Numerical Simulation of Turbulent Non-premixed Combustion Processes for Methane and Dimethyl Ether Binary Fuels

Maoqi Lu, Zhongguang Fu,* Xinkun Yuan, Jiayao Wu, and Syed Waqas Sabir

ABSTRACT: The C_{16} = 1.6 standard k − ε equation combined with the steady flamelet model was applied to a methane/dimethyl ether swirl combustion field, and the effects of the dimethyl ether (DME) blending ratio and operating pressure on the flame behavior, including species variation, reaction zone behavior, and flame entrainment, were investigated. The results demonstrated that selected models could better reproduce the trends of the experimental measurements. The downstream reaction zone achieved better calculation accuracy than the outer shear layer of the first recirculation zone. The addition of DME accelerated the accumulation process of H₂, O, H, and OH radicals. The intermediate radical CH₂O was rapidly developed by the influence of the H extraction rate under a constant fuel volume flow rate. The reaction zone dimensions were approximately linearly and positively correlated with the DME blending ratio, whereas flame entrainment expressed a lower DME concentration dependence in the high-DME mass-dominated system. The operating pressure significantly impacted the distribution of reactive radicals in the turbulent flame; meanwhile, the flame and reaction zone length showed nonlinear inverse behavior with pressure variation, while the thickness of the reaction zone was always linearly and negatively correlated with pressure. Moreover, the peak flame entrainment rate also experienced a nonlinear decline with pressure elevation; however, the peak positions were not sensitive to pressure fluctuation. Concurrently, the response surface functions for the reaction zone dimensions were established covering the range of 0–1 for the DME blending ratio and 1–5 atm operating pressure, which could provide assistance for combustion condition optimization and combustion chamber design.

1. INTRODUCTION

The vigorous development of renewable energy sources has placed greater demands on energy storage technologies, which has led to strong curiosity among researchers around the world about different types of energy storage methods. As of the end of December 2019, the cumulative installed capacity of energy storage projects (including physical-, electrochemical-, and heat-energy storage) commissioned in China was 32.4 GW, up by 3.6% year-on-year. Among them, the cumulative installed capacity of electrochemical energy storage projects increased by 59.4% year-on-year. Advances in electrochemical energy storage technology have given impetus to the development of new green fuels such as hydrogen, alcohols, and ethers.\(^1\)

Dimethyl ether (DME), as the simplest ether, has attracted much attention in recent years due to its excellent performance in terms of ignition,\(^2\) emission,\(^3\) and efficiency. Studies have shown the theoretical feasibility and potential of DME as a novel fuel alternative to traditional fuels such as liquefied petroleum gas (LPG), diesel, and liquefied natural gas (LNG).\(^4\)\(^5\)\(^6\)\(^7\)\(^8\) As an attractive clean alternative fuel, DME can be catalytically prepared on a large scale from waste renewable energy and biomass or fossil fuels\(^5\)\(^6\) while possessing transport safety and convenience similar to LPG, which makes DME promising for large-scale chemical energy storage. Thus, the comprehensive development and utilization of DME play an essential role in further improving China’s energy structure and ecological environment.

The basic combustion characteristics of pure DME and DME blends have been studied by numerous scholars,\(^7\)\(^8\) such as Hashemi et al.\(^7\) who used a flow reactor to study the pyrolysis and oxidation processes of DME and DME/CH₄. Mohammad and Juhany\(^7\) performed experimental measurements and PREMIX code predictions of laminar combustion velocities of DME/CH₄ and air mixtures. Detailed analysis of DME addition to boost the overall reaction activity and combustion rate was carried out with the assistance of the heat release rate, species profiles, and reaction pathway sensitivity. The superior atomization and ignition performance of the DME has enabled it to be extensively investigated in the compression ignition (CI) engine field as well.\(^9\)\(^10\)\(^11\)\(^12\)\(^13\) The homogeneous compression ignition (HCCI) for various proportions of DME/H₂ and DME/CH₄ blend fuels had

Received: November 6, 2020
Accepted: January 12, 2021
Published: March 3, 2021
been investigated through the numerical simulation by Wang et al.\textsuperscript{12} It was found that the ignition delay times of the two blends at 900 K demonstrated an inverse relation to the DME blending ratio. Furthermore, the ignition delay time of DME/CH\textsubscript{4} invariably exceeded that of DME/H\textsubscript{2} due to the stability of CH\textsubscript{4} molecular structure, whereas the delayed ignition time of the two blends presented opposite outcomes along with the decreasing amount of DME blend ratio at 1400 K. Park et al.\textsuperscript{13} comprehensively evaluated a biogas/DME-blended diesel combustion process for various performance indexes, such as the pressure pulsation, heat release rate, ignition delay, combustion emissions, etc. In the field of gas turbines, the possibility of a DME gas turbine development was previously confirmed by Gökalp et al.\textsuperscript{14} upon rationalization of the physicochemical characteristics. This was also supported by the experimental study by Lee et al.\textsuperscript{15,16} on the combustion characteristics of DME and CH\textsubscript{4} in a 60 kW gas turbine in which DME had equivalent NO\textsubscript{x} emissions, lower CO generation, and better combustion stability to CH\textsubscript{4}. Kang et al.\textsuperscript{27} reported large eddy simulation (LES) and Reynolds-averaged Navier–Stokes (RANS) simulation results in a variable geometric swirl number was an effective factor that affected the local extinction phenomena in the steady flamelet model (SFM). A dynamic second-order moment closure combustion model of LES was validated with a CH\textsubscript{4} swirl flame (SM1) by Luo et al.,\textsuperscript{17} and Rohani and Saqr\textsuperscript{30} numerically presented the combustion characteristics for adding H\textsubscript{2} and varying swirl numbers in the SM1 flame. A conditional moment closure (CMC) model was used by Roy and Sreedhar\textsuperscript{a} to evaluate the flame structure and global NO emissions of CH\textsubscript{4} and DME in an exhaust gas recirculation (EGR) environment. Even though the concept of alkane or hydrogen-hydrocarbon swirl flames has been fairly well established by different researchers, the DME or CH\textsubscript{4}/DME swirl flames, especially under high-pressure operating conditions, have not been fully elucidated.

Accordingly, the present work focuses on the effects of DME blending ratios and operating pressures on the combustion behavior of turbulent flames through numerical calculations based on the SM1 flame, which are developed to describe the variation laws applicable to the energy release process of DME combustion in gas turbines. In this paper, the chemical component distribution, reaction zone profile, and flame entrainment of the DME/CH\textsubscript{4} turbulent flame are emphasized. In addition, the reaction zone size under the combined interaction of the blending ratio and operating pressure is constructed as a reference for the design and operation of the DME/CH\textsubscript{4} gas turbine combustion system.

2. NUMERICAL MODELS

2.1. Turbulence Model. The standard $k - \varepsilon$ model is widely applied to resolve turbulent flow problems. Two transport equations in this model, $k$ and $\varepsilon$, are determined by eqs 1 and 2, respectively.

$$\frac{\partial}{\partial x_i}(\rho ku_i) = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \varepsilon$$ (1)

$$\frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) - C_{\mu} \frac{\varepsilon}{k} G_k - C_{\varepsilon} \rho \varepsilon^2$$ (2)

where $G_k$ and $G_b$ are the generation values of turbulence kinetic energy induced by the mean velocity gradients and buoyancy and $C_{\mu}$, $C_{\varepsilon}$, $\sigma_k$ and $\sigma_\varepsilon$ are the default model constants having values of 1.44, 1.92, 1.0, and 1.3, respectively.

Dally et al.\textsuperscript{32} pointed out that $C_{\mu}$ modified from a default value of 1.44 to 1.6 could not only obtain better prediction results in a cold flow field of a bluff body but also enhance the robustness of iterations. Meanwhile, Pope\textsuperscript{35} also proposed that the modified $k - \varepsilon$ model constant with $C_{\mu} = 1.60$ could accurately verify the experimental data of round jet combustion. Therefore, a non-standard model constant with $C_{\mu} = 1.60$ is utilized for the turbulence equation calculation in the current analysis.

2.2. Radiation Model. The radiative transfer equation (RTE)\textsuperscript{36} can be written as eq 3.

$$\frac{dI(r \rightarrow s)}{ds} = (a + 4 \sigma)I(r \rightarrow s) + \frac{\alpha}{4 \pi} \int_0^{2\pi} I(r \rightarrow s) \Phi(s \rightarrow r') \sin \theta ds'$$ (3)

where $a$ is the absorption coefficient and $\sigma$ is the scattering coefficient. The radiation intensity is determined by the absorption and scattering coefficients. RTE, which is a discrete ordinate model (DOM) for describing the spatial and angular
discretization combined with the weighted gray gas model (WSGGM), has a critical role in thermal simulation.

WSGGM\(^{(9)}\) is expressed for calculating the gas absorption coefficient as eq 4:

\[
a_{\nu,i} = \sum_{j=1}^{f} b_{\nu,i,j} T_i^{j-1}
\]  

(4)

Here, \(a_{\nu,i}\) is the emissivity weighting factor of the \(i\)th gray gas and \(b_{\nu,i,j}\) is the emissivity gas temperature polynomial coefficients.

DOM + WSGGM has been applied to combustion systems in several research studies.\(^{(37,38)}\) More recently, Kez et al.\(^{(39)}\) pointed out the adaptability of WSGGM in oxygen-fuel combustion systems at pressures up to 10 bar as a result of comprehensive evaluation of various radiation models. Bordbar et al.\(^{(40)}\) further refined the WSGGM model by introducing higher-degree temperature polynomials.

### 2.3. Combustion Model.

A steady flamelet model (SMF)\(^{(41,42)}\) is adopted for a turbulence-chemistry interaction. A detailed chemical kinetic mechanism is exploited to obtain one-dimensional counter flow flamelet ensembles to represent turbulent flames where data on the thermal state of each component is recorded in the PDF lookup table. The scalar governing equations\(^{(43,44)}\) can be stated as eqs 5 and 6

\[
\frac{\rho \chi}{\partial t} \frac{\partial^2 Y_i}{\partial T^2} + \frac{1}{\rho \chi} \sum_{j=1}^{f} H_j S_j + \frac{\rho \chi}{2 \rho \chi} \left( \frac{\partial \phi_j}{\partial T} \right) - \sum_{i} c_{p,i} \frac{\partial Y_i}{\partial T} \frac{\partial T}{\partial T} = 0
\]

(5)

\[
\frac{\rho \chi}{\partial t} \frac{\partial^2 Y_i}{\partial T^2} + \frac{1}{\rho \chi} \sum_{j=1}^{f} H_j S_j + \frac{\rho \chi}{2 \rho \chi} \left( \frac{\partial \phi_j}{\partial T} \right) - \sum_{i} c_{p,i} \frac{\partial Y_i}{\partial T} \frac{\partial T}{\partial T} = 0
\]

(6)

where \(Y_i\) and \(S_i\) are the \(i\)th species mass fraction and reaction rate, \(f\) is the mixture fraction, \(c_{p,i}\) and \(c_{p,f}\) are the \(i\)th species specific heat and average specific heat, \(H_i\) is the \(i\)th species specific enthalpy.

The scalar dissipation \(\chi\) is given by eq 7

\[
\chi(f) = \frac{a_i}{2 \pi} \left[ \frac{3}{\sqrt{\rho_0 / \rho + 1}} \right] \exp \left\{ -2 (\text{erfc}^{-1}(2f))^2 \right\}
\]

(7)

where \(a_i\) is the characteristic strain rate, \(\text{erfc}^{-1}\) is inverse complementary error function, and \(\rho_0\) is the density of the oxidizer stream. As shown in eq 8, the probability density function (PDF) is utilized for calculating the average scalar properties (mass fraction and temperature):

\[
\bar{\rho} = \int \rho(f, \chi_{at}) p(f, \chi_{at}) df \, d\chi_{at}
\]

(8)

Note that the statistical independence assumption is adapted between \(f\) and \(\chi_{at}\) which are calculated by the eq 9:

\[
p(f, \chi_{at}) = p(f) p(\chi_{at})
\]

(9)

The \(\beta\)-shape PDF is used for \(f\) and \(\chi\). The mean value of the scalar dissipation rate \(\chi_{at}\) is modeled as eq 10

\[
\chi_{at}^{\beta} = \frac{C_p k}{\chi_{at}}^{2}
\]

(10)

where \(C_p\) has a value of 2.0.

In addition, the average enthalpy\(^{(46)}\) of the energy equation is also calculated as shown in eq 11

\[
\frac{\partial}{\partial x_i} \left( \rho u_i T \right) = \frac{\partial}{\partial x_i} \left[ \left( \frac{\mu}{\sigma} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial T}{\partial x_i} \right] + S_{id}
\]

(11)

where \(\sigma\) and \(\sigma_t\) are the laminar Prandtl number and turbulent Prandtl number.

To generate the PDF table, GRI-mech 2.11 for the oxidation of CH\(_4\) (49 species, 277 reactions) was adopted; for the oxidation process of DME, a new detailed chemical kinetic mechanism (53 species and 290 reactions) was proposed by Zhao et al.\(^{(31,47,48)}\), which could better reproduce previously studied shock tube and laminar premixed flame experimental findings. Therefore, the chemical and thermodynamic databases are established by GRI-Mech 2.11 + Zhao’s DME sub-Mech (74 species and 331 reactions) to analyze DME/CH\(_4\) co-combustion.

### 3. COMPUTATIONAL DOMAIN AND CONDITIONS

The selected numerical model is reasonably validated for SM1 flames provided by Sydney Burner. Figure 1 displays the geometry of the entire burner, and a brief description of the burner dimensions is presented in the present work; for details, please refer to the research papers by Kalt et al.,25 Masri et al.,26 and Yasir.49 The burner has a 3.6 mm-diameter central fuel tube with a 50 mm-diameter bluff body surrounding it (\(d = 50\) mm). Swirling air is injected through a 5 mm wide annulus around the bluff body. The burner is centrally located in a 130 × 130 × 350 mm\(^3\) square wind tunnel, which provides co-flow air. To enable fuel and swirl air stream to be fully developed through the tube, these inlets are shifted 50 mm upstream; such an approach has been applied in Yang et al.’s and Kashir et al.’s previous work.27,29

The following parameters are required to determine the flame structure of SM1: the axial velocity of central fuel jet \(U_p\), the velocity of co-flow air provided by the wind tunnel \(U_\infty\), the axial velocity of annular swirl air \(U_a\) and the rotational velocity of annular swirl air \(W_a\). Detailed values\(^{(35,36)}\) for the SM1 case are shown in Table 1. The swirl strength is gauged by the swirl number, defined as the ratio of the tangential momentum to the axial momentum.\(^{51}\) However, the geometric swirl number \(S_g = W_a / U_a\) slightly larger than the actual swirl number) is chosen to evaluate the swirl strength in the current research. In addition, the fuel blending ratio \((V_{DME} / V_{fuel})\) conforms to the bulk flow rate ratio of DME to fuel where \(V_{fuel} = V_{CH_4} + V_{DME}\) and the operating pressure \((P / P_{atm})\) refers to the ratio of the combustion chamber pressure to the atmospheric pressure \(P_{atm} = 101,325\) Pa). Specific setting values are shown in Table 1 for the predicted conditions.
4. NUMERICAL METHODS AND GRID INDEPENDENCY

4.1. Numerical Methods. A steady-state solution of the 3D computational domain is realized by the pressure solver of the Ansys Fluent program. The SIMPLE algorithm is utilized for the pressure−velocity coupling. The PRESTO! scheme is adopted for pressure. Other convective equations are discretized in the second-order upwind scheme to improve the precision, and the second-order central scheme is managed to discretize the diffusion source. The residuals of all governing equations are lower than $10^{-6}$, which determines the convergence of calculation. Meanwhile, the temperature and velocity at the outlet plane are monitored. When the variations are within 1 K and 0.1 m/s, respectively, they are regarded as another criterion for solution convergence.

4.2. Grid Independence. The accuracy of numerical results depends on the grid quality. To obtain more accurate simulation results and a lower calculation cost, the grid independence should be tested. Hexahedral cells are applied to generate fluid domain. Coarse (1.63 million cells), medium (1.97 million cells), and fine (2.31 million cells) meshes are obtained by scaling up the number of nodes on blocks in the reaction zone. A comparison of the axial temperature distributions of the three grid cells is presented within the reaction zone in Figure 2. The axial temperature for all grids has a consistent trend over the range $1 < x/d < 5$, and with encryption of the grids, the temperature distribution comes closer. It is noted that the impact of the coarse grid on axial temperature in the calculation domain differs significantly. Nevertheless, the medium and fine meshes produce nearly identical outputs with a maximum temperature variation of less than 3.5%, which implies that the medium mesh has a sufficient spatial resolution for the current modeling approach and lower computation costs versus the fine mesh. Consequently, the following analysis and discussion sections are all performed on the medium mesh composed of 1.97 million cells.

5. RESULTS AND DISCUSSION

5.1. Numerical Model Validation. In this section, experimental data on the axial velocity, mean mixture fraction,

| SM1 | $V_{DME}/V_{CH4}$ | $U_j$ (m/s) | $U_s$ (m/s) | $W_s$ (m/s) | $U_e$ (m/s) | $P/P_{atm}$ | $T_{inlet}$ (K) |
|-----|-------------------|------------|------------|------------|------------|-------------|---------------|
| C0  | 0                 | 32.7       | 38.2       | 19.1       | 20         | 1           | 293           |
| C1–C10 | 0.1–1          | 32.7       | 38.2       | 19.1       | 20         | 1           | 293           |
| C11–C14 | 0.1            | 32.7       | 38.2       | 19.1       | 20         | 2–5         | 293           |
| C15–C18 | 0.2            | 32.7       | 38.2       | 19.1       | 20         | 2–5         | 293           |
| C19–C22 | 0.3            | 32.7       | 38.2       | 19.1       | 20         | 2–5         | 293           |
| C23–C26 | 0.4            | 32.7       | 38.2       | 19.1       | 20         | 2–5         | 293           |

Figure 2. Grid independency solutions.

Figure 3. Axial velocities profiles at various axial locations.

Figure 4. Mean mixture fraction profiles at various axial locations.

Figure 5. Temperature profiles at various axial locations.
model. Figure 3 indicates the comparison of axial velocity profiles at $x/d \in \{0.136, 0.4, 0.8, 1.4\}$. The predictions coincide well with the experimental data on the general tendency of evolution. The obvious negative axial velocities are captured at $x/d \in \{0.136, 0.4\}$, which corresponds to the first recirculation zone (FRZ) observed experimentally within $x < 43$ mm downstream of the bluff body. However, the predictions overestimate the magnitude of the axial velocity at $x/d = 0.8$, suggesting an underestimation in the FRZ size. Kalt et al. reported that a second recirculation zone (SRZ) with a radius of 10 mm was also found between 65 and 110 mm downstream of the bluff body. At $x/d = 1.4$, the axial velocity...
is between $-0.0281 \text{ m/s}$ and $-0.119 \text{ m/s}$ in $r/d \in (0, 0.04)$, indicating that the incipient part of SRZ can be captured, whereas the numerical values remain a little over-predicted and the dimensions of SRZ are understated. Kashir et al.\textsuperscript{29} suggested that the calculation errors in RANS could be attributed to an inherent shortcoming in simulation of shear flow. Meanwhile, a good prediction of the calculated values for the RANS model has been recorded in the region away from the shear flow, where the average relative error does not exceed 11\% compared with experimental measurements (10.853\%, 4.312\%, 3.408\%, and 10.586\% for $x/d = 0.136, 0.4, 0.8,$ and 1.4 in $0.55 < r/d < 0.8$ zones, respectively). Overall, despite slight deviations in the numerical accuracy of the numerical model, it still provides a good representation of the flow characteristics observed experimentally.

Figure 7. Radial molar fraction prediction profiles of $\text{H}_2 - \text{H}$ (a), $\text{OH} - \text{O}$ (b), $\text{CO} - \text{CH}_2\text{O}$ (c), and $\text{CH}_2 - \text{CH}_3$ (d) at axial positions corresponding to the half-reaction zone length.

Figure 8. Predicted variations of normalized reaction zone boundaries $L_{RN}^N$, length $L_{RN}^N$, and width $W_{RN}^N$ as a function of DME molar fraction in fuel jet.

Figure 9. Flame entrainment ratio ($R_{ent}$) vs normalized axial position ($x/d^*$) for different DME addition conditions.

Figure 10. Normalized flame entrainment rate ($m^*$) profiles at various non-dimensional flame axis locations, $x/L_R$.

The distribution of the mean mixture fraction and temperature at different axial positions are depicted in Figures 4 and 5. Unlike what was previously inferred by Kashir et al.,\textsuperscript{29} the center-line predictions of the mixture fraction in this research are underestimated at $x/d = 0.8$ and slightly overestimated at $x/d = 1.5$, inferring an early jet break-up. There is a degree of under-prediction of the mixture fraction in $x/d = 0.2, 0.1 < r/d < 1$. However, this discrepancy is considerably ameliorated in $x/d \in (0.8, 1.1, 1.5)$. Especially, the average relative error between the model calculations and the experimental values is 8.126\% in $x/d = 1.1, r/d < 0.2$. The above described differences in mixture fraction predictions are
apparently enhanced via the LES + flamellet model by Kempf et al.,\textsuperscript{53} as mentioned above, which may still be traced to an inherent flaw in the RANS simulation of strong shear flows. Since the temperature variation is dependent on mixture fraction profiles, the radial temperature plots display analogous discrepancies at the axial position, as shown in Figure 5. The inadequate prediction of the mean mixture fraction (refer to Figure 4) and the robust non-linear coupling between mixture fraction and temperature disclose the phenomenon that the temperature is overvalued in $x/d = 0.2$, $0.1 < r/d < 0.45$. The center-line temperature predictions at $x/d \in (0.8, 1.5)$ are also subjected to some extent of over- and underestimation, which was also mentioned in the LES study of Luo et al.\textsuperscript{28} Likewise, the predictions are closely matched to the measured values at $x/d \in (0.8, 1.5)$, $0.2 < r/d < 0.5$, away from the nozzle plane, where a relative error of less than 10\% between the model predictions and the experimental measurements is achieved. Specifically, the lowest average relative error is obtained with $x/d = 1.1$, which is just 3.941\%.

The above comparisons of the axial velocity, mean mixing fraction, and temperature indicate that the non-standard constant $k - \varepsilon$ model in combination with the steady flamellet model.

5.2. Effect of Adding DME on the Reaction Zone Evolution. The reaction zone, which is located between the unburned mixture and the flue gas/burnt gas, has a profound impact on the combustion process, and the progress of the reaction zone dominates the flame behavior. Concretely, (1) the location of the reaction zone defines the profile of the flame, and the flame length and width can be easily described through axial and radial dimensional measurements of the reaction zone. (2) The high-temperature section and radical pools’ formation are also placed in the reaction zone, which is the main source of critical phenomena such as fuel oxidation and pollutant generation processes. (3) Residence time of partially pivotal compositions is linked to the size of the reaction zone, which plays an essential role in the formation and destruction processes of these species. Given the significance of the reaction zone on the combustion performance, the reaction zone behaviors, including the inside radical levels as well as the reaction zone size are primarily discussed to facilitate comprehension on the effect of adding DME to the integrated characteristics of the swirl flame.

OH has been commonly cited in previous investigations to display the dimensions and location of the flame reaction zone either in experimental studies with PLIF visualization techniques or numerical simulations.\textsuperscript{54,55} For instance, the $x_{OH} = 0.0005$ contour was found to coincide well with the flame boundary as well as the blue luminous region in an experimental work of Katta et al.\textsuperscript{54} Simultaneously, Kang et al.\textsuperscript{55} confirmed the findings in experimental and numerical tests. The $x_{OH} = 0.0005$ iso-line is also adopted to represent
the reaction zone boundary in the present work, which is marked by an orange dashed line, as shown in Figure 6a, and the area between \(x_{\text{OH}} = 0.0005\) can be viewed as the reaction zone. DME has a higher calorific value per volume than CH\(_4\) due to a fixed fuel volume flow\(^1\) (i.e., \(\dot{U}_f = \text{constant}\)), which induces the peak temperature of the gas in the reaction zone to rise with DME addition, as depicted in Figure 6a. Furthermore, the content of pyrolysis products H\(_2\) and some highly reactive radicals such as OH, H, and O also increase gradually with the rising DME blending ratio, which can enhance the chemical rate and promote the combustion process in the reaction zone, as shown in Figure 6a.

![Figure 12. Predictions of normalized flame length (a), reaction zone length (b), and flame width (c) as a function of operating pressure.](image)

Table 2. Fitting Function Parameters for Normalized Reaction Zone Dimensions

| \(V_{\text{DME}}/V_{\text{CH4}}\) | \(A\) | \(B\) | \(P/P_{\text{atm}}\) | \(n\) | \(m\) |
|---|---|---|---|---|---|
| 0.1 | 4.389 | 0.0461 | 0.1 | 2.341 | -0.108 |
| 0.2 | 4.597 | 0.0418 | 0.2 | 2.480 | -0.108 |
| 0.3 | 4.908 | 0.0258 | 0.3 | 2.748 | -0.134 |
| 0.4 | 5.117 | 0.0227 | 0.4 | 2.886 | -0.130 |

Table 3. Response Surface Functions of Normalized Flame Inner and Outer Boundaries and Reaction Zone Lengths for the Combined Effect of the DME Blending Ratio and Operating Pressure

| \(Y\) | \(A\) | \(B\) | \(C\) | \(P/P_{\text{atm}}\) | \(n\) | \(R^2\) |
|---|---|---|---|---|---|---|
| \(X_{\text{inner position}}\) | 1.233 | 0.478 | 1.642 | 0.173 | 0.993 |
| \(L_f^N\) | 1.685 | 1.119 | 2.549 | 0.0241 | 0.987 |
| \(L_R^N\) | 1.304 | 1.059 | 1.719 | -0.125 | 0.978 |

Table 4. Comparison of Calculated and Simulated Values under Other Operating Conditions

| \(V_{\text{DME}}/V_{\text{CH4}}\) | \(P/P_{\text{atm}}\) | \(X_{\text{inner position}}\) | \(L_f^N\) | \(L_R^N\) | \(X_{\text{inner position}}\) | \(L_f^N\) | \(L_R^N\) |
|---|---|---|---|---|---|---|---|
| 0.6 | 3 | 2.897 | 5.640 | 2.743 | 2.878 | 5.572 | 2.677 |
| 0.7 | 4 | 3.096 | 5.819 | 2.723 | 3.100 | 5.805 | 2.698 |
| 0.8 | 5 | 3.258 | 5.977 | 2.719 | 3.300 | 6.033 | 2.737 |

DME has a higher calorific value per volume than CH\(_4\) due to a fixed fuel volume flow\(^1\) (i.e., \(\dot{U}_f = \text{constant}\)), which induces the peak temperature of the gas in the reaction zone to rise with DME addition, as depicted in Figure 6a. Furthermore, the content of pyrolysis products H\(_2\) and some highly reactive radicals such as OH, H, and O also increase gradually with the rising DME blending ratio, which can enhance the chemical rate and promote the combustion process in the reaction zone, as shown in Figure 6a–d. However, another pyrolysis product, CO\(_2\), has a similar variability in its content because of the rise of C/H in fuel jet. It is notable that the intermediate radical
content, especially the CH₂O radical increased drastically, which is attributed to the low energy of C–O in the DME molecule structure. The R1-dominated decomposition reaction allowed the accumulation of the CH₃ radical pool in response to the increasing DME content followed by the CH₃ and CH₃O H absorption processes (R2R2−R4R4), which is also facilitated by the increase in OH and O radical concentrations, thus boosting the CH₂O radical pool.

\[
\begin{align*}
\text{R1:} & \quad \text{CH}_3\text{OCH}_3 = \text{CH}_3 + \text{CH}_2\text{O} \\
\text{R2:} & \quad \text{CH}_3 + \text{O} = \text{CH}_2\text{O} + \text{H} \\
\text{R3:} & \quad \text{CH}_3\text{O} + \text{O} = \text{CH}_2\text{O} + \text{OH} \\
\end{align*}
\]

To quantitate the effect of DME blending ratios on the chemical components within the reaction zone, the radial distributions of some selected species (H₂, H, O, CO, CH₂O, CH₂ and CH₃) corresponding to the semi-reaction zone lengths are compared in Figure 7a–d. The pyrolysis products such as H₂ and CO are expressed as monotonic curves in these graphs, i.e., peaking near the flame axis, which are also shown in Figure 6d; the active and intermediate radicals show non-monotonic traces, peaking at the stoichiometric profiles of the diffusion flame. Moreover, when the DME concentration goes to quantitate the effect of DME blending ratios on the chemical components within the reaction zone, the radial distributions of some selected species (H₂, H, O, CO, CH₂O, CH₂ and CH₃) corresponding to the semi-reaction zone lengths are compared in Figure 7a–d. The pyrolysis products such as H₂ and CO are expressed as monotonic curves in these graphs, i.e., peaking near the flame axis, which are also shown in Figure 6d; the active and intermediate radicals show non-monotonic traces, peaking at the stoichiometric profiles of the diffusion flame. Moreover, when the DME concentration goes.
up, the peak of the active radicals H, OH, and O also elevate and the peak position moves toward the flame axis’s side, while the intermediate radicals CH₂ and CH₃ exhibit the opposite tendency on the radial distribution that corresponds to the half-reaction zone length. This phenomenon can be explained by the fact that the distributions of the methylene profiles at various DME blending ratios are generally identical (slight variations may exist), i.e., 1.5 < x/d < 2.0 in the axial region and 0.2 < r/d < 0.4 in the radial region with high concentrations. However, the half-reaction zone positions progressively move away from the nozzle plane, which triggers a gradual decrease in the peak methyl (similar to this is methylene and formaldehyde) concentration because of the deviation from the high content intervals. It is notable that the peak concentration of the CH₂O radical tends to progressively move away from the nozzle plane, which triggers the critical conditions in this study in which the CH₄ mass ratio dominates in case 2 and the DME mass ratio dominates in case 3. For cases 0–2, the oxidation of CH₄ plays a major role in the overall combustion process; however, the DME oxidation gradually becomes the dominant process for the combustion reaction with the further enhancement of the blending ratio (cases 3–10). A similar report was provided in an experimental investigation of the DME/CH₄ high temperature ignition delay times by Burke et al. Burke et al.⁶ pointed out that a small amount of DME was added to induce the formation of free radical pools at lower temperatures, which enhanced the combustion rate of CH₄. Concretely, 80CH₄/20DME reduced the ignition delay time by more than five times compared to pure CH₄, while the DME content further expanded to 40%, which only altered the ignition delay time from 152 to 108 μs. Overall, the normalized reaction zone length L_R could still be expressed by a fitting line with R² > 0.98 in the range of variation from pure CH₄ to pure DME, as shown in eq 15. Moreover, straight fitting functions of L^N_R and W^N_f versus DME blend ratios are also obtained, as written in eqs 16 and 17.

$\frac{L^N_R}{L^N_f} = \frac{L^N_R}{L^N_f} = \frac{W^N_f}{W^N_f}$

The dimensions of the reaction zone for the non-premixed turbulent flames solved by the SFM model are governed by molecular diffusion as well as the swirl-mixing interaction. The geometric swirl number fixed at 0.5, this size is more dependent on the fuel properties. Specifically, (1) when the fuel is converted from pure methane to pure dimethyl ether, on the one hand, the fuel density and Reₜ rise, which elevates the flame turbulence intensity; on the other hand, enlargement of the fuel-air momentum ratio, MR (MR = \( \rho f U^f / \rho_a U_a \)), consequently improves the fuel jet penetration. (2) The molecular weight of DME is heavier than CH₄ which also decreases the molecular diffusion coefficient of mixed fuel compared with pure methane; thus, the axial and radial mixing rate of fuel-air will be limited. (3) With the addition of DME, the stoichiometric mixture fraction gradually shifts from 0.055 to 0.1, which implies that an axial position corresponding to the stoichiometric combustion would shift toward the exit plane. It is indicated that the above factors are also confirmed by the plotted curves in Figure 8 in which the axial and radial expansion of the reaction zone is affected by a higher DME blending ratio.

It is interesting to note that L_R has a slightly variable growth rate in the range of 0–20 and 20–100 vol % for DME addition, which is slightly larger for the former than the latter. It can be inferred that the two fuel mass ratios are comparable for a DME/CH₄ mixture at a constant volume flow rate when the blending ratio is 0.258. Thus, case 2 and case 3 represent the critical conditions in this study in which the CH₄ mass ratio dominates in case 2 and the DME mass ratio dominates in case 3. For cases 0–2, the oxidation of CH₄ plays a major role in the overall combustion process; however, the DME oxidation gradually becomes the dominant process for the combustion reaction with the further enhancement of the blending ratio (cases 3–10). A similar report was provided in an experimental investigation of the DME/CH₄ high temperature ignition delay times by Burke et al. Burke et al.⁶ pointed out that a small amount of DME was added to induce the formation of free radical pools at lower temperatures, which enhanced the combustion rate of CH₄. Concretely, 80CH₄/20DME reduced the ignition delay time by more than five times compared to pure CH₄, while the DME content further expanded to 40%, which only altered the ignition delay time from 152 to 108 μs. Overall, the normalized reaction zone length L_R could still be expressed by a fitting line with R² > 0.98 in the range of variation from pure CH₄ to pure DME, as shown in eq 15. Moreover, straight fitting functions of L^N_R and W^N_f versus DME blend ratios are also obtained, as written in eqs 16 and 17.

\[ L^N_R = 1.382V_{DME}/V_{CH_4} + 2.231 \quad (R^2 = 0.98968) \]
\[ L^N_f = 2.029V_{DME}/V_{CH_4} + 4.195 \quad (R^2 = 0.97464) \]
\[ W^N_f = 0.0907V_{DME}/V_{CH_4} + 0.382 \quad (R^2 = 0.99052) \]

### 5.3. Effect of the DME Blending Ratio on Flame Entrainment

Entrainment is the inward radial flux of the ambient fluid drawn into the jet, and its rate controls the mixing degree between the jet and ambient fluid, which impacts the flame residence time and global chemical reaction process.⁶ Thus, the analysis of turbulent flame entrainment supports the design and optimization of the combustion chamber procedure. Many previous publications had extensively discussed diverse parameters affecting flame entrainment rates,⁷⁻⁸ including the reacting or non-reacting jet, heat release, buoyancy, co-flow velocity, etc. However, the relationship between the flame entrainment rate and fuel composition was rarely discussed. Kang et al.⁹ demonstrated that the
different types and ratios of fuel blending caused a drastic change in the density of the mixed fuel jet and consequently in the flow field, which affected the flame entrainment in the diffusion flame of H₂/DME. Thus, flame entrainment ratio characterization is particularly critical for mixed fuel combustion. Referring to the results published by Han and Mungal and Kang et al., the present study defines the flame entrainment ratio ($R_{ent}$) as the mass flow rate flowing across the radial section of the reaction zone to the initial mass flow rate of the fuel jet, as depicted in eq 18.

$$R_{ent} = \int_{0}^{\mu/\rho} 2\pi
$$

where $\rho_r$ represents the fuel density and $\rho$ is the fuel mixture density. Ricous and Spalding defined $C_e$ as the entrainment coefficient. $d^a$ is the momentum diameter of the fuel injection, as shown in eq 19.

$$d^a = \left( \frac{\rho_f}{\rho_{\infty}} \right)^{0.5}$$

where $\rho_{\infty}$ is the air density.

The distributions of $R_{ent}$ at normalized axial positions ($x/d^a$) are plotted in Figure 9. The trend of $R_{ent}$ variations at different DME blending ratios is similar, showing a double-peak behavior, which corresponds to the temperature distribution of the first recirculation zone and the reaction zone in Figure 6a. $R_{ent}$ is almost linear at the initial stage of the reaction zone with $20 < x/d^a < 33$ for each case, and the entrainment coefficient $C_e$ varies between 0.41 and 0.5 for each flame. It is noted that the $R_{ent}$ curves tend to coincide when the DME blending ratio is more than 30%, showing a smaller amplitude of $C_e$ fluctuation and converging to 0.43–0.46, which demonstrates the minor dependence of flame entrainment on the DME blending ratio in the DME mass-dominated systems. The $R_{ent}$ reaches its maximum value at the position of $x/d^a = 39$ for pure methane, and the position of $x/d^a$ corresponding to the $R_{ent}$ maximum value gradually moves upstream of the nozzle to $x/d^a = 30$ with the increment in the DME blending ratio. Meanwhile, the $R_{ent}$ peak exhibits a non-linear behavior. The reason for this is that the stoichiometric air/fuel mass ratio presents a negative exponential power function variation in the $V_{DME}/V_{fuel} = 0$ to 1 interval, as shown in the embedded graph in Figure 9. In addition, with the normalized axial position gradually shifting toward the exit plane, the chain termination reaction progresses and the reaction zone converges to the flame axis, which leads to a parabolic decline of the $R_{ent}$ curves.

Considering the $R_{ent}$ peak affected by the stoichiometric air/fuel mass ratio ($S$). Yang and Blasiak proposed that the flame entrainment ratio is normalized using the stoichiometric air/fuel mass ratio, as shown in eq 20.

$$m^* = \frac{R_{ent}}{S + 1}$$

The normalized flame entrainment ratio ($m^*$) versus the non-dimensional flame axis position ($x/L_R$) is plotted in Figure 10. It is revealed that $m^*$ lies approximately on a single curve, i.e., the normalized entrainment rates remain highly similar for all conditions, especially for the DME mass-dominant systems where all attain a maximum value around $x/L_R = 0.4$. The fitting curve of $m^*$ in respect to $x/L_R$ is given in eq 21, which can provide certain assistance for the combustion chamber design and optimization.

$$m^* = -0.00253 + 3.527 \left( \frac{x}{L_R} \right) - 66.75x \left( \frac{x}{L_R} \right)^2 + 522.04x \left( \frac{x}{L_R} \right)^3 - 1586.98x \left( \frac{x}{L_R} \right)^4 + 2289.06x \left( \frac{x}{L_R} \right)^5 - 1591.95x \left( \frac{x}{L_R} \right)^6 + 431.14x \left( \frac{x}{L_R} \right)^7$$

(21)

5.4. Effect of the Operating Pressure on the Reaction Zone Behavior. The species profiles at 1–5 atm for $V_{DME}/V_{fuel} = 0.1$ and 0.3 are illustrated in Figure 11a,b. Activated radicals are highly sensitive to pressure changes in all conditions, whether CH₄ mass-dominated or DME mass-dominated, especially H and O radicals, whose peak levels decline rapidly with rising pressure. It is in accordance with the observations of Zhou et al., which could be explained by the fact that the collision of molecules with free radicals was more frequent at the elevated pressure, which allowed for the enhancement of the chemical reactivity of R5–R7. However, the three-body reactions induced by R8–R10 also played an essential role with increasing pressure by allowing reduction in the active radical pool and generation of some relatively inactive radicals such as HO₂, meaning that a hindrance was exerted on the whole reaction process. The reduced peak CH₃ radical content can be attributed to an altered kinetic mechanism at high pressure that inhibits the dissociation reaction of the fuel in a sense that R111 is driven by pressure and competes with other DME reactions.

$$H + O_2 = O + OH$$

(R5)

$$CO + OH = CO_2 + H$$

(R6)

$$CH_3 + O = CH_2O + H$$

(R7)

$$H + OH(+)M \leftrightarrow H_2O(+)M$$

(R8)

$$H + O_2(+)M \leftrightarrow HO_2(+)M$$

(R9)

$$CH_3 + H(+)M \leftrightarrow CH_2(+)H$$

(R10)

The flame and reaction zone lengths indicated by $x_{OH} = 0.0005$ are producing non-linear evolution/progress/growth depending on the pressure as illustrated in Figure 12a,b. The flame length increment gradually diminishes with pressure elevation when transitioning from CH₄ mass-dominated to DME mass-dominated conditions, which implies that the sensitivity of flame length to pressure progressively drops as the DME blending ratio increases. Nevertheless, the reaction zone length exhibits an opposite variation trend regardless of whether CH₄ or DME mass-dominated, revealing that the inner flame boundary position is significantly impacted by pressure. It could be explained that the process from pyrolysis to oxidation of the fuel may be decelerated with the reduced reactive radical content and inhibited dissociation reaction, which creates the phenomenon of axial stretching at inner flame boundaries. It should be mentioned that the reaction zone thickness for all test conditions thins linearly. Tu et al. reported that high operating pressure caused the reaction zone...
to move from the oxidant side to the fuel side. The chemical acceleration behavior of HCO + O → HO2 + CO, CH2 + O2 → 2H + CO2, and CH3 + O2 → OH + H + CO under high-pressure conditions enhanced the overall rate of O2 consumption. Both were directly related to reaction zone thinning. Furthermore, the reaction zone dimensions are fitted as a function of operating pressure, as presented in Table 2. The $L_d^N$ and $L_R^N$ power exponents ($n, m$) appear to drop at $V_{DME}/V_{fuel} = 0.2 \rightarrow 0.3$, which also represents the pressure-dependent distinction between the CH4 mass-dominant and DME mass-dominant system responses.

The DME mixing ratio and operating pressure both have a great impact on the structure of the reaction zone. To construct the variation of the reaction zone size under the joint effect of them, a multivariate nonlinear fitting scheme is adopted to establish the response surface function, and the formula is presented as eq 22 where the unknown parameter values are listed in Table 3. The fitting curves ($R^2$) are greater than 0.97 for all reaction zone sizes, indicating the feasibility of the fitting scheme. Moreover, a comparison between the simulated and calculated values of high-pressure combustion at other blending ratios is presented in Table 4, which demonstrates that the fitting function could be extended to a larger adaptation range.

\[ Y = A \times (B \times V_{DME}/V_{fuel} + C) \times (P/P_{atm})^n \]  
\[ \text{eq } 22 \]

Thus, the response surface images of the inner and outer flame boundaries and the reaction zone length with respect to the above factors are established for the $V_{DME}/V_{fuel}$ = 0–1 and $P/P_{atm}$ = 1–5, as shown in Figure 13a–c. This provides assistance in dealing with optimization of combustion conditions and combustion chamber retrofitting for engineering applications.

5.5. Effect of Operating Pressure on the Flame Entrainment Rate. Figure 14 displays the $R_{ent}$ distribution of each normalized axial positions ($x/d_*$) for $V_{DME}/V_{fuel} = 0.1$ and $P/P_{atm} = 1–5$. The $R_{ent}$ peak as well as the amplitude of the peak variation decreases with pressure increments, whereas there is only a slight movement to the right for the $R_{ent}$ position, which demonstrates that the $R_{ent}$ peak position is lower than the peak magnitude. Meanwhile, the reduced radial inward flux of ambient fluids into the reaction zone would remain less sensitive under higher-pressure operating conditions.

The relationship between the normalized flame entrainment rate ($m^*$) and the dimensionless flame axis position ($x/L_R$) is illustrated in Figure 15. The normalized flame entrainment rate distribution trend is consistent for different pressures. Unfortunately, $m^*$ is unable to obtain a uniform fit curve, which is mainly caused by the fact that the $(S + 1)$ values for the test conditions are the same, and thus the data distribution of $m^* = x/L_R$ is highly similar to that of $R_{ent} = x/d_*$. It can also be observed that, similar to $R_{ent}$, $m^*$ reaches a peak at $x/L_R = 0.42–0.48$ and then declines in a parabolic pattern. The $m^*$–$x/L_R$ functional dependence for the test conditions could be expressed by eq 23, as shown in Table 5. Correlation coefficients exceeding 0.97 also suggest a favorable quintic polynomial correlation for $m^* = x/L_R$.

\[ m^* = A_0 + A_1 \left( \frac{x}{L_R} \right) + A_2 \left( \frac{x}{L_R} \right)^2 + A_3 \left( \frac{x}{L_R} \right)^3 + A_4 \left( \frac{x}{L_R} \right)^4 \]
\[ + A_5 \left( \frac{x}{L_R} \right)^5 \]  
\[ \text{eq } 23 \]

6. CONCLUSIONS

For investigation of the evolution/progress of the energy release process of CH4/DME in gas turbines, the effects of the DME blending ratio and operating pressure on the combustion process of the CH4/DME binary fuel were numerically investigated in this paper. The specific conclusions are as follows:

(1) The non-standard constant $k = \varepsilon^* model in combination with the SFM model was numerically validated for the methane turbulent flame, and the findings indicated that there was some under-prediction in the region of the strong shear flow with $x/d < 0.8$; however, the prediction accuracy was significantly improved in the downstream reaction region with $x/d > 1.1$. Meanwhile, the trends of the radial distributions of the flow field, temperature field, and mixing fraction at different axial positions were also well predicted.

(2) When the fuel stream transitioned from pure methane to pure DME at atmospheric pressure, the peak molar fraction of H2 and highly reactive radicals O, H, and OH increased by 51% to 173%, while the peak CH2O increased by 72.8 times, indicating the high sensitivity of DME addition to CH2O content variations. The phenomenon of axial stretch and radial expansion for the reaction zone size maintained a highly linear dependence. The difference between the CH4 mass-dominant chemical reaction and the DME mass-dominant chemical reaction led to a slightly higher growth rate of 0.545 for the former reaction zone length than the latter.

(3) The flame entrainment rate was also affected by the fuel mass ratio of different components. When the DME mass ratio was higher than 25.8%, the entrainment rate curves had a coincident trend and the $C_i$ fluctuation narrowed between 0.43 and 0.46, which revealed that the dependence of flame entrainment on DME blending in the DME mass-dominant system was minor.

(4) Whether CH4 or DME mass-dominant, the operating pressure was doubled and the peak content of highly reactive CH4/DME binary fuel were numerically validated for the methane turbulent flame, and the findings indicated that there was some under-prediction in the region of the strong shear flow with $x/d < 0.8$; however, the prediction accuracy was significantly improved in the downstream reaction region with $x/d > 1.1$. Meanwhile, the trends of the radial distributions of the flow field, temperature field, and mixing fraction at different axial positions were also well predicted.

(5) The response surface function for the reaction zone dimensions under the combined effect of the DME blending ratio and pressure was established, which could accurately describe the reaction zone dimensions in the range of $V_{DME}/V_{CH4} = 0–1$ and $P/P_{atm} = 1–5$. This could provide some assistance for combustion-condition optimization and combustion chamber design.
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