & Lung, 1989; Buckmaster, 1985). In this diagram, both Damköhler and turbulent Reynolds numbers characterize combustion regimes. The distributed reaction regime is characterized by low Damköhler number (Da < 1), where the reaction rate is lower than the turbulent mixing rate, such that the combustion behavior is dictated by mixing rather than kinetics.

Therefore, and to further explain and confirm the previous results regarding the role of heat transfer in sustaining flameless combustion under elevated pressure conditions, both Damköhler and turbulent Reynolds numbers are calculated for all reacting cases investigated under adiabatic and isothermal conditions. These cases are then pinpointed on Borghi diagram to identify their corresponding combustion regime.

Damköhler number is a ratio between the chemical reaction rate and the mixing rate:

\[
Da = \frac{\text{Reaction rate}}{\text{Mixing rate}}
\]  

Both of these rates can be given by Khalil and Gupta (2017):

\[
\text{Reaction rate} = \frac{u_f}{\delta_f}
\]  

\[
\text{Mixing rate} = \frac{\epsilon}{k}
\]

Where \(u_f\) is the laminar flame speed, \(\delta_f\) is the laminar flame thickness, \(\epsilon\) is the eddy dissipation rate, and \(k\) is the turbulent kinetic energy.

The laminar flame speed is estimated using the empirical correlation first developed by Metghalchi and Keck (1980), and further tuned by Stone, Clarke, and Beckwith...
Following the previous procedure, the reaction and turbulence parameters are estimated for both adiabatic and isothermal cases as follows:

### 3.4.1. For the adiabatic case

Table 5 shows the calculated parameters necessary to identify the combustion regime for the adiabatic case. It can be noted that, in the adiabatic case, the unburnt gas temperature increases with increasing pressure due to mixing with hot product gases. The latter is of increased temperature following the increase in combustion temperature with pressure resulted by the more concentrated reaction zone and high heat of reaction as noticed in Figures 9 and 10 respectively. The diluent percentage in the unburnt gases is noticed to decrease significantly with increasing pressure leading to an increase in the laminar flame speed, the latter is noticed to decrease significantly with increasing pressure. This complies with the noticed decrease in recirculation ratio (Figure 8), following the increase in product gases temperature and decreased density as explained before. Although increasing unburnt gases temperature and decreasing diluent level should lead to an increase in the laminar flame speed, the latter is noticed to decrease significantly with increasing pressure. This demonstrates the dominant effect of pressure on laminar flame speed, which outweighs the effects of both unburnt gases temperature and diluent level. Consequently, chemical reaction rate is noticed to decrease significantly with pressure. From another side, increasing the pressure is found to reduce the turbulent kinetic energy significantly which complies with the previous results noted in Figure 7. Consequently, mixing rate is substantially decreased with increasing pressure leading to a final increase in Damköhler number and a decrease in turbulent Reynolds number.

### Table 4. Parameters for the laminar flame speed correlation of Methane/Air/Diluent mixtures.

| $S_{u,0}$ | $S_{u,1}$ | $S_{u,2}$ | $S_{u,3}$ | $S_{u,4}$ | $\alpha_0$ | $\alpha_1$ | $\beta_0$ | $\beta_1$ | $g$ | $h$ | $i$ |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|-----|-----|-----|
| 0.376   | 0.151   | −2.21   | −0.458  | 3.58    | 1.42    | −1.98   | −0.314  | 0.608   | 2.046| 0.730| 0.447|

### Table 5. Calculated parameters for the combustion regime identification of the adiabatic case.

| Pressure [atm.] | 1 | 3 | 5 | 10 | 15 |
|-----------------|---|---|---|----|----|
| Unburnt temperature ($T_u$) [K] | 950 | 960 | 968 | 978 | 985 |
| Oxygen percentage [%] | 20.35 | 20.4 | 20.47 | 20.54 | 20.6 |
| Diluent percentage (X) [%] | 3.1 | 2.85 | 2.5 | 2.2 | 1.9 |
| Laminar flame speed ($u_f$) [m/s] | 0.21 | 0.1 | 0.07 | 0.05 | 0.04 |
| Thermal conductivity ($k$) [W/mK] | 0.0454 | 0.0454 | 0.0454 | 0.0454 | 0.0454 |
| Density of air ($\rho$) [kg/m³] | 1253.72 | 1256.98 | 1257.34 | 1255.26 | 1255.3 |
| Specific heat capacity ($C_p$) [J/kgK] | 0.0454 | 0.0454 | 0.0454 | 0.0454 | 0.0454 |
| Laminar flame thickness ($\delta_f$) [mm] | 0.821 | 0.578 | 0.494 | 0.357 | 0.288 |
| Chemical reaction rate ($R_c$) [s⁻¹] | 255.74 | 173.04 | 141.81 | 139.97 | 138.69 |
| Mixing rate (Integral) [s⁻¹] | 66539.65 | 2447.96 | 524.68 | 67.08 | 19.84 |
| Turbulent energy ($\epsilon$) | 1090.46 | 365.82 | 219.75 | 109.88 | 73.32 |
| Damköhler number ($Da$) | 0.2 | 0.5 | 0.6 | 1.3 | 1.9 |
| Turbulent Reynolds Number (Re) | 5.48 | 5.46 | 5.42 | 5.41 | 5.37 |

(1998):

$$u_f = \left[ S_{u,0} + S_{u,1}(\Phi - 1) + S_{u,2}(\Phi - 1)^2 + S_{u,3}(\Phi - 1)^3 \right] \times \left[ T^0 p^0 \right] \times \left[ 1 - gX^{(h+i(\Phi-1))} \right]$$

(14)

Here, $\Phi$ is the fuel/air equivalence ratio, $X$ is the diluent level, $g$, $h$, $i$ are coefficients associated with the diluent level, $S_{u,0}$, $S_{u,1}$, $S_{u,2}$, $S_{u,3}$, $S_{u,4}$ are empirical coefficients associated with equivalence ratio, $\alpha = \alpha_0 + (\Phi - 1)\alpha_1$, $\beta = \beta_0 + (\Phi - 1)\beta_1$, $\alpha_0$ is the stoichiometric temperature exponent, $\beta_0$ is the stoichiometric pressure exponent, and $\alpha_1$ and $\beta_1$ show the equivalence ratio dependency.

$T$ and $P$ are the dimensionless temperature and pressure and are given by:

$$T = \frac{T_u}{T_0}$$

(15)

$$P = \frac{P_u}{P_0}$$

(16)

where $T_u$ and $P_u$ are the unburnt temperature and pressure respectively, $T_0$ is the reference temperature (298 K), and $P_0$ is the reference pressure (1 atm.).

The values for the above mentioned coefficients are obtained from (Stone et al., 1998) and are summarized in the table below: Table 4.

The laminar flame thickness can be estimated from the following equation (Khalil & Gupta, 2017):

$$\delta_f = \frac{2k}{\rho_u C_p u_f}$$

(17)

In this equation, $k$ is the thermal conductivity, $\rho_u$ is the unburnt gases density, $C_p$ is the specific heat capacity, and $u_f$ is the laminar flame speed.
Table 6. Calculated parameters for the combustion regime identification of the isothermal case.

| Pressure [atm.] | 1    | 3    | 5    | 10   | 15   |
|-----------------|------|------|------|------|------|
| Unburnt temperature \((T_{u})\) [K] | 470  | 467  | 466  | 466  | 466  |
| Oxygen percentage (%) | 19.65| 19.6 | 19.58| 19.58| 19.58|
| Diluent percentage (X) [%] | 6.4  | 6.7  | 6.76 | 6.76 | 6.76 |
| Laminar flame speed \((u_{f})\) [m/s] | 0.15 | 0.076| 0.053| 0.034| 0.027|
| Unburnt gases density \((\rho_{u})\) [kg/m³] | 0.422| 1.27 | 2.12 | 4.26 | 6.4  |
| Thermal conductivity (k) | 0.0454| 0.0454| 0.0454| 0.0454| 0.0454|
| Specific heat capacity \((C_{p})\) | 1234.82| 1232.25| 1229.89| 1229.26| 1228.90|
| Laminar flame thickness \((\delta)\) [mm] | 1.162| 0.763| 0.657| 0.51 | 0.428|
| Chemical reaction rate \((s^{-1})\) | 129.13| 99.55| 80.66| 66.67| 63.15|
| Turbulent kinetic energy (k) | 99.67| 11.70| 4.42 | 1.12 | 0.50 |
| Turbulent eddy dissipation rate (\(\epsilon\)) | 109932.7| 4309.44| 979.43| 124.13| 37.01|
| Mixing Rate \((Integral)\) [s⁻¹] | 1103| 368.38| 221.46| 110.79| 73.89|
| Damköhler number \((Da)\) | 0.12| 0.27 | 0.36 | 0.60 | 0.85 |
| Turbulent Reynolds Number \((Re)\) | 2.09| 1.97 | 1.88 | 1.85 | 1.84 |

3.4.2. For the isothermal case

Table 6 shows the calculated parameters necessary to identify the combustion regime for the isothermal case. In the isothermal case, the unburnt gas temperature is noticed to decrease with increasing the pressure from 1 to 5 atm. before it becomes nearly constant for pressures above 5 atm. As mentioned before, the unburnt gases temperature is controlled through the product gases temperature which in turn controlled by the combustion temperature. Consequently, this behavior complies with the previously noticed decrease in combustion temperature with increasing pressure from 1 to 5 atm. and the nearly constant temperature for pressures above this value, see Figure 20. As previously explained in Section 3.3, maximum temperature is noticed to decrease slightly with increasing the pressure from 1 to 5 atm. due to the dominant effect of increasing heat transfer. Further increase in pressure has no apparent effect on temperature, which may be attributed to the equal but opposite effects of pressure and heat transfer increase on temperature. This variation of temperature with pressure explains the noticed trend of diluent level with pressure, which also complies, with the previously noticed trend of recirculation ratio, see Figure 15. Similar to the adiabatic case, the laminar flame speed is noticed to decrease significantly with increasing pressure. Consequently, chemical reaction rate is noticed to decrease significantly with pressure. From another side, increasing the pressure is found to reduce the turbulent kinetic energy significantly which complies with the previous results noted in Figure 14. Consequently, mixing rate is substantially decreased with increasing pressure leading to a final increase in Damköhler number and a decrease in turbulent Reynolds number. However, it should be noted that both the laminar flame speed and reaction rate for the isothermal case are considerably lower than their counterparts in the adiabatic case for all pressures investigated. This can be attributed to the considerably lower unburnt gases temperature in the former case than in the latter case due to the heat transfer effect. Consequently, Damköhler number for the isothermal case is considerably lower than the adiabatic case for all pressures investigated which favors distributed reaction.

Figure 22 shows a comparison between the predicted contours of Damköhler number under adiabatic and isothermal conditions. It can be noted from the figure that the reaction zone (identified by regions where \(Da > 0\)) is far more distributed under isothermal wall conditions compared with the adiabatic wall conditions for all pressure studied. It is also apparent that, in the isothermal case, within the area of reaction, Damköhler number is lower than one for all pressures investigated which reflects the sustained flameless mode of combustion. In the adiabatic case, Damköhler number is relatively higher and reaches twice its value in the isothermal case. This complies with the transition to the conventional concentrated mode of combustion in the adiabatic case with elevated pressures.

Finally, Figure 23 shows the locations of the above-investigated cases on Borghi diagram. Circles in blue color represent the isothermal cases while circles in red color represent the adiabatic cases. Pressure for each case is shown inside the circle. It can be noted from the figure that, of all adiabatic cases, only the one under atmospheric pressure is located in the distributed regime. The adiabatic case with pressure of 3 atm. represents a transition state. Further increase in pressure above 3 atm. leads to combustion transition from the distributed regime to the flamelet in eddies regime. From another side, all isothermal cases (cases with heat transfer incorporated) are located in the distributed combustion regime. This complies with the previously demonstrated contours of temperature, and OH and CO mole fractions in sections 3.2, and 3.3.

Finally, it is noteworthy to mention that enlarging heat transfer on the combustor walls might decrease the enthalpy of the combustor hot products as expected. This
might have a negative effect on gas turbine thermal efficiency. However, this effect can be considered similar to the effect of the dilution air in conventional combustors, which is added to the hot products so that the exit temperature becomes appropriate for turbine blades material. In addition, this heat is not necessarily being lost. The combustion air can pass over the combustor walls for cooling them while it is being preheated at the same time. Using the heat transfer across the combustor walls to preheat combustion air might increase the gas turbine thermal efficiency.

4. Conclusion

Combined effects of pressure and increasing heat transfer on flameless combustion mode were investigated in a 10 kW flameless combustor with coaxial methane and air jets arrangement. Operating pressures covered in the current study are in the range from 1 to 15 atm. Heat transfer across the combustor wall is increased through keeping the combustor wall temperature at a value (1173 K) that is well below the combustor operating temperature. Two-dimensional axisymmetric computations were performed under reacting conditions using ANSYS Fluent 17. DRM22 mechanism is tuned for improved CO predictions. The effect of pressure on mixing and recirculation ratio, reaction zone location and spread, global flame characteristics, and emissions was investigated. Results were reported for both adiabatic and isothermal
combustor wall conditions. Following conclusions are made:

- Under adiabatic combustor wall conditions, increasing the pressure results in a more concentrated reaction zone, and a subsequent increase in the heat of reaction. A transition from flameless to conventional combustion modes eventually occurs at 3 atm. The calculated Damköhler number is noticed to increase from 0.2 to 1.9, while the turbulence Reynolds number decreases from 5.48 to 5.37. As peak temperature increases from 1840 to 1940 K, NOx emissions increases subsequently from 10 to 78 ppm. The majority of the predicted NOx are generated via the thermal route (nearly 90%).

- Under isothermal combustor wall conditions, increased heat transfer is noticed to limit the increase in heat of reaction and temperature with pressure. Peak temperatures remains in the range (1350–1400 K) for all pressures investigated. The calculated Damköhler number is noticed to increase from 0.12 to 0.85, which is nearly half the values encountered under adiabatic conditions. Moreover, turbulence Reynolds number decreases from 2.09 to 1.84. These results demonstrate a distributed reaction under all pressures investigated. Finally, predicted NOx emissions are found below 5 ppm for all conditions.

Enlarging heat transfer on the combustor walls might decrease the enthalpy of the combustor hot products as expected. This might have a negative effect on gas turbine thermal efficiency. However, this effect can be considered similar to the effect of the dilution air in conventional combustors, which is added to the hot products so that the exit temperature becomes appropriate for turbine blades material. In addition, this heat is not necessarily being lost. The combustion air can pass over the combustor walls for cooling while it is being preheated at the same time. Using the heat transfer across the combustor walls to preheat combustion air might increase the gas turbine thermal efficiency.

Finally, the numerical predictions were generally in fairly good agreement with the experimental measurements despite some discrepancies between the CO predictions and the experiments. These discrepancies in CO predictions are still noted despite the previous tuning of the reduced chemical reaction mechanism. The main reason for this might be the limited ability of the current chemical reaction mechanism to predict all CO consumption and production routes in flameless combustion. The DRM22 reduced mechanism is derived from the GRI-MECH 1.2 which was primarily developed for conventional combustion. Thus, future work will focus on the development of new mechanisms for this purpose.

Disclosure statement

No potential conflict of interest was reported by the authors.

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