Characterization of MILD Combustion of a Premixed CH₄/Air Jet Flame versus Its Conventional Counterpart

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ABSTRACT: This study is performed to characterize moderate or intense low-oxygen dilution (MILD) combustion (MC) versus conventional combustion (CC) of a premixed CH₄/air jet flame in a hot coflow under identical inlet and ambient conditions. The present CC and MC correspond to the cases using a bluff-body (BB) and a no bluff-body (NBB), respectively. It is demonstrated that the NBB combustion develops by entraining ambient hot low-oxygen gas so as to dilute the reactant mixture and simultaneously heat up beyond the minimum autoignition temperature (Tₐᵢ), leading to the MC. By contrast, in the BB case, the conventional flame is established and stabilized by a steady heat source of the recirculation zone (RZ) behind the BB with highly intense mixing and rapid ignition. A large reaction zone with uniform temperature distribution (i.e., low temperature rise) is found in the MC mode, while the CC has a much smaller size of the intense reaction zone with the concentrated high temperature and species distributions. Significantly, it has been first revealed that, in the BB case, there is a secondary combustion in the MC mode formed far downstream from the BB flame under the environmental condition of a high-temperature hot coflow.

1. INTRODUCTION

Conventional combustion (CC) of fossil fuels has been continuously emitting carbon dioxide (CO₂), nitric oxides (NOₓ), and fine particles (PM), causing a serious threat to human life. This calls for an urgent action to take for avoiding or reducing such a threat! Moderate or intense low-oxygen dilution (MILD) combustion (MC) has been found to be one of the most promising technologies to support this action. This mode of combustion can achieve high thermal efficiency of combustion systems and simultaneously low pollutant emissions. Of note, the like of MC may be named flameless oxidation (FLOX) or high-temperature air combustion (HiTAC). Despite being differently named, they are all similarly realized by re-circulating combustion products into the incoming fresh air and fuel efficiently. Relative to the conventional combustion (CC), a strong mixing between reactants and flue gases slows down various combustion reactions, thus substantially dropping local peak temperatures of combustion, thereby reducing NOₓ emissions. Other distinct characteristics, such as no visible flame and enhanced radiation efficiency, are also found in this mode of combustion.

To differentiate MC and CC in the flame establishment, combustion characteristics, and pollution emissions clearly, a number of previous investigations have been carried out experimentally and numerically since the discovery of MC. Wünning et al. defined MC as a low NOₓ emission technology by experiment. They also distinguished MC and CC by the exhaust gas recirculation rate Kₑ and furnace temperature Tₑᵣₙ (or combustion system temperature), where Kₑ is defined as

\[ Kₑ = \frac{mₑ}{mᵣ + mₑ} \]

Here, mᵣ, mₑ, and mᵣ are the mass fluxes of the recirculated exhaust gas, oxidant, and fuel, respectively. Wünning et al. found that, for the methane combustion, MC can be established only when two conditions are satisfied: (i) \( Kₑ > 3.5 \) and (ii) \( Tₑᵣₙ > 850 \, °C \). By contrast, CC is for \( Kₑ < 0.75 \). It followed that Plessing et al. realized MC in a combustion chamber with highly preheated air and strong exhaust gas recirculation. Using ambient air (≈300 K) at high recirculation rates, Kumar et al. achieved MC at high heat release rate up to 10 MW/m³ in a 3 kW furnace. They also proposed a new scaling criterion for the burners operated in MC mode based on the heat release rate and reactant mixing time. Dally et al. studied MC in a CH₄/H₂ jet in hot coflow (JHC) burner and found that the MC could be established with a low-oxygen hot coflow. Then, Dally et al. and Szegö et al. investigated MC in lab-scale furnaces under different fuel dilution, air preheating, and heat extraction conditions. They found that dilution of the fuel jet with inert gas (CO₂ or N₂) could help achieve MC and reduce NOₓ emissions due to the high scalar dissipation near the fuel jet. Besides, the fuel jet momentum was found to be dominant for the MC establishment in their experiments. Mi et al. then achieved the premixed MC by increasing the momentum rate of the fully/partially premixed reactant jet in the same furnace as in Szegö et al. They discovered that there was a critical inlet jet momentum rate for the geometry used by them, below which MC cannot be established.

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achieved. Recently, Cheong et al.\textsuperscript{13} found through experiments that the distance between fuel and air jet nozzles is also crucial for realizing MC in the furnace. The separation controls both the mixing of the fuel and oxidant jets themselves and their mixing with the flue gas, thus influencing combustion reaction rates.

In a separate study, Cavaliere et al.\textsuperscript{2} compared MC and CC in a well-stirred reactor (WSR) by varying the inflow temperature ($T_{in}$). They defined the MC mode as a combustion process where $T_{in} > T_{air}$. $\Delta T_{max}$, in which $T_{air}$ is the autoignition temperature and $\Delta T_{max} = T_{max} - T_{in}$ is the maximum temperature rise due to combustion. Wang et al.\textsuperscript{14} developed this definition to classify the combustion of a CH$_4$/O$_2$/N$_2$ mixture in a WSR into several regimes (CC, MC, high-temperature combustion (HTC), etc.) based on a three-dimensional plot of $T_{max}$, N$_2$ mole fraction (X$_{N2}$), and equivalence ratio ($\Phi$). They\textsuperscript{15} also used this method to identify MC and TC in the JHC burner of Dally et al.\textsuperscript{6} based on the coflow temperature ($T_C$) and oxygen mole fraction (X$_{O2}$). Mei et al.\textsuperscript{16,17} investigated the reaction zone dimensions of MC and TC in the same JHC burner by varying $T_{air}$, X$_{O2, coflow}$, coflow velocity ($V_C$), and coflow diluent (N$_2$ and CO$_2$). They pointed out that MC is characterized by a large reaction zone and weak chemical reactions and the oxy-fuel (CO$_2$-diluted) reaction zone is much larger than the air-fuel (N$_2$-diluted) counterpart. More recently, large eddy simulation (LES)\textsuperscript{18,19} and direct numerical simulation (DNS)\textsuperscript{20,21} were also utilized to differentiate the small-scale characteristics of MC and TC by varying the dilution level, and it was found that MC is characterized by autoignition, a small scalar gradient, and distributed reactions, while TC has a larger scalar gradient and thin flame sheets.

The previous studies\textsuperscript{22–25} mainly focused on how external conditions, such as jet conditions (e.g., fuel type, oxygen mole fraction, temperature, inlet momentum rate, nozzle separation, etc.) and outer boundary wall conditions (e.g., temperature, heat transfer rate), would influence the combustion. It may lead to the misconception that these two modes of combustion are so distinct that they cannot be achieved under the same inlet and environmental conditions. This stimulates this work to study whether a change of internal flow structure individually, without changing inlet and boundary conditions, can cause differences in the flame mode. Previously, the internal flow structure was always treated as a dependent variable that changes with varying jet and coflow conditions.\textsuperscript{3–25} In this sense, the effect of the flow structure on the establishment of both combustion modes under identical conditions deserves a study. Moreover, in the past studies,\textsuperscript{25–27} CC was realized by reducing the jet momentum rate or reducing the diluent or even eliminating it. However, in practical applications, CC is commonly achieved by flame stabilizers such as a bluff-body (BB) or swirler.\textsuperscript{22–27} In addition, previous works were focused mainly on nonpremixed MC,\textsuperscript{5,14,15,18–20} while a few works have been performed on premixed MC in hot (flue gas) coflow. Note that the premixed combustion is very important in fundamental research and applications. Therefore, in this work, MC and CC in a premixed JHC burner are investigated together. Specifically, a bluff-body (BB) is placed downstream near the nozzle exit to vary the internal flow structure to realize CC, while it is taken away to develop MC, both under identical inlet and ambient conditions.

When the BB is set near the nozzle exit, the premixed reactant jet will rapidly slow down and a recirculation zone (RZ) with negative velocity will develop behind the BB. In this situation, when the mixture in the RZ is ignited with an external heat source (e.g., spark electrode), the strong mixing between the RZ and the oncoming premixed reactants in the shear layer will be continuously ignited, finally developing a conventional BB flame.\textsuperscript{22–24} Without BB, the mixture jet will directly flow downstream and be gradually diluted and heated by entraining the surrounding exhaust gas with low oxygen, finally establishing MC.\textsuperscript{3,15–17}

In this context, this work investigates these two modes of combustion (MC and CC) with the same inlet and outer surrounding conditions. Specifically, the aim of the investigation is to distinguish the two modes in the flow field, combustion establishment process, and spatial distributions of the mean temperature and various species concentrations.

2. COMPUTATIONAL DETAILS

2.1. Numerical Conditions. Present numerical calculations are partly validated using the experimental results of Cabra et al.\textsuperscript{26} who measured the temperature and various species (O$_2$, CH$_4$, N$_2$, H$_2$, CO, OH, etc.) of a premixed CH$_4$/air jet flame in a hot vitiated coflow. Their combustion was not in the MC mode but developed through autoignition,\textsuperscript{25} whose ignition mechanism is very similar to that of MC. Therefore, this configuration is suitable not only for the validation of the present modeling but also for the comparison between turbulent premixed MC and CC of a jet flame. The Cabra burner\textsuperscript{28} consisted of a central jet nozzle of inner diameter $d = 4.57$ mm surrounded by a hot vitiated coflow, which initially flowed in an annular tube of diameter 210 mm. The jet exit velocity was 100 m/s, corresponding to a Reynolds number ($Re$) of about 28 000. The vitiated coflow, with temperature 1350 K and velocity 5.4 m/s, was the combustion product of 2200 lean premixed H$_2$/air flames generated from a perforated plate in the annular tube. Thus, it was a mixture of O$_2$, N$_2$, and H$_2$O.

Moreover, to examine the applicability of the present numerical models to BB flames, the premixed BB flame experiments conducted by Kariuki et al.\textsuperscript{29} are also considered. In this configuration, the premixed jet nozzle has a diameter of 35 mm and a 45° half-angle BB (diameter $d_B = 25$ mm) at the nozzle exit and was put in static ambient air at room temperature (300 K). The bulk velocity at the nozzle exit was 21.6 m/s and the corresponding Reynolds number was about 34 000, comparable with that of the Cabra experiments.\textsuperscript{28}

The Cabra burner\textsuperscript{28} is chosen for numerical simulations of this work for comparing MC and CC, while a conical BB is set at 1.0d behind the jet exit to create a RZ and realize the CC in the BB case. The velocities of the central jet and the hot coflow are reduced to 50 and 1 m/s, to avoid blowing off. Moreover, the coflow oxygen concentration is decreased to 6% to establish MC in the no bluff-body (NBB) case. Table 1 shows all of the detailed conditions of the central premixed jet and the hot coflow for the present calculations and those experiments.\textsuperscript{26,28}

Due to the symmetry of the combustion systems, a two-dimensional computational domain, shown in Figure 1, is selected for the present calculations to save the cost of computation. The radial length of the computational domain is 200 mm, and the axial length is 1000 mm downstream from the jet inlet. The zero-shear stress wall boundary is set at the
sides, and the pressure boundary of 1 atm is set at the outlet. After verifying the grid independency, a structured mesh with about 14,000 cells is chosen for the model validation of the Cabra experiments\textsuperscript{28} and the NBB case, and a mesh with about 20,000 cells is chosen for the BB case. Note that the grid number of the latter is comparable with that for the validation of the Kariuki experiments,\textsuperscript{26} indicating that 20,000 cells are sufficient for modeling the flow and combustion in such unconfined BB flames. The minimum mesh scale in the BB case is $0.033 \text{ mm} \times 0.044 \text{ mm}$ and $0.285 \text{ mm} \times 0.42 \text{ mm}$ in the NBB case.

### 2.2. Computational Models

To predict the turbulence, reaction, and their interactions correctly in the two combustion regimes, we require appropriate models for turbulence, species transport, radiation, and chemical reactions. Based on the past studies,\textsuperscript{15−17,28−42} the models chosen presently are shown below.

#### In consideration of the accuracy and cost of calculations, one of the two-equation turbulent models, i.e., the $k$–$\varepsilon$ model,\textsuperscript{30} is commonly used in numerical simulations. However, previous studies\textsuperscript{15−17} found that the standard $k$–$\varepsilon$ model cannot achieve ideal results for turbulent round jets. Thus, this study adjusts the constant $C_{\varepsilon}$ from 1.44 to 1.6, which has been proved feasible for a better prediction for such turbulent round jet flows.\textsuperscript{31}

The compositional probability density function (PDF) model is used as the combustion model, which can well describe the interactions between turbulence and chemical reactions in both MC\textsuperscript{34,35} and CC.\textsuperscript{36,37} In this model, the joint PDF is applied to the Reynolds-averaged species and energy equations. The PDF equations derived from the N–S equations are shown below

\[
\frac{\partial}{\partial t} \left( \rho P \right) + \frac{\partial}{\partial x_i} \left( V_i \rho P \right) + \frac{\partial}{\partial y_k} \left[ S_{ij} \rho P \right] = -\frac{\partial}{\partial x_i} \left( \rho \left( \bar{v}_i \psi \right) P \right) + \frac{\partial}{\partial y_k} \left( \rho \left( \frac{1}{\rho} \frac{\partial J_{ik}}{\partial y_k} \psi \right) P \right) \tag{2}
\]

where $P$ is the Favre joint PDF composition, $\rho$ is the fluid density, $V_i$ is the mean fluid velocity along the $i$ direction, $S_{ij}$ is the reaction rate for species $k$, $\psi$ is the composition space vector, $v_i'$ is the velocity fluctuation vector along the $i$ direction, and $J_{ik}$ is the vector for molecular diffusion flux. In eq 2, the three terms on the left-hand side are closed, while the terms on the right-hand side are not and require modeling. The turbulent scalar flux (first term on the right) is closed by the gradient-diffusion assumption

\[
-\frac{\partial}{\partial x_i} \left( \rho \left( \bar{v}_i \psi \right) P \right) = \frac{\rho h_i}{S_{\psi}} \frac{\partial P}{\partial x_i} \tag{3}
\]

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<th>Karuki experiments\textsuperscript{26}</th>
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#### Table 1. Central Jet and Coflow Conditions of the Experiments and the Calculations

![Figure 1. Computational domains and structured meshes for (a) experimental validation of Cabra et al.\textsuperscript{28} and the NBB case and (b) BB case and (c) experimental validation of Kariuki et al.\textsuperscript{26} The unit is millimeter.](image-url)
where $\mu_t$ and $S_c$ are turbulent viscosity and Schmidt number, respectively. The second term on the right-hand side of eq 2 is the molecular mixing term, which also needs to be closed. Compared with the interaction by exchange with the mean (IEM)\textsuperscript{38} and the Euclidean minimum spanning tree (EMST)\textsuperscript{38} models, modified curl (M-Curl)\textsuperscript{39} mixing model was found to be a better choice for modeling the molecular mixing for turbulent combustion.\textsuperscript{28,29} This is also confirmed by the present calculations in Section 3. To reduce the computational cost, the in situ adaptive tabulation (ISAT) model\textsuperscript{40} is used, and the ISAT error tolerance is set at $10^{-6}$ to ensure the accuracy of the calculations. Besides, the number of particles in each cell is set to 30. For the M-Curl model, some of the particle pairs are selected randomly from all of the particles in a cell, and its Favre-mean composition $\phi$ is changed as

\begin{equation}
\phi_i^j = (1 - \epsilon)\phi_i^0 + \xi \frac{(\phi_i^0 m_i + \phi_j^0 m_j)}{(m_i + m_j)}
\end{equation}

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\end{equation}

where $\phi_i$ and $\phi_j$ are compositional vectors, $m$ is the mass for each particle, and $\xi$ is a number selected randomly.

This study applies DRM-22, a chemical kinetic mechanism\textsuperscript{41} simplified from GRI-Mech 1.2, a detailed mechanism;\textsuperscript{42} note that DRM-22 contains 22 species and 104 reversible reactions. This simplified mechanism was found\textsuperscript{41} to predict adiabatic flame propagation velocity and ignition delay well. In addition,
and $H_2$) along the jet centerline. Note that the mixture fraction $x$ and its root-mean-square (rms) value ($\bar{x}'$), mixture fraction ($f$), and species concentrations ($Y_m$ where $m = CH_4, O_2, CO, CO_2, OH,$ and $H_2$) along the jet centerline. Note that the mixture fraction was defined by Bilger et al. as

$$f = \frac{2(Y_C - Y_{C,2})/M_C + (Y_{H} - Y_{H,2})/2M_H - (Y_O - Y_{O,2})/M_O}{2(Y_{C,1} - Y_{C,2})/M_C + (Y_{H,1} - Y_{H,2})/2M_H - (Y_{O,1} - Y_{O,2})/M_O}$$

where $M$ stands for the elemental mass and $Y$ represents the mass fraction of these elements (carbon, hydrogen, and oxygen). The subscripts 1 and 2 denote those quantities related to the central jet and annular coflow, respectively.

Evidently, in Figure 2, the use of the M-Curl model predicts better than the other two mixing models, with respect to the measurements. Specifically, in the EMST and IEM models, the earlier occurrence of combustion reactions is predicted, hence leading to earlier growths of the centerline temperature, $CO, CO_2, \text{and } H_2$. Perhaps, due to the overestimation of the mixing rate, the simulated temperatures from the EMST and IEM models are higher in the mixing layer, hence causing early ignition. In this context, the M-Curl model is chosen as the mixing model for this study, whose results are presented below and in the next section.

Using the M-Curl model, the predictions of the centerline $T$, $T'$, and $Y_m$ (where $m = CH_4, O_2, CO, CO_2, OH,$ and $H_2$) can act to validate the modeling. To enhance the validation, Figure 3 presents the radial profiles of the predicted and measured $T$, $T'$, and $f$ at $x/d = 15, 30, 40, 50,$ and $70$. In general, the simulations agree reasonably well with the measurements. Specifically, the predictions of the centerline $T$, $f$, $Y_{CO}, Y_{CH_4}, \text{and } Y_{O_2}$ nearly perfectly match their measured values at $x/d \leq 80$. By comparison, the centerline profiles of $T'$, $Y_{CO}, Y_{CH_4}, \text{and } Y_{O_2}$ are not predicted so well. Overestimations of $Y_{CO}, Y_{CH_4}, \text{and } Y_{O_2}$ occur at $x/d > 60$. At $x/d > 80$, due to the coflow velocity decay, outer cold air can enter the inner combustion region, thus causing a lower measured temperature and higher values of $Y_{O_2}$. The dilution effect of outer air would also reduce the measured concentrations of minor species.

In addition, the present model is also validated by the premixed BB flame of Kariuki et al. Figure 4 presents the radial profiles of the calculated and measured axial velocity $V_x$ and progress variable defined by $C = Y_{CO}/Y_{CO,p}$ where $Y_{CO,p}$ is the mass fraction of $CO_2$ in the complete combustion products. Apparently, the present model slightly underestimates $V_x$ at $0 \leq r/d_k \leq 0.4$ and $x/d_k = 0.4$ and 0.8, while $C$ is also underestimated at $x/d_k < 1.6$, relative to the measurements. Despite the above, the calculations of $V_x$ and $C$ overall agree reasonably well with their experimental data. Thus, the Reynolds average Navier Stokes (RANS)-PDF model is also applicable for premixed BB flames.

To conclude, the computational models of RANS-PDF (with the M-Curl mixing model) work appropriately in simulating the premixed JHC flame and premixed bluff-body flame, so they are adequate for use in this study.

3. VALIDATION OF THE COMPUTATIONAL MODELS

Figure 2 displays the numerical predictions of the centerline temperatures and concentrations of some typical species using the M-Curl, EMST, and IEM models against the experimental results of Cabra et al. Presented on the plots are the results of the Favre-averaged temperature ($\bar{T}$) and its root-mean-square (rms) value ($\bar{T}'$), mixture fraction ($\bar{f}$), and species concentrations ($\bar{Y}_m$ where $m = CH_4, O_2, CO, CO_2, OH,$ and $H_2$) along the jet centerline. Note that the mixture fraction was defined by Bilger et al. as

$$f = \frac{2(Y_C - Y_{C,2})/M_C + (Y_H - Y_{H,2})/2M_H - (Y_O - Y_{O,2})/M_O}{2(Y_{C,1} - Y_{C,2})/M_C + (Y_{H,1} - Y_{H,2})/2M_H - (Y_{O,1} - Y_{O,2})/M_O}$$

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the velocity decreasing slowly as $x/d$ increases. By contrast, the flow field changes dramatically once a bluff-body is placed near the nozzle exit to make the BB case. The central premixed reactant mixture flows around the BB, being first divided and then merged together. A large recirculation zone (RZ; about $5.69d$ long) is formed behind the BB, thus changing the flow direction and velocity distribution significantly. Downstream from the RZ, the central jet velocity first recovers until its local maximum returns back to locate on the centerline at $x/d \geq 20$ and then turns to decay farther downstream. To quantitatively show the fundamental difference in the velocity field, Figure 7 presents the centerline axial velocity variations for the NBB and BB cases. It is evident that the two jets are totally different at $x/d < 30$ and appear to become similar at $x/d > 50$ gradually. At $x/d > 80$, the centerline axial velocity is nearly equal for the two cases. Similar results can be found in previous studies.\(^{46,47}\) Esquiva-Dano et al.\(^{48}\) also concluded that under different jet velocities and BB shapes, the centerline axial boundary of the RZ. In contrast, the MC develops far downstream and distributes volumetrically with a quasiningiform temperature distribution of no obvious temperature peaks. Overall, these two modes of combustion are greatly distinct. The specific differences between the NBB and BB cases in the flow field, flame establishment, and combustion characteristics are presented below.

4.1. Difference between the NBB and BB Cases in the Flow Field. Figure 6 shows the axial velocity ($V_x$) fields of the NBB and BB cases together with the lateral profiles of $V_x$ at $x/d$ = 4, 12, 20, and 60 and a few streamlines. Evidently, in the NBB case, the central jet flow gradually develops downstream, with the velocity decreasing slowly as $x$ increases. By contrast, the flow field changes dramatically once a bluff-body is placed near the nozzle exit to make the BB case. The central premixed reactant mixture flows around the BB, being first divided and then merged together. A large recirculation zone (RZ; about $5.69d$ long) is formed behind the BB, thus changing the flow direction and velocity distribution significantly. Downstream from the RZ, the central jet velocity first recovers until its local maximum returns back to locate on the centerline at $x/d \geq 20$ and then turns to decay farther downstream. To quantitatively show the fundamental difference in the velocity field, Figure 7 presents the centerline axial velocity variations for the NBB and BB cases. It is evident that the two jets are totally different at $x/d < 30$ and appear to become similar at $x/d > 50$ gradually. At $x/d > 80$, the centerline axial velocity is nearly equal for the two cases. Similar results can be found in previous studies.\(^{46,47}\) Esquiva-Dano et al.\(^{48}\) also concluded that under different jet velocities and BB shapes, the centerline axial velocity (normalized by the jet exit velocity) in the far downstream area is almost the same. This can be explained. For an ideal fluid flow around a BB, the flow field can be decomposed to a free flow without BB and a potential flow caused by the BB (e.g., for cylinder BB, the potential flow is a dipole flow).\(^{48}\) The potential flow affects only the flow near the BB and thus the downstream flow is dominated by the free flow. It can be inferred that for the actual viscous premixed jet, the effect of BB should also be reasonably weak in the far downstream area; thus, the centerline axial velocity is very similar for the cases of NBB and BB with different shapes and jet velocities. The results here and in refs 46 and 47 confirm this point.

Figure 8 shows contours of the nondimensional velocity gradient $G \equiv |V \cdot \nabla d/V|$ (upper half) and turbulent intensity $I \equiv \nu/V$ (lower half) in the (a) NBB and (b) BB cases. Large velocity gradients occur in the shear layers between the central jet and outer coflow and between the jet and the RZ. Careful inspections indicate that, in the CC case, $G$ and $I$ near the RZ boundary are both much larger than those between the central jet and coflow. In other words, the maxima of $G$ and $I$ are much greater in the CC case than in the MC case where no BB exists. Higher velocity gradients are usually supposed to cause a higher turbulent shear rate and thus stronger molecular-level mixing.\(^{49}\) The mixing intensity may be reflected by the turbulence intensity $I$. In the CC case, the mixing between the reactant mixture and combustion product mixture from the RZ is more intense ($I_{\text{max}} \approx 12.0$) than that between the central jet and hot coflow ($I_{\text{max}} \approx 7.0$) in the MC case. Namely, relative to the CC case, the mixing occurring between the “cold” premixed reactants and co-flowing hot flue gases is far weaker in the MC case.

Figure 9 shows the contours of the mixture fraction ($f$) for the NBB and BB cases. The mixture fraction, as defined in eq 6, describes the mixing between the central jet and the coflow.

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Figure 5. Contour distributions of the Favre-averaged temperature ($T$) in the (a) NBB and (b) BB cases.

Figure 6. Contour distributions of the axial velocity ($V_x$) in the (a) NBB and (b) BB cases. The solid black lines mark streamlines. The red lines represent lateral distributions of the axial velocity at $x/d = 4, 12, 20, \text{ and } 60$.

Figure 7. Centerline axial velocity ($V_x$) in the NBB and BB cases.

Figure 8. Contour distributions of the nondimensional velocity gradient $G \equiv |V \cdot \nabla d/V$ (upper half) and turbulent intensity $I \equiv \nu/V$ (lower half) in the (a) NBB and (b) BB cases.
In general, the lower the mixture fraction is, the more the premixed reactant mixture is diluted by the coflow. In the NBB or MC case, \( f \) is quite low (<0.3) in the reaction zone, which means that the reactant mixture is highly diluted. This also indicates that the mixedness between the jet and low-oxygen coflow is the main factor for the MC “flame”.

By comparison, in the BB or CC case, the mixture fraction is substantially higher (>0.5) in the reaction zone, especially, \( f > 0.7 \) in the RZ, revealing that the CC flame has little to do with the mixing process between the central jet and the hot coflow. The CC flame depends almost solely on the mixing between the premixed reactants and the combustion products in the RZ. The reasons for the above differences will be explained in the next section.

Overall, the presence of a bluff-body changes the flow field considerably, particularly forming a strong recirculation and thus the reverse flow region. The strong turbulence mixing between the upcoming reactant mixture, which slows down due to the BB, and the burning product mixture in the RZ enables both the flame stabilization and rapid combustion. Nevertheless, the lifted MC flame results merely from the reactants being mixed and heated by the hot coflow.

### 4.2. Difference between the NBB and BB Cases in the Establishment of Combustion

To identify the difference between the MC and CC in their combustion establishment, Figure 11 shows the difference between the turbulent flame speed \( S_f \) and local axial velocity \( V_x \), i.e., \( (S_f - V_x) \), in the reaction zone. The turbulent flame can be stabilized by the balance of its propagation or autoignition. For the flame propagation, the flame is stabilized in the region where \( (S_f - V_x) \approx 0 \). Otherwise, it will propagate upstream or downstream. For autoignition, the reactant temperature should be higher than \( T_{ai} \). In the NBB case, the turbulent flame speed is never larger than the local velocity \( S_f < V_x \). The flame front (if any) propagates only downstream or “blows out” and is never stabilized. Therefore, the lifted flame can be stabilized only by autoignition far downstream from the nozzle. In the BB case, the flame speed behind the BB is much larger than the local speed \( S_f \gg V_x \). The flame propagates upstream to ignite the upcoming reactant mixture. Note that the reactant temperature is below \( T_{ai} \) upstream of the flame front (see Figure 5). Thus, the flame is stabilized by flame propagation. There are two reasons for the differences in flame stabilization between the two cases. First, the flame temper-
ature in the BB case is much higher than that in the NBB case, which leads to a larger flame speed (S_f) for the CC. Second, as is described in Section 4.1, the central velocity decays much more rapidly in the BB case due to the BB.

To differentiate the flame establishments of the two cases, we carried out the unsteady RANS-PDF calculations for the NBB and BB cases (Figure 12 shows some of the results). The time step of the calculation is set as 1 × 10^{-4} s, with other numerical settings being identical to the steady RANS calculations. In each case, a small region (1.5 < x/d < 3, 0 < r/d < 1) is initialized with 1700 K at t = 0 s, the same as for the steady RANS-PDF calculations of the BB case. This external “spark” is necessary to establish the BB combustion 50 but unnecessary for the NBB case or MC. It is found that both cases have nearly reached their statistical steady state at t = 0.1 s.

Figure 12 shows the instantaneous temperature distributions at several consecutive time instants in the two cases. In the NBB case (Figure 12a), a temperature increment for (T − T_C) ≥ 10 K does not appear, and no combustion is supposed to occur, at t ≤ 0.01 s. The initial heat patched in the tiny region at t = 0 quickly spreads out and downstream, causing a rapid drop in temperature to T_C = 1250 K. No ignition occurs due to the initial spark anywhere in the computational domain. As time goes on, combustion develops and takes place solely due to autoignition at x/d ≈ 50–60 or the time t < 0.02 s, which is the minimum τ_q calculated from WSR (see Figure 10). In the WSR system, where reactants are perfectly mixed, only chemical reactions are simulated, in contrast to the present BB and NBB cases where the mixing and reaction processes happen simultaneously. Once the autoignition has occurred, the combustion zone spreads downstream instead of propagating upstream, as shown at t = 0.02 and 0.03 s, and gradually reaches its steady state. The initial patch of a tiny high-temperature (1700 K) area has no impact on the final establishment of a stable MILD combustion (MC).

However, in the BB case, see Figure 12b, a visible combustion zone or flame is established in a different way. After initializing a small region with a high temperature of 1700 K or “sparking” behind the BB, a flame develops gradually downstream of the BB. Then, the upcoming reactant mixture is ignited rapidly and continuously. It is interesting to find that, at t = 0.0001 s, the high-temperature region behind the BB is very tiny but sufficient to establish the combustion process. That is, sparking with some heat greater than the minimum ignition energy can successfully ignite the reactant mixture when there is a BB. In other words, the key reason for the establishment of this conventional combustion (CC) is the presence of the BB, behind which a recirculation zone (RZ) is formed, acting as a heat source for continuous ignition and a flame stabilizer to avoid the flame being blown off.

Moreover, Figure 12b demonstrates that at t = 0.025 and 0.03 s some temperature rise takes place in the mixing layer between the jet and coflow at x/d ≈ 80. That is, in the BB case, there is also a secondary combustion developing far downstream due to autoignition, which is similar to that in the NBB case. However, it takes longer for this ignition because the upstream CC flame consumes most of the reactants. Presumably, if the CC flame is blown off, the MC should develop quite far downstream as stable as in the NBB case. It seems that a balance between these two combustion processes would control the flame characteristics of the BB case. If the conventional flame behind the BB cannot consume most reactants, the remainder would be consumed by the downstream MC. When the CC can no longer be stabilized due to some reasons (e.g., a sufficiently high jet momentum to blow...
off the flame), the entire combustion would take place downstream in the MC mode, like the NBB case. Nevertheless, despite its interestingness, this issue is out of the scope of this work.

To summarize, in the NBB case, the central high-velocity cold reactant mixture entrains and mixes with the ambient hot flue-gas mixture (coflow). The reactant mixture is thus gradually heated beyond its autoignition temperature ($T_{\text{auto}}$) sufficiently downstream, and consequently, the stable MILD combustion is established slowly and sustains due to autoignition. In contrast, in the BB case, where an ignition is forced initially, highly strong mixing between the cold reactant mixture and very hot species in the RZ is the key factor for establishing a stable CC flame. Combustion takes place rapidly behind the BB due to extremely fast ignition by the recirculated high-temperature combustion products. Besides, the CC flame has to be integrated with the downstream secondary combustion of the MC mode. The finding of the secondary combustion in the MC mode has never been reported in the literature before for the BB case. With this finding, the use of a BB nozzle is expected to be able to produce the MC by adding some diluents (exhaust gas) to increase the reactant momentum so that the BB flame is blown off. In other words, the BB nozzle may achieve both combustion modes by varying the premixed reactant momentum.

4.3. Difference between the NBB and BB Cases in the Combustion Characteristics. The Favre-averaged temperature distributions for both MC and CC are shown in Figure 5. Evidently, the high-temperature reaction zone for the CC is concentrated in the RZ behind the BB, while the temperature over the reaction zone is more uniform for the MC. In particular, the maximum temperature for the CC is 2497 K, which is about 900 K higher than that for the MC. The rapid ignition process along with fast reactions and rapid heat release behind the BB is the reason for the concentrated high-temperature distribution for the CC. In comparison for the MC or NBB case, the process of establishing combustion is slow due to slow mixing and sufficient dilution of reactants before combustion takes place, leading to low reaction rates. The decreased reaction rates bring about a low heat release rate per volume, which is the reason for more uniform temperature distribution.

The Favre-averaged mass fractions ($Y_\text{OH}$, $Y_\text{CH}_2\text{O}$, and $Y_\text{CO}$) of the species OH, CH$_2$O, and CO are shown in Figure 13. Evidently, high values of $Y_\text{OH}$, $Y_\text{CH}_2\text{O}$, and $Y_\text{CO}$ are more concentrated in the BB case. Moreover, the maximum values for $Y_\text{OH}$ and $Y_\text{CO}$ in the BB case are about 40 times larger than those for the NBB case. As discussed above, those intermediate species are produced and destroyed at low rates for the MC due to the dilution effect and slow ignition process, while, for the CC, chemical reactions take place violently behind the BB, leading to more intermediate species per unit volume.

Comparison of Figures 5 and 14 suggests that the high OH and high-temperature regions are overlapped. That is, the generation of OH is strongly correlated with high temperature. The generation and consumption of OH are mainly controlled by these reactions: (I) H + O$_2$ → OH + O and (II) CO + OH → CO$_2$ + H. Moreover, reaction I has a high activation energy (60.2 kJ/mol) and therefore requires a high temperature to ensue. Besides, the distributions of CH$_2$O and OH are almost in a complementary relationship, signifying that the two species hardly coexist, whatever the mode of combustion is. For consumption of CH$_2$O, the most important reaction is CH$_2$O + OH → CHO + H$_2$O whose activation energy is very low (about 1.9 kJ/mol) or the reaction temperature is low. In the MC, because of the low temperature rise, the maximum OH value is reduced largely, and especially CH$_2$O is distributed widely, versus a highly concentrated CH$_2$O region in the CC. These differences characterize the two combustion modes, as demonstrated in Figure 14. This figure shows the contours of the species mass fractions of 5% of their maxima (i.e., $Y_{\text{max}} \geq 5\%$), which represent the regions of significant intermediate species CH$_3$, CH$_2$O, CHO, CO, OH, and CH$_4$.

Distinct distributions of CH$_4$ and the other five intermediate species are obvious for the NBB and BB cases. The regions of $Y_{\text{max}} \geq 5\%$ of the intermediate species (CH$_3$, CH$_2$O, CHO, CO, and OH) for the MC are much larger than those for the CC. This means that the oxidation of MC is much slower than that of CC. Because of a strong dilution of the hot coflow, various reactions for MC are greatly restrained, causing both low reaction rates and a large reaction zone simultaneously. Although the length of the reaction zone (the same definition as above) of the MC is about 2 times greater than that of the CC, the former is much larger than the latter in volume by 10–20 times. Note that, in the CC, only CO and OH distribute over significant downstream distances. That is, the related reactions of OH and CO are slower or occur later than those of other species shown in Figure 14. In fact, the reaction CO +
OH → CO₂ + H is one of the latest reactions for CH₄ oxidation. Besides, this reaction is the most important one to determine the oxidation rate of CC. However, in the MC, all intermediate carbon-related species appear to distribute similarly or not much differently; see Figure 14. That is, the reactions associated with these species are all important for the oxidation of MC. Moreover, in the MC, the distribution regions of CO and OH are much different and especially the OH-related reactions seem to continue even at the end of the computational domain (200d).

5. CONCLUDING REMARKS
This study has been carried out to address the lack of comparison, in the literature, between the MILD combustion (MC) and typical conventional combustion (CC) of the bluff-body (BB) flame of a premixed CH₄/air jet in a hot coflow (simulating the furnace gas) under identical inlet and ambient conditions. This work is distinct from the previous work, comparing the establishment conditions and reaction characteristics of MC and CC through differing inlet and ambient conditions, i.e., nozzle size and ejection angle, inlet temperature and velocity, fuel type, fuel/oxidant diluting type and dilution level, coflow oxygen level and temperature, etc. In this study, a BB is placed near the nozzle exit as a flame stabilizer to differentiate MC and CC of a practical BB flame. The MC and CC have been characterized in terms of their flow fields, combustion establishments, mean temperatures, and species concentrations in Section 4, from which the main conclusions can be drawn below:

(1) The MC and CC modes are fundamentally distinct. In the CC case, the conventional flame is established and stabilized by a steady heat source of the recirculation zone (RZ) behind the BB with highly intense mixing and rapid burning. By contrast, the MC is a slow combustion mode that develops (and sustains) by entraining and mixing the hot “flue gas” so as to heat the premixed reactant mixture gradually beyond the autoignition temperature (Tₐ). In other words, relative to the CC, the MC depresses nearly all combustion-related chemical reactions and thus reduces local burning peak temperatures and mass fractions of main intermediate species. As a consequence, a large reaction zone with uniform temperature distribution (i.e., low temperature rise) is found in the MC mode, while the CC has a much smaller reaction zone with concentrated high temperature and species distributions.

(2) Under the same inlet and boundary conditions, MC and CC may be switched only by changing the inner flow structure through a BB. This proves that the BB has a great impact on changing the combustion mode without varying the ambient oxygen level and temperature or others.

(3) In the CC case, a secondary combustion zone is formed far downstream under the ambient condition of high-temperature (above autoignition) hot coflow. This observation has never been reported in the literature before and therefore is a new finding. With this finding, it is postulated that the use of a BB nozzle can also produce the MC mode. In other words, the BB nozzle may achieve both combustion modes by varying the premixed reactant momentum. This interesting issue will be left for another study in the near future.

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■ NOMENCLATURE

Symbols

\begin{align*}
C & \quad \text{progress variable} \\
 d & \quad \text{diameter of the premixed jet nozzle in Cabra burner} \\
 d_k & \quad \text{diameter of the bluff-body cone end in Kariuki burner} \\
f & \quad \text{mixture fraction} \\
 G & \quad \text{nondimensional velocity gradient} \\
 I & \quad \text{turbulence intensity} \\
k & \quad \text{turbulent kinetic energy} \\
 K_r & \quad \text{recirculation rate} \\
 S_f & \quad \text{turbulent flame speed} \\
 T & \quad \text{Favre-averaged temperature} \\
 T' & \quad \text{root-mean-square (rms) temperature} \\
 T_{\text{ai}} & \quad \text{autoignition temperature of the reactants} \\
 T_c & \quad \text{coflow temperature in the jet flame} \\
 T_{\text{max}} & \quad \text{maximum temperature due to combustion} \\
 T_{\text{mix}} & \quad \text{mixing temperature of the premixed jet with the coflow} \\
 T_{\text{in}} & \quad \text{inflow temperature in the WSR} \\
 \Delta T_{\text{max}} & \quad \text{maximum temperature rise due to combustion} \\
 V & \quad \text{velocity magnitude} \\
 V_c & \quad \text{coflow velocity} \\
 v^r & \quad \text{rms velocity} \\
 V_a & \quad \text{axial velocity} \\
 X_m & \quad \text{mole fraction for species} \\
 X_{m,c} & \quad \text{mole fraction for species} \\
 Y_m & \quad \text{mass fraction for species} \\
 Y_{m,\text{max}} & \quad \text{maximum mass fraction for species} \\
\end{align*}

\begin{align*}
\tau_{\text{ig}} & \quad \text{ignition delay time} \\
\epsilon & \quad \text{turbulent dissipation rate} \\
\end{align*}

■ GREEK LETTERS

\begin{align*}
\tau_{\text{ig}} & \quad \text{ignition delay time} \\
\epsilon & \quad \text{turbulent dissipation rate} \\
\end{align*}

■ ABBREVIATIONS

\begin{align*}
\text{BB} & \quad \text{bluff-body} \\
\text{CC} & \quad \text{conventional combustion} \\
\text{JHC} & \quad \text{jet in a hot coflow} \\
\text{MC} & \quad \text{moderate or intense low-oxygen dilution (MILD) combustion} \\
\text{NBB} & \quad \text{no bluff-body} \\
\text{PDF} & \quad \text{probability density function} \\
\text{RANS} & \quad \text{Reynolds average Navier Stokes} \\
\text{rms} & \quad \text{root mean square} \\
\text{RZ} & \quad \text{Reynolds average Navier Stokes} \\
\text{WSR} & \quad \text{well-stirred reactor}
\end{align*}
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