Analysis of Highly CO₂-Diluted Oxy-propane Flames Stabilized over a Multihole Burner of a Model Gas Turbine Combustor

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ABSTRACT: Premixed oxy-propane flames are investigated numerically in a multihole model gas turbine combustor at various inlet mixture compositions over a range of equivalence ratios (Ω: 0.241–0.500), oxygen fractions (OF: 32.4–60.0%), and adiabatic flame temperatures (T_{ad}: 1600–1900 K) at a constant bulk throat velocity of 5.2 m/s. The flames in multihole combustors are highly influenced by their corresponding adiabatic flame temperatures. Similar flame shapes are observed at constant T_{ad} where cases with (Ω = 0.241, OF = 60%) and (Ω = 0.50, OF = 32.4%) both represent lifted flames at T_{ad} = 1600 K, anchored flames in (Ω = 0.276, OF = 60%) and (Ω = 0.50, OF = 36.6%) at T_{ad} = 1750 K, and anchored stronger flames in cases (Ω = 0.313, OF = 60%), (Ω = 0.392, OF = 50%), and (Ω = 0.50, OF = 40.8%) at T_{ad} = 1900 K. Flames in a multihole combustor are characterized by the presence of an outer recirculation zone (ORZ) only. In comparison with a swirl-stabilized combustor in identical inlet conditions, flames in a multihole combustor demonstrate a lower Damköhler number (Da), higher flame thickness, elevated pattern factor, and increased CO emission. Due to the reduced vorticity level because of the absence of swirl motion, the multihole flames have higher axial temperature than the swirl-stabilized ones.

1. INTRODUCTION

The global fossil fuel crisis and strict environmental regulations call for a more effective power generation process. With the continuously growing energy demand, relying on renewable energy is not entirely possible and requires a more efficient combustion system with reduced fossil fuel consumption. Lean-premixed (LPM) is one of the popular combustion modes with inherent low NOx emission characteristics used in current air-fuel gas turbine combustors. Operation in a fuel-lean environment, however, makes the flames susceptible to blowoff due to the competing influences of a reduced flow time scale and elevated chemical time scale. Oxyfuel combustion is another combustion technique that is often used for low-emission combustion applications. In oxy-combustion, fuel is burned in a nitrogen-free environment, which results in almost no NOx in the exhaust. The high temperature generated in a nitrogen-free environment can be controlled by recirculating CO₂ from the exhaust gas, which also reduces the overall carbon emission as well.

In addition to the operating flow conditions, the burner configuration also impacts flame stability. The burner should be designed to prevent the flashback and flame instabilities and at the same time should be flexible enough to operate with a wide range of fuels. Aside from the commonly used swirl-stabilized combustors, multihole combustors are recently gaining traction due to their improved combustion stability and fuel flexibility. Multihole combustors typically house multiple short mixing tubes where the fuel and oxidizer get mixed at a microscale. Operating on LPM mode, the multihole burner directs the incoming fuel-oxidizer stream through the mixing tubes and divides the flame into several small flamelets. Multihole burner technology has been examined by some gas turbine manufacturers and has been proven effective against flashback prevention. In addition, the spacings between the inlets in multihole combustor act as hot anchor points between the flamelets and aides in flame stabilization.

Few experimental and numerical works have been carried out to study the flame behavior of the multihole combustor. Funke et al. experimentally examined the performances of two micromix type multihole combustors with nozzle diameters of 0.3 mm (1600 nozzles) and 0.84 mm (300 nozzles) in hydrogen-enriched methane air combustion. They reported an approximately 390% increase in power output with 0.84 mm size nozzles as compared to the 0.3 mm counterpart. The emission of NOx was found below 2.5 ppm with both combustors. Asai et al. investigated the multihole

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burners in a multican DLN combustor. Hydrogen-rich syngas was studied in the combustors in various combustion modes, where a significant reduction in NOx emission was observed. For all the studied combustion modes, NOx emission was recorded to be less than 10.9 ppm after O$_2$ correction. Aliyu et al.\textsuperscript{11} examined the flame characteristics of CH$_4$/O$_2$/CO$_2$ flames in a multihole burner. The stability limits of CO$_2$-diluted oxy-methane flames were mapped in the experimental work. Combustor stability and combustor temperature distribution in their study were found to be strongly controlled by adiabatic flame temperature ($T_{ad}$) and equivalence ratio ($\phi$), respectively. Santavicca and Lieuwen\textsuperscript{17} studied the combustion dynamics with high hydrogen fuel in a multinozzle combustor. The study reported that the asymmetric behaviors of acoustic forcing and the flow field can considerably impact the flame response in a multinozzle combustor.

Abdelmaged et al.\textsuperscript{12} investigated the hydrogen fraction (HF), $\phi$ and OF, and hydrogen fraction (HF) in partially-premixed natural gas/H$_2$/O$_2$/CO$_2$ flames on a perforated plate burner. Hussain et al.\textsuperscript{3} qualified the stability limit in a multihole combustor for hydrogen-enriched oxy-methane flames with CO$_2$ dilution. They reported an improved stability limit in the fuel-lean condition where the stable flame was observed with the H$_2$-enrichment (65% HF) at lower OF (13% OF) than the flame without H$_2$-enrichment (OF = 21%). Dhineshkumar et al.\textsuperscript{18} numerically examined a perforated plate (multihole) gas turbine burner using liquid fuel-air combustion. They reported jet mixing with enhanced turbulence with
the perforated plate combustor. They observed similar performance between the perforated plate burner and swirl-stabilized counterpart with identical combustor power (1 MW). Abdelhafez et al. 13 experimentally investigated the jet spacing and jet diameter in the multihole combustor and reported that an increase in both these parameters unfavorably affects the flame stability. Araoye et al. 14 studied the CH4/H2/O2 flames in a multihole combustor through both experimental and numerical analyses. The study reported that the Damköhler number (Da) and Karlovitz number increases with the increase in HF. Hydrogen enrichment also shortens both the primary and secondary reaction zones in the multihole burner.

Based on the literature review, natural gas (CH4) and syngas fuels have been examined in multihole burners, but liquefied petroleum gas (LPG) and C-MAX fuels, which are mostly propane (C3H8), have not. Propane can also be present in liquefied natural gas (LNG), 15 used in different fuel blends, and can be an alternative to ‘Jet A’ fuel for turboshift engines. 20 Also from a preliminary study done by the authors, it is observed that oxy-propane flames are capable of providing slightly higher power density that methane and syngas counterparts at identical bulk inlet velocity. 21 Thus, understanding propane combustion is necessary for its possible application. The study of oxy-propane flames in this specific burner has not been performed so far. Thus, with an aim to address this research gap, this work numerically examines the oxy-propane combustion (C3H8/O2/CO2) to provide an initial assessment on oxy-propane flames in a multihole combustor under atmospheric conditions. Combustion and emission characteristics of CO2-diluted oxy-propane flames are analyzed in this study in different inlet mixture compositions at a fixed flow velocity in terms of flow, combustion, and emission behaviors. A range of cases has been selected within the stable combustion zone (observed from Ali et al. 22) for oxy-propane flames under fixed flow velocity of 5.2 m/s to be investigated computationally. Lastly, a comparison is also presented between the multihole and a model swirl-stabilized burner. In order to compare the two burners in identical conditions, the same power density (8.36 MW/m3/bar) among the combustors is considered.

2. NUMERICAL MODELING

2.1. Combustor Description. Premixed oxy-fuel flames of propane have been examined in this study in a multihole gas turbine combustor. The multihole combustor houses 61 inlet holes of 3.175 mm (1/8") diameter spaced at 5.5 mm on a hexagonal pattern. The burner is surrounded by a steel base plate while the combustion zone is enclosed with a 6 mm-thick quartz tube with a 76 mm inner diameter. Unlike a typical micromixer type multihole burner, the burner presented here does not premix the fuel and oxidizer streams in the burner itself; rather, a separate meter-long cylindrical chamber takes care of the pre-mixing and then feeds the premixed mixture into the burner. Figure 2 illustrates the schematic diagram of the multihole combustor setup modeled in this work, while Figure 2 depicts the multihole combustor geometry. Since the inlet holes are distributed in a hexagonal manner, 1/6th of the combustor volume has been considered as a computational domain for numerical analysis to reduce the computational time, as shown in Figure 2a. A complete description of the combustor can be obtained from the previous experimental works by Hussain et al. 3 and Aliyu et al. 11, 23 The results will be presented here in a dimensionless manner in both axial and radial directions, as depicted in Figure 2b. The terms Z/D and r/R are used to express the axial and radial positions, respectively. Here, Z, r, R, and D correspond to axial distance, radial distance, combustor radius, and diameter, respectively. The negative term for r/R is used to indicate the direction. Furthermore, the contours for various parameters examined in the study are presented on a centerline plane inside the combustor as illustrated in Figure 2b.

The inlet mixture for CO2-diluted oxy-propane constitutes C3H8, O2, and CO2 where the mixture composition is varied by changing the equivalence ratio (Ø) and oxygen fraction (OF). The expressions for Ø and OF are presented in eqs 1 and 2, respectively. Inlet gas mixtures for the simulations are considered premixed, which eliminates the localized hotspots by ensuring fuel-lean conditions inside the combustor. The CO2 dilution imitates the recirculation of exhaust CO2 in order to control the combustion temperature. Along with the temperature control, exhaust gas recirculation (EGR) also aids in carbon capture processes in practical cases, making zero-emission combustion more convenient than the air-combustion counterpart. The level of CO2 dilution or O2 concentration in oxidizer mixture is varied by changing the oxygen fraction (OF) in the O2–CO2 oxidizer mixture. This EGR feature is a vital addition for modern oxy-fuel gas turbines with carbon-capture capabilities. The exhaust mainly comprises CO2 and H2O. However, a small amount of CO may exist in the exhaust due to the variation in Ø and OF.

\[ \Phi = \frac{\text{(Oxidizer to fuel ratio) actual}}{\text{(Oxidizer to fuel ratio) stoichiometric}} \]  

Figure 2. (a) Schematic diagram of the combustor area for the multihole burner with highlighted computational domain and boundary conditions, and (b) centerline plane in the combustor considered for contour illustrations.
2.2. Governing Equations. 2.2.1. Adiabatic Flame Temperature $T_{ad}$. Thermodynamic analysis of oxy-propane combustion equation (presented in Eq 3 in terms of $\Theta$ and OF) has been performed using the standard enthalpy of formation and sensible enthalpy data to determine corresponding values of $T_{ad}$ for CH$_3$H$_8$/O$_2$/CO$_2$ flames. These enthalpy values have been obtained from thermodynamic textbooks.\textsuperscript{24,25} Following assumptions have been made evaluating the $T_{ad}$ values:

(a) Complete combustion is considered, as a fuel-lean (i.e., $O < 1$) inlet mixture is used in all the studied cases. This also simplifies the thermodynamic calculations.

(b) The dissociation of CO$_2$ is considered marginal and thus is excluded from the thermodynamic analysis.

\[
\text{C}_3\text{H}_8 + \frac{5}{1} \left[ \text{O}_2 + \left( \frac{1}{\text{OF}} - 1 \right) \text{CO}_2 \right] \\
\rightarrow \left[ 3 + \frac{5}{1} \left( \frac{1}{\text{OF}} - 1 \right) \right] \text{CO}_2 + 4\text{H}_2\text{O} + \left( \frac{1}{\text{OF}} - 1 \right) \text{O}_2
\]

(3)

2.2.2. Turbulence Model. The Reynolds-averaged Navier–Stokes (RANS) turbulence model (i.e., standard $k-\epsilon$) has been incorporated in simulating the three-dimensional LPM combustion of oxy-propane using commercial code ANSYS Fluent 19R3. Steady-state conditions with a gravitational effect is considered in the modeling. The SIMPLE algorithm is considered to couple the pressure and velocity fields. The least-square cell-based gradient is selected with second-order discretization for the governing equations. The residuals for all equations are set at $10^{-6}$ to achieve a more precise solution.

The kinetic energy ($k$) and dissipation rate ($\epsilon$) are determined by solving eqs 4 and 5, respectively. Since a steady state is considered in this study, the time-dependent components in both the equations will be zero. Here, $G_k$ and $G_\epsilon$ represent turbulence kinetic energy generation as a result of velocity gradients and buoyancy, which $Y_M$ refers to the contribution of fluctuating dilatation in the compressible turbulence to the overall rate of dissipation. The terms $C_{1k}$, $C_{2k}$, and $C_{3k}$ are constants, whereas $\sigma_k$ and $\sigma_\epsilon$ correspond to Prandtl numbers for both $k$ and $\epsilon$, respectively. Lastly, the turbulent viscosity ($\mu_t$) is evaluated by combining the $k$ and $\epsilon$, as presented in Eq 6.\textsuperscript{26,27}

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right] + G_k + G_\epsilon - \rho \epsilon - Y_M + S_k
\]

(4)

\[
\frac{\partial (\rho \epsilon)}{\partial t} + \frac{\partial (\rho \epsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \mu + \frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} G_k + C_{3\epsilon} G_\epsilon - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon
\]

(5)

2.2.3. Radiation Model. Discrete ordinate (DO) modeling is used to account for radiative heat transfer. The DO scheme is valid for a wide range of optical thicknesses and is recommended in simulating oxy-combustion flames.\textsuperscript{28} One radiative iteration is performed for every ten energy iterations. The weighted sum of the gray gas model (WSGGM) is considered to determine the absorption coefficient of the gas mixture, which is verified over a wide range of operating conditions.\textsuperscript{29} The total emissivity ($\epsilon$), in terms of the weighted sum of gray gases, is calculated using eq 7, where $\alpha$, $k$, $P$, and $L$ correspond to the emissivity weighting factor for the gray gas at temperature $T$, adsorption coefficient, partial pressure of the absorbing gases, and gas layer thickness (or path length), respectively.

\[
\epsilon = \sum_{i=0}^{\text{mol}} \alpha_{i}(T)[1 - e^{-k_{pl}L}]
\]

(7)

2.2.4. Reaction Model. Oxy-fuel combustion with CO$_2$ dilution is realized using the partially premixed combustion model, which is a combination of both diffused and completely premixed combustion models in ANSYS Fluent and allows the model to have fewer limitations compared to the predecessor models used separately. The partially premixed model also allows more control over the reactions and species than the completely premixed model (which does not solve for species concentration).\textsuperscript{26} Hence, the partially premixed reaction model has been modified to accommodate fully premixed combustion by defining the fuel mass fraction in the inlet mixture (i.e., mean mixture fraction) and mixture fraction variance (the value is specified as 0 to keep the $\Phi$ fixed at the inlet). Moreover, chemical equilibrium is assumed and the Zimont model is incorporated for evaluating the turbulent flame speed in the partially premixed reaction scheme.

Transport equations for mean mixture fraction ($\bar{\phi}$), mean reaction progress variable ($\bar{\xi}$), and mixture fraction variance ($\bar{\phi}''$) have been solved to obtain other scalar variables. Mixture fraction can be determined from eq 8, where $s$ refers to the oxygen to fuel ratio, $Y_{fr}$ represents the mass fraction of fuel, and $Y_{ox}$ represents the mass fraction of oxygen. Moreover, the subscripts 0 and 1 correspond to the inlet stream of the oxidizer and fuel.

\[
f = \frac{sY_{fr} - Y_{ox} + Y_{ox,0}}{sY_{fr,1} + Y_{ox,0}}
\]

(8)

The progress variable is presented in terms of species mass fraction as shown in eq 9, where $Y_i$ and $Y_i,ad$ are the mass fraction of product species and the mass fraction of species after complete combustion, respectively. The progress variable ranges from 0 to 1.0; 0 represents an unburnt mixture, whereas 1 represents a completely burnt mixture.

\[
\xi = \frac{\sum_{i=1}^{\text{species}} Y_i}{\sum_{i=1}^{\text{species}} Y_{i,ad}}
\]

(9)

Progress variable and probability density function (PDF) are used to evaluate the temperature and species fractions, i.e., density-weighted average scalars, as expressed in Eq 10. Here, the subscripts u and b refer to unburnt and burnt mixtures, respectively.
\[ \Phi = \tau \int_0^1 \Omega_k(f)p(f)df + (1 - \tau) \int_0^1 \Omega_p(f)p(f)df \]  

(10)

The product formation rate (PFR) refers to the rate at which the products are formed. Product formation rate can be evaluated using eq 11.

\[ \text{PFR} = \frac{\Delta [\text{Products}]}{\Delta t} \]  

(11)

Flame thickness (\(\delta\)) can be determined from eq 12, where \(\lambda_u\), \(\rho_u\), \(c_p\), and \(S_L\) symbolize thermal conductivity, density, specific heat capacity, and laminar flame speed, respectively.

\[ \delta = \frac{\lambda_u}{\rho_u c_p S_L} \]  

(12)

The Damköhler number (\(Da\)) refers to the ratio of reaction rate to diffusion rate (in other words, ratio between flow time scale and chemical time scale) and can be evaluated from eq 14.

\[ Da = \frac{l_i u'}{S_L} \]  

(13)

The pattern factor as provided in eq 15 corresponds to the temperature uniformity at the combustor outlet, where \(T_{\text{maximum}}\) and \(T_{\text{average}}\) are the maximum and average temperatures at the outlet of the combustor, respectively.

\[ \text{pattern factor} = \frac{T_{\text{maximum}} - T_{\text{average}}}{T_{\text{average}} - T_{\text{inlet}}} \]  

(14)

2.3. Boundary Conditions. A velocity inlet boundary condition is employed in the inlets in such a way that all the inlet holes supply a fuel–oxidizer mixture at a bulk velocity of 5.2 m/s. Regulating inlet flow velocity is a common practice in gas turbine operation, to achieve a desired pressure drop across the combustor headend. Furthermore, this study is based on a model gas turbine combustor; hence, in order to maintain similar Reynolds numbers in actual GT combustors with a fixed pressure drop, the bulk velocity at the inlet of the combustor is fixed to 5.2 m/s. The inlet composition is defined by specifying the mean mixture fractions and OFs for each case. The base steel plate is considered as a no-slip wall with adiabatic thermal condition. Since there is no swirling component along the azimuthal direction, no pressure drop is considered in that direction, which allows the use of a rotational periodic condition for the two cut-surfaces of the computational domain to accurately calculate for the interaction in the cut-faces. The no-slip condition is considered for the quartz tube where a semitransparent condition is employed to incorporate the radiation and convection heat transfer to the environment. These heat transfer processes are considered at 300 K surrounding (external) radiation temperature and 290 K freestream temperature, whereas the external convection heat transfer coefficient is specified at 20 W/m² K. The selected boundary conditions for different surfaces of the geometry are illustrated in Figure 2a above while the summary of the boundary conditions is presented in Table 1.

| boundary | boundary conditions employed | parameter (values) |
|----------|-----------------------------|--------------------|
| inlet    | • velocity-inlet            | - 5.2 m/s inlet velocity |
|          | • fuel mass fraction in the inlet mixture | |
|          | • 300 K inlet mixture temperature | |
|          | • backflow progress variable (1), assuming completely burnt mixture at the combustor outlet | |
| outlet   | • pressure-outlet            | - stationary wall |
|          | • no slip shear condition    | - mixed thermal condition |
|          | • material (quartz)          | - wall thickness (6 mm) |
|          | • external heat transfer coefficient (20 W/m² K) | |
|          | • free-stream temperature (290 K) | |
|          | • external-radiation temperature (300 K) | |
|          | • semi-transparent boundary with diffuse fraction (0.9) | |
| steel base | • adiabatic wall            | - stationary wall |
|          | • no slip shear condition    | - adiabatic thermal condition |
|          | • material (steel)           | - wall thickness (10 mm) |
| cut-faces | • periodic boundary         | - rotational periodic surfaces |
|          | (symmetry)                  |                    |

Several assumptions have been made to simplify the numerical model. These assumptions also aid in reducing the computational time.

- Steady-state condition.
- Chemical equilibrium is considered during combustion.
- Completely burnt mixture is assumed at the outlet boundary condition (i.e., progress variable = 1).
- No heat transfer through the steel base.
- No fluctuation in pressure due to the rotational boundary condition.
- Exhaust gas recirculation contains CO₂ stream only.

3. MESHING, SENSITIVITY ANALYSIS, AND MODEL VALIDATION

The hex-dominant element type has been incorporated in meshing with finer elements near the burner region (i.e., near inlet holes), as illustrated in Figure 3. This approach allows more mesh elements to be congregated near the inlet, resulting in a more detailed calculation in the region where the highest product formation (rates and gradients) from the unburnt to the products are formed. Product formation rate can be evaluated using eq 11.

Further details on \(S_L\) calculation can be found in Göttgens et al. The Damköhler number (\(Da\)) refers to the ratio of reaction rate to diffusion rate (in other words, ratio between flow time scale and chemical time scale) and can be evaluated from eq 14. The terms \(l_i\) and \(u'\) correspond to the integral length scale and root mean square (RMS) of velocity fluctuation. The Damköhler number (\(Da\)) refers to the ratio of reaction rate to diffusion rate (in other words, ratio between flow time scale and chemical time scale) and can be evaluated from eq 14. The terms \(l_i\) and \(u'\) correspond to the integral length scale and root mean square (RMS) of velocity fluctuation. The Damköhler number (\(Da\)) refers to the ratio of reaction rate to diffusion rate (in other words, ratio between flow time scale and chemical time scale) and can be evaluated from eq 14. The terms \(l_i\) and \(u'\) correspond to the integral length scale and root mean square (RMS) of velocity fluctuation. The Damköhler number (\(Da\)) refers to the ratio of reaction rate to diffusion rate (in other words, ratio between flow time scale and chemical time scale) and can be evaluated from eq 14. The terms \(l_i\) and \(u'\) correspond to the integral length scale and root mean square (RMS) of velocity fluctuation.
independence test is carried out to eliminate the dependency of numerical results on mesh size. Table 2 presents the variation in combustor temperatures and CO mole fractions at the combustor outlet, for different mesh sizes. Average overall combustor temperatures, axial temperature, and outlet temperatures show a less than 0.5% difference among the tested mesh sizes. The mole fractions of CO at the combustor outlet, on the other hand, demonstrated a maximum of 3.55% variation with different mesh sizes. The meshes are further examined in terms of their axial (centerline axis of the combustor) temperature distributions, as depicted in Figure 4, where the mean difference of less than 1% (∼0.07%) from the previous mesh was observed from mesh size of 164k. Thus, considering the variation in the studied parameters, the mesh configuration with 164k elements has been selected for the numerical analysis.

The numerical model is validated using experimental oxy-propane combustion temperatures from Ali et al.\textsuperscript{22} The flame temperatures in ref \textsuperscript{22} are presented in the static state form and from there the case with $\Phi = 89\%$ and OF = 0.30 has been considered for the comparison. The value of the external convection heat transfer coefficient ($20$ W/m$^2$ K) for the quartz wall is selected in such a way that the numerical temperatures become as close to the experimentally obtained ones as possible. Model and experimental temperatures are contrasted in terms of axial (at combustor centerline) temperature profiles, presented in Figure 5. A marginal variation in experimental and model temperatures was observed between the computational and experimental temperatures that resulted in an acceptable mean error of 0.98% and illustrated the similarity between the model and experiment.

### 4. RESULTS AND DISCUSSION

A range of inlet composition has been investigated numerically for the oxy-propane flames in the multihole burner with CO$_2$-dilution. The test matrix considered in this study is listed in Table 3, where cases 1–3 are considered at constant 60% OF, cases 3–5 at fixed adiabatic flame temperature of 1900 K, and cases 5–7 at constant $\Theta = 0.50$. The effects of these parameters are studied in terms of flame shapes, temperature and vorticity distributions, velocity streamlines, combustion, and emission attributes. Furthermore, the combustion characteristics in the multihole combustor is compared with that in the model swirl-stabilized gas turbine combustor at $\Theta = 0.50$ and OF = 60%.

#### 4.1. Global Flame Behavior

Premixed C$_4$H$_{10}$/O$_2$/CO$_2$ flames in the multihole burner are examined initially in terms of their flame shapes, which is a good indicator of combustion behavior and stability. Typically, the OH$^*$ chemiluminescence approach is employed to characterize flame structure, heat release, and reaction characteristics in premixed flames.\textsuperscript{56} In order to make the study on par with the experimental approaches, the flame shapes in this study are represented using their respective OH contours. Figure 6 shows the contours of OH radicals in the combustion zone for the studied cases, as listed in Table 3, while the corresponding laminar flame speeds are presented in Figure 7. For a fixed OF = 60%, with the increase in $\Theta$ (and $T_{ad}$), the OH concentrations increase making the flame stronger with a higher heat release rate and elevated laminar flame speed (in Figure 7). Case 1 illustrates a weaker flame near the blowout limit, which is attributed to the reduced OH concentration in the middle of the combustion chamber within 0.1 ≤ Z/D ≤ 1.7. Low OH concentrations in 0 ≤ Z/D ≤ 0.1 are due to the inlet flow of the individual flamelets since majority of the product formation takes place after Z/D ≥ 0.1 (discussed in Figures 10 and 13 below). The flames assume similar shapes in constant $T_{ad}$, nevertheless, the OH intensity decreases slightly as OF is reduced and $\Theta$ is increased at constant $T_{ad}$. The reduced oxygen concentration at constant $T_{ad}$ in cases 3–5 makes the mixture more fuel-rich, subsequently increasing the laminar flame speed. At constant equivalence ratio ($\Theta = 0.5$) in cases 5–7, OH concentration and laminar flame speed are reduced with OF and $T_{ad}$. Similar to case 1, case 7 also demonstrates a weaker lifted flame in lower $T_{ad}$ near the blowout limit. Furthermore, in all cases, a lower presence of OH radicals is observed in the corner of the combustor, indicating the limited reaction in the outer recirculation zone (ORZ), which is further explained in Figure 9.

#### Table 2. Combustor Temperatures and CO Emission in Different Mesh Sizes

| mesh size            | average combustor temperature (K) | percentage difference from previous mesh size (%) | percentage difference from previous mesh size (%) | percentage difference from previous mesh size (%) | percentage difference from previous mesh size (%) | avg. outlet CO mole fraction at combustor exhaust (%) | percentage difference from previous mesh size (%) |
|----------------------|-----------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| 1,06,141 (106k)      | 1522.99                           | 0.002823                                      | 0.030459                                      | 0.07%                                         | 1.92 × 10$^{-6}$                               | 1.945920                                      | 0.98%                                         |
| 1,23,845 (124k)      | 1523.03                           | 0.10023                                       | 0.274156                                      | 0.191736                                      | 1.88 × 10$^{-6}$                               | 2.037669                                      | 0.98%                                         |
| 1,63,778 (164k)      | 1521.50                           | 0.060832                                      | 0.191736                                      | 0.191736                                      | 1.84 × 10$^{-6}$                               | 1.78 × 10$^{-6}$                              | 0.98%                                         |
| 2,06,645 (207k)      | 1520.58                           | 0.030459                                      | 0.191736                                      | 0.191736                                      | 1.84 × 10$^{-6}$                               | 1.78 × 10$^{-6}$                              | 0.98%                                         |

4.1. Global Flame Behavior. Premixed C$_4$H$_{10}$/O$_2$/CO$_2$ flames in the multihole burner are examined initially in terms of their flame shapes, which is a good indicator of combustion behavior and stability. Typically, the OH$^*$ chemiluminescence approach is employed to characterize flame structure, heat release, and reaction characteristics in premixed flames.\textsuperscript{56} In order to make the study on par with the experimental approaches, the flame shapes in this study are represented using their respective OH contours. Figure 6 shows the contours of OH radicals in the combustion zone for the studied cases, as listed in Table 3, while the corresponding laminar flame speeds are presented in Figure 7. For a fixed OF = 60%, with the increase in $\Theta$ (and $T_{ad}$), the OH concentrations increase making the flame stronger with a higher heat release rate and elevated laminar flame speed (in Figure 7). Case 1 illustrates a weaker flame near the blowout limit, which is attributed to the reduced OH concentration in the middle of the combustion chamber within 0.1 ≤ Z/D ≤ 1.7. Low OH concentrations in 0 ≤ Z/D ≤ 0.1 are due to the inlet flow of the individual flamelets since majority of the product formation takes place after Z/D ≥ 0.1 (discussed in Figures 10 and 13 below). The flames assume similar shapes in constant $T_{ad}$, nevertheless, the OH intensity decreases slightly as OF is reduced and $\Theta$ is increased at constant $T_{ad}$. The reduced oxygen concentration at constant $T_{ad}$ in cases 3–5 makes the mixture more fuel-rich, subsequently increasing the laminar flame speed. At constant equivalence ratio ($\Theta = 0.5$) in cases 5–7, OH concentration and laminar flame speed are reduced with OF and $T_{ad}$. Similar to case 1, case 7 also demonstrates a weaker lifted flame in lower $T_{ad}$ near the blowout limit. Furthermore, in all cases, a lower presence of OH radicals is observed in the corner of the combustor, indicating the limited reaction in the outer recirculation zone (ORZ), which is further explained in Figure 9.
4.2. Temperature and Flow-Field Structure. Flame temperatures and velocity streamlines provide insight into comprehending the flow field and heat release. Figure 8 illustrates the temperature distribution inside the combustor. The temperature increases as the Ø is increased at a constant OF from cases 1 to 3 and decreases as the OF is increased at a constant Ø from cases 5 to 7. At constant \( T_{ad} \), however, insignificant changes are observed in the combustor temperature with no discernible change trends, which agrees with the findings of Aliyu et al.\(^{11,23}\) and Abdelhafez et al.\(^{34,38}\) for natural-gas flames. Temperature is observed to be significantly lower in the ranges \(-0.8 \leq r/R \leq 0.8\) and \(0 \leq Z/D \leq 2\) as the flame approaches the blowout limit (i.e., cases 1 & 7). A temperature gradient along the radial direction is seen for weaker flames in the multihole combustor due to flame lift-off, which reduces at higher Ø, OF, and consequently \( T_{ad} \).

Figure 9 shows the velocity streamlines mapped over the temperature contour at the centerline plane of the combustor in Ø = 0.313, OF = 60%, \( T_{ad} = 1900\) K. Unlike the swirl-stabilized \( \text{C}_3\text{H}_8/\text{O}_2/\text{CO}_2 \) flames, examined in the earlier study by Nemittallah et al.,\(^{37}\) where the flames are characterized by two recirculation zones, the inner recirculation zone (IRZ) and outer recirculation zone (ORZ), the flow-field in the multihole combustor can be characterized by the presence of the ORZ only. Here, the IRZ (or central recirculation zone) is the recirculation at the combustor center induced by the swirl effect that broadens the blowoff limit through reutilizing the active chemical species and heat to the flame root in the exit of the combustor. On the other hand, the outer recirculation zone (or corner recirculation zone) is the recirculating flow between the outer shear layer and the combustor wall.\(^{34,38}\) A similar finding was also reported in the experimental study involving \( \text{CH}_4/\text{O}_2/\text{CO}_2 \) flames in a multihole combustor by Hussain et al.\(^{1}\) Further comparisons between the multihole and swirl-stabilized combustors are presented in section 4.4 below.

4.3. Combustion and Emission Characteristics. Combustion and emission attributes of \( \text{C}_3\text{H}_8/\text{O}_2/\text{CO}_2 \) flames in the multihole combustor are examined in this section in terms of product formation rate (PFR), progress variable (PV), Damköhler number (\( D_a \)), flame thickness, distribution of species mole fractions, and CO emission in ppm. The terms PFR corresponds to the rate at which the products are formed, PV refers to the transition from unburnt reactants to fully burnt products, whereas \( D_a \) is the ratio of the reaction rate and the diffusion rate.

Figures 10 and 11 illustrate the PFR and PV in the combustor. The reaction zone exists between the inner shear layer (ISL) and outer shear layer (OSL) for each flamelet, and the flamelets are stabilized on both ISL and OSL. For the flames near the blowout limit in Figure 10, i.e., cases 1 & 7, the middle flamelets are lifted significantly and thus, the production formation occurs within \(0 \leq Z/D \leq 0.35\). This lifted flame is attributed to the reduced fuel–oxidizer ratio, which makes the flame anchoring week at the defined mixture flow velocity.\(^{39}\) For the rest of the flames, i.e., cases 2–6, the reaction zone is observed within \(0 \leq Z/D \leq 2.5\). This transition requires more axial distance to fully turn into product species in flames near the blowout

Table 3. Test Matrix for \( \text{C}_3\text{H}_8/\text{O}_2/\text{CO}_2 \) Flames in a Multihole Combustor\(^a\)

| cases | equivalence ratio (Ø) | oxygen fraction (OF) | adiabatic flame temperature \( T_{ad} \), K |
|-------|-----------------------|----------------------|--------------------------------------------|
| 1     | 0.241                 | 60.0%                | 1600                                       |
| 2     | 0.276                 | 60.0%                | 1750                                       |
| 3     | 0.313                 | 60.0%                | 1900                                       |
| 4     | 0.392                 | 50.0%                | 1900                                       |
| 5     | 0.500                 | 40.8%                | 1900                                       |
| 6     | 0.500                 | 36.6%                | 1750                                       |
| 7     | 0.500                 | 32.4%                | 1600                                       |

\(^a\)Fuel contains 100% \( \text{C}_3\text{H}_8 \).
limit, which is $0 \leq Z/D \leq 2.2$ for case 1 and $0 \leq Z/D \leq 2.4$ for case 7. The PFR and PV distributions of cases 3–5 again demonstrate insignificant changes with no discernable change trends, which strengthens the findings of Figure 8.

Figure 6. Flame shapes based on OH contours for the selected cases.

Figure 7. Laminar flame speeds for C$_3$H$_8$/O$_2$/CO$_2$ flames.

Figure 8. Temperature contours for C$_3$H$_8$/O$_2$/CO$_2$ flames in different inlet compositions.
Figure 12 depicts the $Da$ and flame thickness for the oxy-propane flames. The values of $Da$ in Figure 12a are greater than unity, thus implying that the reaction rate in the combustor is generally dominant over the diffusion rate. $Da$ increases with the increase in $\Omega$ at constant OF and with higher OF at constant $\Omega$. At constant $T_{ad}$ $Da$ depends on the fuel–oxidizer composition, where $Da$ decreases from cases 3–5 with the drop in OF and rise in $\Omega$. The fact that case 5 has more fuel than case 3 increases the diffusion rate since the reaction mechanism of $C_3H_8$ has numerous intermediate species that enhance the diffusion rate, thus reducing the $Da$ as $\Omega$ is increased at constant $T_{ad}$. The change in flame thickness, on the other hand, shows an opposite behavior to the $Da$, as shown in Figure 12b. As the flames get stronger, the flame becomes compact consequently, which reduces the flame thickness.

Figures 13 and 14 present the distributions of $C_3H_8$ and CO mole fractions within the combustor. As shown in Figure 13, the concentration of $C_3H_8$ is higher at the inlet and reacts with oxygen to form the product gases within the axial distance $0 \leq Z/D \leq 0.3$ for cases 2–6. Due to the lower PFR in the middle flamelets in cases 1 and 7 and the transition from reactants to products taking place within $0 \leq Z/D \leq 2.1$, the presence of $C_3H_8$ is observed within axial distance $0 \leq Z/D \leq 2.4$ in these two near-blowout cases. The mole fraction of CO in Figure 14 mainly depends on the axial combustor temperature, the availability of oxygen and fuel concentration. CO increases from cases 1 to 3 with the increase in $\Omega$, as expected. CO also increases from cases 3 to 5, as $\Omega$ is increased at the expense of OF. At higher OF and lower $\Omega$ (case 3), more oxygen is available compared to the fuel in the combustion chamber, which oxidizes the generated CO rapidly and produces $CO_2$. Alternatively, at lower OF and higher $\Omega$ (case 5), the oxygen content is not high enough to oxidize CO rapidly, which increases its concentration in the combustor. Lastly, the CO concentration is observed to be decreasing from cases 5 to 7 with the OF. This can be attributed to the declining flame temperature, which reduces the dissociation of $CO_2$ to CO. This lower dissociation results in decreased CO concentration from cases 5–7. The variation of CO in the combustion chamber is also reflected in the CO emission at the combustor outlet, shown in Figure 15.

4.4. Multihole and Swirl-Stabilized Burners. The oxy-propane flame in the present multihole combustor is compared with a swirl-stabilized combustor (used in ref 22) in this section under identical mixture composition ($\Omega = 0.313$, OF = 60%, $T_{ad} = 1900$ K). The swirl-stabilized burner contrasted here encompasses a swirler setup with 8 vanes angled at 55°. Since these combustors have different cross-sectional areas for the fuel–oxidizer inlet, a fixed inlet velocity (5.2 m/s) would result in variation in total mass flow rates. Thus, to maintain an identical power density (8.36 MW/m³/bar) among the combustors, the mass fluxes are fixed, ensuring identical fuel mass flow rate supply to the combustor. A detailed description of the experimental setup and CFD model for the compared swirl-stabilized combustor are presented in the authors’ earlier studies.22,37

Figure 16 depicts the comparison between multihole and swirl-stabilized combustors in terms of temperature distribution, streamlines, vorticity, and CO formation within the combustion chamber. A high-temperature zone is observed in
the middle of the multihole combustor near inlets with only the ORZ at the corner of the combustor. On the other hand, high-temperature areas are observed near the combustor wall due to the swirling motion of the flow with both the IRZ and ORZ present in the chamber in the swirl-stabilized combustor assuming a characteristic 'V'-type flame shape, which can form...
as a combined effect of flame front curvature, flow straining, and heat loss to the base (in some cases without heat loss to the flame holding base). The highest flame core temperatures are comparable in both the multihole (1882 K) and swirl-stabilized (1892 K) combustor. The axial temperatures are slightly higher in the multihole combustor than the swirl-stabilized counterpart. The increased temperature in the centerline axis of the combustor in multihole arrangement is due to the absence of the swirling effect. Unlike the multihole burner, the flow is pushed toward the combustor wall in the swirl-stabilized burner, which reduces the axial temperature. Figure 17 shows the temperature along combustor length for both types of burners. A sharp increase in temperature is observed within $0 \leq Z/D \leq 0.28$ and $0 \leq Z/D \leq 0.09$ for multihole and swirl-stabilized combustors, respectively. The temperature decreases gradually as the flow progresses.
in mean and maximum outlet temperatures is due to heat loss through the quartz wall by means of both convection and radiation heat transfer. Furthermore, the swirl effect allows increases in residence time and reduction in flame temperature as reported in earlier studies.42,43

Maximum vorticity in the multihole combustor is observed at 3928.24 s⁻¹, while the corresponding value is considerably higher (46394.8 s⁻¹) in the swirl-stabilized burner. Lower vorticity in the multihole burner indicates its lower circulation tendency compared to the swirl-stabilized burner. Although the maximum CO concentration is higher in the swirl-stabilized burner, it oxidizes this CO faster, thus resulting in lower CO emission at the outlet, as shown in Figure 19c. Da is lower in the multihole combustor (Figure 19a), which implies reduced reaction rate over diffusion rate, compared to that of the swirl-stabilized counterpart. The reduced reaction rate of the multihole burner is reflected in its greater flame thickness, as shown in Figure 19b.

5. CONCLUSIONS

Lean premixed oxy-propane (C₃H₈/O₂/CO₂) flames have been studied numerically for combustion in a multihole model gas turbine combustor. The effect of inlet composition has been investigated over various Ø (0.241–0.50), OF (32.4–60%), and Tₐd (1600–1900 K) under atmospheric conditions at a constant bulk flow velocity of 5.2 m/s. Furthermore, the oxy-propane flame in the multihole combustor is compared with a swirl-stabilized combustor in identical flow conditions (Ø = 0.313, OF = 60%, and Tₐd = 1900 K) and power densities (8.36 MW/m²/bar). The following conclusions have been outlined based on the results of this study:

Similar to swirl-stabilized flames, multihole-stabilized flames are also heavily influenced by Tₐd, where flame at (Ø = 0.241, OF = 60%) and (Ø = 0.50, OF = 32.4%) demonstrate comparable lifted flame at Tₐd = 1600 K, similar almost-anchored flames at (Ø = 0.276, OF = 60%) and (Ø = 0.50, OF = 36.6%) at Tₐd = 1750 K, and lastly, similar stronger anchored flames in cases with (Ø = 0.313, OF = 60%), (Ø = 0.392, OF = 50%), and (Ø = 0.50, OF = 40.8%) at Tₐd = 1900 K.

Due to the absence of a swirling motion, only the ORZ has been observed in the multihole combustor, which is located at the corner of the combustor between the quartz tube wall and the peripheral inlet holes. Reaction zones in the multihole burner exist between the ISL and OSL of each flamelet. The product formation zone for the lifted flames is observed within 0 ≤ Z/D ≤ 2.4 for the lifted flames near the blowout, which is considerably shortened in more stable anchored flames 0 ≤ Z/D ≤ 0.35.

In comparison with the swirl-stabilized flames, multihole flames do not have IRZs, which significantly reduces the mixing of CO and available O₂ and increases the outlet temperature distribution, causing an increase in the pattern factor. Even though the CO mole fraction is lower in the combustion chamber in the multihole case, the CO emission at the outlet is lower at the outlet of the swirl-stabilized combustor due to re-oxidation of CO with enhanced mixing of species at elevated vorticity. Axial temperatures and flame thickness are higher with reduced Da in multihole flames than the corresponding swirl-stabilized case, which indicates higher reaction rates in the swirl-stabilized combustor.

Since this study encompasses C₃H₈/O₂/CO₂ combustion in the steady state and within stable combustion regime at a fixed inlet flow velocity, the effect of other inlet conditions such as Reynolds number, power density, and mass flow rate should also be examined. In addition, the mechanism behind blowout and
flashback along with acoustic instabilities should be investigated in the transient flow state.

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**NOMENCLATURE**

| Symbol | Description |
|--------|-------------|
| 3D     | three-dimensional |
| $\bar{\theta}$ | mean reaction progress variable |
| $C_3H_8$ | propane |
| CO     | carbon monoxide |
| $CO_2$ | carbon dioxide |
| $c_p$  | specific heat capacity |
| D      | combustor diameter |
| $Da$   | Damköhler number |
| DO     | discrete ordinate |
| EGR    | exhaust gas recirculation |
| $f$    | mean mixture fraction |
| $f'$   | mixture fraction variance |
| $H_2$  | hydrogen |
| $H_2O$ | water (vapor) |
| IRZ    | inner recirculation zone |
| $L$    | gas layer thickness |
| LPM    | lean premixed |
| NOx    | nitrogen oxides |
| $O_2$  | oxygen |
| OF     | oxygen fraction (volumetric concentration of $O_2$ in the $O_2/CO_2$ oxidizer) |
| ORZ    | outer recirculation zone |
| P      | partial pressure of the absorbing gases |
| PDF    | probability density function |
| PIV    | particle image velocimetry |
| PF     | pattern factor |
| PV     | progress variable |
| r      | radial location inside combustor |
| $R$    | combustor radius |
| $S_{eq}$ | source term |
| $S_L$  | laminar flame speed (LFS) |
| $T_{ad}$ | adiabatic flame temperature |
| $T_0$  | temperature of the unburnt reactant mixture |

**Figure 19.** Comparison of flames in the multihole and swirl-stabilized combustor in terms (a) $Da$, (b) flame thickness, and (c) CO emission at 0.313 Ø and 60% OF under atmospheric conditions.
u′, root mean square (RMS) of velocity fluctuation
υ, velocity component along j direction
WSGGM, weighted sum of gray gas model
Yf, mass fraction of fuel
Yp, mass fraction of product species
Y_{f, ap}, mass fraction of species after complete combustion
Y_{o, ap}, mass fraction of oxygen
z, axial location inside the combustor

Greek symbols
α, emissivity weighting factor for the gray gas i at temperature T
δ, flame thickness
κ, adsorption coefficient
λ, unburnt thermal conductivity
μ, turbulent viscosity
ρ, density
Φ, equivalence ratio

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