Large eddy simulation of a supersonic lifted hydrogen flame: Impacts of Lewis, turbulent Schmidt and Prandtl numbers

Ruixuan Zhu (朱芮萱) ; Zhiwei Huang (黄志伟) ; Chao Xu (徐超) ; Xiaohang Fang (方晓航) ; Huangwei Zhang (张黄伟) ; Martin Davy

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Large eddy simulation of a supersonic lifted hydrogen flame: Impacts of Lewis, turbulent Schmidt and Prandtl numbers

Ruixuan Zhu, Zhiwei Huang, Chao Xu, Xiaohang Fang, Huangwei Zhang, and Martin Davy

AFFILIATIONS
1Department of Engineering Science, University of Oxford, Oxford OX1 3PJ, United Kingdom
2School of Aeronautics and Astronautics, Shanghai Jiao Tong University, Shanghai 200240, China
3Transportation and Power Systems Division, Argonne National Laboratory, Lemont, Illinois 60439, USA
4Department of Mechanical & Manufacturing Engineering, Schulich School of Engineering, University of Calgary, Calgary, Alberta T2L 1Y6, Canada
5Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117576, Singapore

ABSTRACT
Parametric large eddy simulations (LES) of a supersonic lifted hydrogen flame are reported. The emphases are on two aspects: impacts of (1) Lewis number ($Le_i$, of the $i$th species) and (2) turbulent Schmidt and Prandtl numbers ($Sc_i$ and $Pr_i$) on supersonic turbulent flame and flow structures. Five cases are considered: species-specific $Le_i$, $Sc_i = Pr_i = 1.0$ ($C_0$); unity $Le_i$, $Sc_i = Pr_i = 1.0$ ($C_1$); species-specific $Le_i$, $Sc_i = 0.5$, $Pr_i = 1.0$ ($C_2$); species-specific $Le_i$, $Sc_i = 1.0$, $Pr_i = 0.5$ ($C_3$); and species-specific $Le_i$, $Sc_i = Pr_i = 0.5$ ($C_4$). Numerical results of instantaneous and/or time-averaged species mole fractions, mixture fraction, heat release rate, flame base location, and mixed modes of premixed and diffusion combustion are compared between cases $C_0$ and $C_1$. Differences in auto-ignition locations and strengths and flame structures and stabilization specify the impacts of Lewis number. They are triggered by different predictions of species mass and thermal diffusions at fuel-coflow and/or coflow-ambient air mixing layers. These differences are rationalized by a scale analysis of mass/thermal diffusion and convection for case $C_0$, which suggests the relatively low but non-negligible former against the latter. Cases $C_0$ and $C_2$, $C_3$, $C_4$ barely see differences in terms of instantaneous and/or time-averaged temperature, velocity, and mixed combustion modes except for further downstream areas where combustion occurs. Both $Sc_i$ and $Pr_i$ impose less significant influences than Lewis number, as sub-grid scale mass/thermal diffusion is subordinate to its resolved counterpart according to their scale analysis for case $C_4$.

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I. INTRODUCTION
In recent years, the rapid, ongoing development of hypersonic propulsion systems, such as scramjet engines, has sparked research interest in supersonic turbulent flames. Supersonic turbulent flames typically encounter strong shock-wave compression resulting in high-enthalpy gas environments. Experimental studies under such high-enthalpy conditions are challenging using ground-based combustion facilities.1 Huge capital investments are required to tackle numerous practical difficulties in facility setup.2 To reduce the cost, computational fluid dynamics (CFD) can play a significantly important role during the design stage by providing fundamental understandings of supersonic turbulent flames, particularly, with the rapid advances in high-performance computing, large eddy simulation (LES) is able to provide detailed spatiotemporal information of the structure and dynamics of the flow and flame in a computationally affordable way.3 Improving the numerical accuracy of LES, e.g., in the modeling of supersonic turbulent flames, is one of the current interest of industry and government organizations.4

The experiment of a supersonic lifted hydrogen flame by Cheng et al.,5 termed as Cheng supersonic flame hereafter, provides a reliable...
set of data for flow dynamics, mixing, temperature, and species concentrations. This dataset has been widely used as a reference in exploring the accuracy of LES studies on supersonic turbulent flames. Table I summarizes past LES studies on Cheng supersonic flame. Most of these investigations have focused on improving the sub-grid scale (SGS) turbulent combustion model for capturing unresolved turbulence-chemistry interactions, instead of other unclosed terms in the filtered transport equations of LES, including mass and thermal diffusion fluxes, $J_i$ and $J_h$. These two terms are typically approximated as

$$J_i = -\bar{\rho}(D_i + D_{sgs}) \nabla \bar{Y}_i,$$  
(1)

$$J_h = -\bar{\rho}(z + x_{sgs}) \nabla \bar{h}_s,$$  
(2)

where $\bar{\rho}$ is the filtered density, $D_i$ and $\bar{Y}_i$ refer to the mass diffusivity and fraction of the $i$th species, $z$ is the thermal diffusivity, and $\bar{h}_s$ is the sensible enthalpy. $D_{sgs}$ and $x_{sgs}$ are the SGS mass and thermal diffusivities, which read

$$D_{sgs} = \frac{\mu_{sgs}}{\rho S_{Cl}},$$  
(3)

$$x_{sgs} = \frac{\mu_{sgs}}{\rho P_{rt}},$$  
(4)

where $\mu_{sgs}$ is the SGS dynamic viscosity, and $S_{Cl}$ and $P_{rt}$ are turbulent Schmidt and Prandtl numbers, respectively.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Computational domain</th>
<th>Mesh resolution</th>
<th>Chemistry</th>
<th>Combustion model</th>
<th>Main focus</th>
</tr>
</thead>
<tbody>
<tr>
<td>Daupertain et al.</td>
<td>Hemisphere, $70D_f$ in radius</td>
<td>$0.81 \times 10^6$ cells, 25–30 nodes in the diameter of both fuel an oxidizer jets</td>
<td>4 species, 2 reactions</td>
<td>QLC</td>
<td>Application of LES</td>
</tr>
<tr>
<td>Wang et al.</td>
<td>Cylindrical, $43D_f$ in length and $30D_f$ in radius</td>
<td>Main mesh divided into 13 blocks, each of $31 \times 31 \times 161$ nodes</td>
<td>9 species, 19 reactions</td>
<td>PDF</td>
<td>Development of a hybrid LES/assumed sub-grid PDF model</td>
</tr>
<tr>
<td>Boivin et al.</td>
<td>Hemisphere, $10,000D_f$ in radius</td>
<td>$6.6 \times 10^5$ cells, minimum volume of $8 \times 10^{-12} \text{m}^3$</td>
<td>6 species, 3 reactions</td>
<td>QLC</td>
<td>Validation of a reduced chemistry and analysis of flame stabilization</td>
</tr>
<tr>
<td>Moule et al.</td>
<td>Cylindrical, $60D_f$ in length and $20D_f$ in radius</td>
<td>$31 \times 10^6$ cells, minimum size of $0.1–0.2 \text{mm}$</td>
<td>9 species, 19 reactions</td>
<td>Unsteady PaSR</td>
<td>Capability of unsteady PaSR closure and analysis of flame structure and associated stabilization zone</td>
</tr>
<tr>
<td>Ribert et al.</td>
<td>Cylindrical, $70D_f$ in length</td>
<td>Three meshes of 2, 30, and $113 \times 10^6$ cells</td>
<td>6 species, 3 reactions</td>
<td>QLC</td>
<td>Effect of shear layer prediction on flame stabilization position</td>
</tr>
<tr>
<td>Bouheraoua et al.</td>
<td>Cylindrical, $70D_f$ in length and $30D_f$ in radius</td>
<td>Three meshes of 4, 32, and $268 \times 10^6$ cells, minimum sizes of $0.24, 0.12$ and $0.06 \text{mm}$</td>
<td>6 species, 3 reactions</td>
<td>QLC</td>
<td>Mechanism driving flame stabilization</td>
</tr>
<tr>
<td>Paixão de Almeida et al.</td>
<td>Cylindrical, $70D_f$ in length and $30D_f$ in radius</td>
<td>Two meshes of 0.2 and $2 \times 10^6$ cells</td>
<td>9 species, 19 reactions</td>
<td>PDF</td>
<td>Performance of a joint scalar-enthalpy PDF model and a joint velocity-scalar-energy PDF model</td>
</tr>
<tr>
<td>Chen et al.</td>
<td>Cylindrical, $240 \text{mm}$ in length and $50 \text{mm}$ in radius</td>
<td>Three meshes of 10, 20, and $30 \times 10^6$ cells</td>
<td>11 species, 23 reactions</td>
<td>PaSR</td>
<td>Influence of compressibility on reaction rates and sub-grid stress</td>
</tr>
<tr>
<td>Zhang et al.</td>
<td>Cylindrical, $100D_f$ in length and $30D_f$ in radius</td>
<td>$26 \times 10^6$ cells, minimum size of 0.16 mm</td>
<td>9 species, 19 reactions</td>
<td>QLC</td>
<td>Accuracy of LES with a high-fidelity numerical solver</td>
</tr>
<tr>
<td>Zhao et al.</td>
<td>Cylindrical, $100D_f$ in length and $30D_f$ in radius</td>
<td>$26 \times 10^6$ cells, minimum size of 0.16 mm</td>
<td>9 species, 19 reactions</td>
<td>PSR</td>
<td>Assessment of LES-PSR model including viscous heating and compressibility effects</td>
</tr>
<tr>
<td>Huang et al.</td>
<td>Cylindrical, $70D_f$ in length and $30D_f$ in radius</td>
<td>$12.2 \times 10^6$ cells, minimum size of $0.05/0.12 \text{mm}$ in $x$-directions</td>
<td>9 species, 19 reactions</td>
<td>MMC</td>
<td>Examination of LES-MMC model including pressure work and viscous heating</td>
</tr>
</tbody>
</table>
Various approaches have been used for calculating the mass and thermal diffusivities on both filtered scale ($D_i$ and $\chi$) and SGS ($D_{sgs}$ and $\chi_{sgs}$) in the LES studies on Cheng supersonic flame (Table I). For example, Chen et al.17 used the mixture-averaged diffusion model to calculate $D_i$ and $\chi$, together with the molecular dynamic viscosity, $\mu$. The mixture-averaged diffusion model assumes that $D_i$ is computed from binary diffusivities between the $i$th species and the rest of species in the mixture and that $\chi$ and $\mu$ of a mixture are evaluated using an averaging formula combining the corresponding values from all individual pure species. In Refs. 2, 3, and 13, $\mu$ is predicted using Sutherland’s law, $\chi$ is renewed from the thermal conductivity, $\chi$ is calculated using the Eucken approximation with $\mu$ involved, and $D_i$ is computed via a computationally more efficient assumption of unity Lewis number. The Lewis number of the $i$th species, $Le_i$ is defined as the ratio of $\chi$ and $D_i$. The mass diffusivities of all species are equal to $\chi$ in the unity-Lewis number assumption. For the computations of $D_{sgs}$ and $\chi_{sgs}$, a wide span of $Sc_i$ and $Prt_i$ values has been used in the literature, e.g., unity in Refs. 10, 11, and 13 and sub-unity in Refs. 2 and 3. The optimal choice of Lewis, turbulent Schmidt, and Prandtl numbers that balances numerical accuracy and computational efficiency, hence, has not been well understood for the LES of the Cheng supersonic flame, and more broadly, any supersonic turbulent flame.

A particular modeling challenge for the Cheng supersonic flame is associated with the light species H$_2$ and H. The mass diffusivities of H$_2$ and H are much higher than those of relatively heavy species, e.g., O$_2$ and H$_2$O$_2$, referring to the differential diffusion effect. The mass diffusivities of H$_2$ and H are also higher than the thermal diffusivity, resulting in the preferential diffusion effect. The Lewis numbers of individual species in a mixture quantitatively characterize differential and preferential diffusion effects. As turbulent hydrogen flames involve profound differential and preferential diffusion effects, extensive numerical studies have been focused on the impacts of Lewis number. For example, Lee et al.18 performed direct numerical simulation (DNS) in highly turbulent lean hydrogen–air flames. The turbulent burning velocity, $U_T$, was observed to significantly increase with the incorporation of species-specific Lewis numbers but be minorly influenced by the preferential diffusion effect. In the LES, the mass diffusivities on the filtered scale can become comparable to the SGS turbulent viscosity, i.e., $\mu_{sgs}/\rho$, especially in regions close to the flame front when the LES computational grid is fine.19 The use of non-equal Lewis numbers for different species has also been found critical in the modeling of localized scalar mixing, auto-ignition, extinction, and re-ignition.20–23 Previous LES studies have unveiled the necessity of accounting for the differential diffusion effect in the modeling of a H$_2$/N$_2$ lifted turbulent flame21 and a jet-in-hot-coflow CH$_4$/H$_2$ flame.24 The LES study of a lean-premixed H$_2$/air low-swirl lifted flame showed improved predictions on velocities and species distributions near the flame front by considering preferential diffusion effects.25 While these LES studies mainly focused on subsonic turbulent hydrogen flames, this work aims to assess the importance of incorporating differential and preferential effects, i.e., the impacts of Lewis number, in depicting supersonic turbulent flame and flow structures with LES. The LES results of Cheng supersonic flame using the mixture-averaged diffusion model are compared to those using the unity-Lewis number assumption. The mixture-averaged diffusion model employs both differential and preferential diffusion effects via species-specific Lewis numbers. It is relatively less computationally time-consuming but has been proven to show comparable accuracy against the most precise and sophisticated multi-component diffusion model in the modeling of both turbulent and laminar flames.4,26

The impacts of Lewis number on the LES of Cheng supersonic flame are embodied in the calculations of mass and thermal diffusivities on the filtered scale. This work also aims to optimize the LES of Cheng supersonic flame regarding the calculations of SGS mass and thermal diffusivities, i.e., $D_{sgs}$ and $\chi_{sgs}$. Based on Eqs. (3) and (4), $D_{sgs}$ and $\chi_{sgs}$ are determined by the turbulent Schmidt and Prandtl numbers, i.e., $Sc_i$ and $Prt_i$, respectively, with the SGS dynamic viscosity, i.e., $\mu_{sgs}$ involved. The values of $Sc_i$ and $Prt_i$ characterize turbulent scalar transfers of species mass fractions and energy from turbulent momentum transfer, respectively. They can impose influences on numerical predictions of turbulence/chemistry interactions and, thus, flame and flow structures. The impacts of $Sc_i$ and $Prt_i$ have been extensively studied in Reynolds-averaged Navier–Stokes (RANS) simulations of supersonic turbulent flames while less in LES. Eklund and Baurle27 concluded that a low $Sc_i$ can numerically result in unstart phenomena in an ethylene-fueled scramjet combustor, while high $Sc_i$ can lead to flame blowout using RANS simulations. Xiao et al.28 developed a turbulence model in RANS simulations with variable $Sc_i$ and $Prt_i$ as part of the solution and applied it into scramjet non-reacting and H$_2$/air reacting flows. Numerical results with variable $Sc_i$ and $Prt_i$ show better agreement with corresponding experimental data. Zheng and Yan29 performed sensitivity analysis of $Sc_i$ and $Prt_i$ between 0.5 and 0.9 using RANS simulations of two supersonic hydrogen flames: Burrows–Kurkov case30 and DLR case,31 where ignition locations vary with the two parameters. In the LES context, Ingenito and Bruno32 performed the LES of a supersonic H$_2$/air combustor with three different $Sc_i$ of 0.4, 0.6, and 0.7. The flame was observed to oscillate with $Sc_i = 0.7$ but be stable with $Sc_i = 0.4$ and 0.6, and it becomes less stratified and no longer confined to the H$_2$/air interface as $Sc_i$ decreases. A variable $Sc_i$ was also implemented into a new SGS turbulence model, and this parameter turned out to vary from 0.4 to 1.0 and be particularly low where combustion occurs in the LES study. While LES studies on the impacts of $Sc_i$ and $Prt_i$ on supersonic turbulent flames are still scarce, those of Cheng supersonic flame with different combinations of the two parameters are performed in this work. Based on the aforementioned RANS and LES studies, the values of $Sc_i$ and $Prt_i$ equal to 0.5 or 1.0 are applied.

The objectives of this work are twofold as stated above. The first is the impacts of Lewis number and the other is those of turbulent Schmidt and Prandtl numbers on the LES of supersonic turbulent flames. The rest of this paper is organized as below. The LES governing equations and a newly developed numerical solver used to solve these equations are detailed in Sec. II. The target Cheng supersonic flame and computational configuration are introduced in Sec. III. The numerical results, including flame and flow structures and statistics of scalars and velocity, from present simulations are discussed against corresponding experimental data in Sec. IV. The conclusions are summarized in Sec. V.

II. MODELING DETAILS

A. LES governing equations

The filtered fully compressible Navier–Stokes equations, i.e., continuity, momentum, species mass fractions, and sensible enthalpy,
coupled with the ideal gas equation of state, are solved in this work. They, respectively, read
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (5)
\]
\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p - \nabla \cdot \mathbf{\tau} - \nabla \cdot \mathbf{\tau}_{sgs} = 0, \quad (6)
\]
\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) + \nabla \cdot \mathbf{J}_i = \bar{\omega}_i, \quad (i = 1, 2, ..., N - 1), \quad (7)
\]
\[
\frac{\partial (\rho h_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h_i) - \frac{Dp}{Dt} + \nabla \cdot \mathbf{\Phi}_T = \bar{\omega}_T, \quad (8)
\]
\[
\bar{\rho} = p \left( R_e T \sum_i Y_i / W_i \right). \quad (9)
\]

Here, the mass and thermal diffusion fluxes, i.e., \( \mathbf{J}_i \) in Eq. (7) and \( \mathbf{\Phi}_T \) in Eq. (8), have been given in Eqs. (1)–(4). The filtered density, i.e., \( \bar{\rho} \), the mass fraction of the \( i \)-th species, i.e., \( Y_i \), and the sensible enthalpy, i.e., \( h_i \), have been referred to in Eqs. (1) and (2), \( t \) is the time; \( \overline{\rho} \) is the filtered pressure; and \( \mathbf{u} T \) state for the velocity vector and temperature, respectively. \( \mathbf{\tau} \) and \( \mathbf{\tau}_{sgs} \) in Eq. (6) denote the filtered and SGS viscous stress tensors, respectively, computed by
\[
\mathbf{\tau} = \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) I \right], \quad (10)
\]
\[
\mathbf{\tau}_{sgs} = \mu_{sgs} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) I \right], \quad (11)
\]
where \( I \) is the identity matrix and the superscript \( T \) indicates matrix transposition. The molecular dynamic viscosity, i.e., \( \mu \) in Eq. (10), is calculated together with the mass and thermal diffusivities, i.e., \( D_i \) in Eq. (1) and \( \chi \) in Eq. (2), using either the mixture-averaged diffusion model with a mixture-averaged formula or a combination of the Sutherland’s law, Eucken approximation, and unity-Lewis number assumption. The SGS dynamic viscosity, i.e., \( \mu_{sgs} \) in Eq. (11), is estimated using the constant Smagorinsky turbulence model. The SGS mass and thermal diffusivities, \( D_{mg} \) in Eq. (3) and \( D_{th} \) in Eq. (4), are accordingly determined by the turbulent Schmidt and Prandtl numbers, i.e., \( Sc \) and \( Pr_T \), as constants of 0.5 or 1.0.

In Eq. (7), \( \bar{\omega}_i \) refers to the chemical net production rate of the \( i \)-th species, and \( N \) denotes the number of species. Equation (7) is solved for all the species except the \( \text{N}_2 \) species, an “inert species,” e.g., nitrogen (\( \text{N}_2 \)) here, whose mass fraction is computed by subtracting the mass fractions of all other species from unity. \( \bar{\omega}_T \) in Eq. (8) is the heat release rate from chemical reactions. Radiative heat transfer, Soret and Dufour effects play secondary roles and are, thus, not included in Eqs. (7) and (8). Note that the real gas effect on supersonic turbulent flames is also not referred to in this work. In Eq. (9), \( R_g \) is the universal gas constant and \( W_i \) is the mole weight of the \( i \)-th species.

B. Numerical solver and method

The LES governing equations are solved using a density-based multi-component reactive flow solver, AHISDetFoam, within the OpenFOAM 6.0 framework. The AHISDetFoam solver is customized from the OpenFOAM built-in non-reactive rhoCentralFoam solver. It uses the cell-centered finite volume method (FVM) to discretize Eqs. (5)–(8). A first-order splitting scheme separates the solutions of chemical and non-chemical terms. The chemical terms, i.e., \( \bar{\omega}_i \) in Eq. (7) and \( \bar{\omega}_T \) in Eq. (8), are first solved over one time step using a sparse stiff chemistry solver based on dynamic adaptive hybrid integration (AHIS-S) and the quasi-laminar chemistry (QLC) closure. The AHIS-S solver combines a sparse matrix technique with the dynamic adaptive hybrid integration method to speed up the finite-stiff chemistry integration. The non-chemical terms are then integrated over the time step along with the chemical terms calculated from the first step, with the second-order implicit Crank–Nicolson scheme applied for time discretization. AHISDetFoam inherits the following numerical approaches from rhoCentralFoam to solve the non-chemical terms. An operator-splitting approach is used to solve the transport terms in Eqs. (6) and (8). Specifically, an explicit predictor equation is first solved for the convected of conserved variables, and an implicit corrector equation is then solved for the diffusion of primitive variables. The convection terms in Eqs. (5), (6), and (8) are solved using the second-order semi-discrete, non-staggered, and central-upwind Kurganov, Noelle, and Petrova (KNSP) scheme with a van Leer flux limiter. For the convective term in Eq. (7), a total variation diminishing (TVD) scheme is used to ensure the scalar boundedness. The diffusion terms in Eqs. (6)–(8) are split into orthogonal and non-orthogonal parts to minimize the non-orthogonality error. The second-order Gauss scheme with linear interpolation and the surface interpolation of variable normal gradients are applied for the orthogonal and non-orthogonal parts, respectively.

The performance of the AHIS-S chemistry solver in terms of accuracy and efficiency has been extensively demonstrated in the simulations of 0D auto-ignition systems and unsteady perfectly stirred reactors (PSR), as well as 1D laminar flames and detonation problems. Similar computational costs to those of fully explicit chemistry solvers are achieved, with accuracy being comparable to those of fully implicit chemistry solvers guaranteed. The rhoCentralFoam solver has been validated with non-reactive benchmark cases, including 1D shock tube, 2D forward-facing step, supersonic jet, and hypersonic flow over a biconic. Some reactive flow solvers coupling rhoCentralFoam and other chemistry solvers (from OpenFOAM standard libraries), e.g., rhoCentralRIFoam and RYrhoCentralFoam, are increasingly used in the combustion research community. They have shown capabilities in accurately capturing flow discontinuities from shock and expansion waves, shock–flame interactions, and auto-ignition in supersonic shock-laden reactive flows. The rhoCentralRIFoam and RYrhoCentralFoam solvers function well on computing the overall characteristics of detonative combustion and/or the transient behaviors of rotating detonation. The accuracy of LES studies on Cheng supersonic flame and a model supersonic hydrogen combusor using RYrhoCentralFoam has been confirmed. The statistics of velocity and reactive scalar fields predicted numerically are in good agreement with the corresponding experimental measurements.

III. CHENG SUPERSONIC FLAME

A. Experimental configuration

Figure 1(a) shows the schematic of Cheng supersonic flame burner. A sonic round jet of hydrogen (\( \text{H}_2 \)) is injected as the fuel from a central pipe with a diameter, \( D_f \) of 2.36 mm, surrounded by an annular jet of hot, vitiated air stream at Mach 2 as the coflow. The coflow is generated by an upstream lean combustor where hydrogen
burns with air with excess oxygen (O₂). The inner and outer diameters of the annular coflow jet are Di = 3.81 and Do = 17.78 mm, respectively. The flow conditions of fuel and coflow jets at the Cheng supersonic flame burner exit are given in Table II. The liftoff height of Cheng supersonic flame is about 25Df, see Fig. 1(b), which shows an experimental photograph of flame luminosity.14 The experimental measurements in Refs. 14 and 54 reported radial profiles of mean axial velocity, ⟨u⟩, temperature, ⟨T⟩, mixture fraction, ⟨Z⟩, and some species mole fractions, including ⟨X_O2⟩, ⟨X_H₂O⟩, ⟨X_N₂⟩, ⟨X_H₂⟩, and ⟨X_OH⟩, at all or parts of seven downstream distances, i.e., x/Df = 0.85, 10.8, 21.5, 32.3, 43.1, 64.7, and 86.1. They are referred to in comparison with subsequent LES studies in this work.

B. Computational configuration

Figure 1(c) shows the schematic of the cylindrical computational domain for the LES of Cheng supersonic flame on the central plane of symmetry.13 Above the coordinate origin, O, located at the center of the fuel jet at the burner exit, it has a length of 70Df along the streamwise x-direction, with a radius of 30Df along the radial r-direction. It also extends 1.5Df upstream into the fuel and coflow pipes. The mesh consists of 12 175 200 hexahedral cells with radially localized refinement around the fuel and coflow inlets and their shear layers, marked with a dashed box where the distribution of cells is enlarged and demonstrated in Fig. 1(d).3 The minimum cell sizes along x- and r-directions are 118 and 50 μm, respectively. Note that the Kolmogorov and integral length scales of Cheng supersonic flame estimated experimentally fall in ranges of 8–35 and 3400–7400 μm, respectively.

The boundary conditions of the cylindrical computational domain are listed in Table III. The “decayingTurbulenceInflowGenerator” boundary condition,54,56 which specifies a synthetic inflow turbulence, is applied for velocity fields at the fuel and coflow inlets. In this manner, the representation of the velocity field reads the sum of vortons induced by a collection of randomly placed spots; the fluctuations of velocity distribution inside each spot possess prescribed statistical properties, including integral length scale and symmetric Reynolds-stress tensor. The integral length scale is approximated from hydraulic diameters of fuel and coflow pipes, i.e., Df and [Do − Di], respectively. The symmetric Reynolds-stress tensor is expressed by combining both the fuel and coflow inlets as round jet flows.54 The correlations between its six components of normal and shear stresses are given following the method of Masri et al.58 The normal and shear stresses are related to the axial velocity fluctuation and, thus, the mean velocity along x-direction and turbulent intensities at the jet center and circumference based on Refs. 55 and 56. The mean velocities of fuel and coflow jets along x-direction, Uf and Uc, are 1780 and 1420 m/s, respectively. For the round fuel jet, the turbulent intensities are assumed to be If,cen = 5% and If,cir = 18% at its center and circumference; for the annular coflow jet, its central circumference with a diameter of (Di + Do)/2 has the lowest turbulent intensity, Ic,con, of 5%, while the highest turbulent intensities, Ic, cir, are assumed to be 22% at both its inner and outer circumferences. The “fixedValue” boundary condition is applied for other variables of fuel and coflow inlets, whose magnitudes are set consistent with the experimental flow conditions at the burner exit, given in Table II. The fuel and coflow pipes are all slip and adiabatic walls with “slip” and “zeroGradient” boundary conditions specified for velocity and other variables, respectively. The computational domain is open to the atmosphere (1 atm, 298 K) at lateral and outlet boundaries, which are assumed to be non-reflective with “waveTransmissive” and “zeroGradient” boundary conditions specified for pressure and other variables, respectively. It is closed at the annular plane at x = 0 with inner and outer diameters as Di and 30Df, respectively, where velocity is set as “fixedValue” of zero and other variables with the “zeroGradient” boundary condition.
IV. RESULTS AND DISCUSSION

The parametric LES studies on Cheng supersonic flame, summarized in Table IV, are performed on the University of Oxford Advanced Research Computing (ARC) facility in this work. A detailed chemical mechanism for hydrogen combustion with 9 species and 19 reactions is used. The Courant–Friedrich–Lewy (CFL) number is set as 0.3, and accordingly, the physical time step, Δt, is approximately \(4 \times 10^{-9}\) s. The computation on 336 processors for each LES takes about 15,961 CPU-hours per characteristic flow-through time which is the ratio of computational domain length, i.e., 70D\(_f\), and coflow mean velocity along x-direction, i.e., \(U_i\). Each LES collects the statistics on average over 0.25 ms as in Ref. 10, longer than two characteristic flow-through times, after a statistically transient flow period of 0.5 ms. The quality and reliability of the present LES studies are evaluated via a posteriori analysis of mesh resolution, provided in the supplementary material.

A. Impacts of Lewis number

The impacts of Lewis number on the LES of Cheng supersonic flame are assessed by comparing numerical results solved using the mixture-averaged diffusion model, i.e., Case \(C_0\) and the unity-Lewis number assumption, i.e., Case \(C_1\). Figures 2(a)–2(e) and 2(f) depict mean and instantaneous distributions of some species mole fractions and mixture fraction, respectively. Each frame shows a 2D cut on the symmetry plane in the central region of 70D\(_f\) \(\times 10D_f\) \(\times 2\pi\). The time-averaged and instantaneous filtered quantities, on the left and right sides of each frame, respectively, are represented by angle brackets, i.e., \(\langle X_{H_i}\rangle\), \(\langle X_{O_i}\rangle\), \(\langle X_{H_2O}\rangle\), \(\langle X_{N_i}\rangle\), \(\langle X_{OH}\rangle\), and \(\langle Z\rangle\), and tilde, i.e., \(\tilde{X}_{H_i}\), \(\tilde{X}_{O_i}\), \(\tilde{X}_{H_2O}\), \(\tilde{X}_{N_i}\), \(\tilde{X}_{OH}\), and \(\tilde{Z}\). Both diffusion models numerically capture turbulent eddies on a range of scales which are intrinsic characteristics of fuel and coflow jets and their mixing layers in the instantaneous contours. Localized differences between the two instantaneous predictions are observed though with identical initial conditions. They are amplified by the turbulence. The contours of mean species mole fractions predicted by the two diffusion models demonstrate differences mostly in the flame regions with significantly reduced reactants of \(H_2\) and \(O_2\) but increased product of \(H_2O\). Mean flame liftoff heights, i.e., \(l_{f0}\) at 38D\(_f\) and \(l_{f1}\) at 33.7D\(_f\) marked in Figs. 2(a1) and 2(e2), respectively, are identified by \(\langle X_{OH}\rangle = 0.008\) using the method in Refs. 3 and 11. Note that other criteria, e.g., mean temperature \((T) = 1600K\) from Ref. 2, yield nearly identical results. Those between 24.4D\(_f\) and 32.4D\(_f\) have been reported in the literature,\(^3\),\(^6\),\(^9\),\(^11\) while the experimentally measured value is 25D\(_f\).\(^6\) Both \(l_{f0}\) and \(l_{f1}\) are overestimated as such, while \(l_{f1}\) is closer to the experimental value. The different mean flame liftoff heights obtained experimentally and numerically are likely associated with the absence of combustion models in the present simulations,\(^3\),\(^6\),\(^9\),\(^11\) which is not the main focus of this work. Note that unexpected turbulence from unaligned fuel/colow axes and early ignition from radicals, e.g., \(OH\), in the coflow in the experiments are not mimicked. The two factors may also play a part in the mismatched experimental and numerical results, as referred to by Huang et al.\(^9\). The predictions of \(\langle Z\rangle\) using the two diffusion models show qualitative agreement.

The time-averaged statistics, i.e., \(\langle X_{H_i}\rangle\), \(\langle X_{O_i}\rangle\), \(\langle X_{H_2O}\rangle\), \(\langle X_{N_i}\rangle\), \(\langle X_{OH}\rangle\), and \(\langle Z\rangle\), for cases \(C_0\) and \(C_1\) are presented in Figs. 3–5 in a quantitative way. Their radial profiles at selected streamwise distances are compared to the experimental data from Ref. 14. At \(x/D_f = 32.3\) in Fig. 3, the two numerical predictions are in line. \(\langle X_{OH}\rangle\) is nearly unchanged at zero along the radial direction. Its experimental profile, whereas, reaches local maxima near the jet symmetry. Accordingly, the little consumption of \(H_2\) and generation of \(H_2O\) lead to the overestimation of \(\langle X_{H_i}\rangle\) and underestimations of \(\langle X_{H_2O}\rangle\) in the central jet. Using either diffusion model, combustion occurs at \(x/D_f = 43.1\) downstream of both \(l_{f0}\) and \(l_{f1}\). As Fig. 4 shows, the numerical over-prediction of \(\langle X_{H_i}\rangle\) and under-prediction of \(\langle X_{OH}\rangle\) and \(\langle X_{H_2O}\rangle\) in the central jet are less significant, especially using the unity-Lewis number assumption. In the flame regions at \(x/D_f = 64.7\) in Fig. 5, the mixture-averaged diffusion model achieves better accuracy in predicting \(\langle X_{OH}\rangle\) and \(\langle X_{H_2O}\rangle\) against the experimental data. The two numerical radial profiles of \(\langle X_{H_i}\rangle\) deviate from the experimental ones in the central jet. Those of \(\langle X_{N_i}\rangle\) are slightly underestimated near the jet symmetry with the dilution effects of unconsumed \(H_2\). Overall, these statistics, especially \(\langle X_{O_i}\rangle\), \(\langle X_{N_i}\rangle\), and \(\langle Z\rangle\), are well reproduced numerically at all the three streamwise distances using both diffusion models, considering uncertainties of asymmetric experimental profiles due to the imperfect burner orientation.\(^11\)

Figure 6 shows the profiles of \(\langle Z\rangle\) along the centerline. Excellent agreement is observed between the numerical results of cases \(C_0\) and \(C_1\) and their experimental counterparts, consistent with the findings in Figs. 3–5. The mixing of reactants, i.e., \(H_2\) and \(O_2\), is accurately predicted by either diffusion model as such, on which the differences in Lewis numbers impose limited influences.

### Table III: Boundary conditions of the cylindrical computational domain. \(p\) is the pressure; \(T\) is the temperature; \(u\) is the velocity; \(O_2\), \(H_2O\), \(N_2\), and \(H_2\) are species.

<table>
<thead>
<tr>
<th>Boundary Conditions</th>
<th>(p)</th>
<th>(T)</th>
<th>(u)</th>
<th>(O_2), (H_2O), (N_2) and (H_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel and coflow inlet</td>
<td>fixedValue</td>
<td>fixedValue</td>
<td>decayingTurbulenceInflowGenerator</td>
<td>fixedValue</td>
</tr>
<tr>
<td>Fuel and coflow pipe</td>
<td>zeroGradient</td>
<td>fixedValue</td>
<td>slip</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>Lateral and outlet boundary</td>
<td>waveTransmissive</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>Annular plane at (x = 0)</td>
<td>zeroGradient</td>
<td>fixedValue</td>
<td>fixedValue</td>
<td>zeroGradient</td>
</tr>
</tbody>
</table>

### Table IV: Parametric LES of Cheng supersonic flame. \(L_e\) is Lewis number of \(i\)th species; \(S_c\) is turbulent Schmidt number; and \(P_r\) is turbulent Prandtl number.

<table>
<thead>
<tr>
<th>Case ID</th>
<th>(L_e)</th>
<th>(S_c)</th>
<th>(P_r)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C_0)</td>
<td>Species-specific</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>(C_1)</td>
<td>Unity</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>(C_2)</td>
<td>Species-specific</td>
<td>0.5</td>
<td>1.0</td>
</tr>
<tr>
<td>(C_3)</td>
<td>Species-specific</td>
<td>1.0</td>
<td>0.5</td>
</tr>
<tr>
<td>(C_4)</td>
<td>Species-specific</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>
The role that the differences in Lewis numbers play in numerically capturing auto-ignition and flame stabilization is then described. Time sequences of heat release rate fields, i.e., $\dot{\omega}_T$, on the symmetry plane in the central region of $70D_f \times 10D_f \times 2\pi$. Case ID: $C_0$ (top) and $C_1$ (bottom).

FIG. 2. Mean (left) and instantaneous (right) distributions of species mole fraction for (a1) and (a2) $H_2$, (b1) and (b2) $O_2$, (c1) and (c2) $H_2O$, (d1) and (d2) $N_2$, (e1) and (e2) $OH$, and (f1) and (f2) mixture fraction on the symmetry plane in the central region of $70D_f \times 10D_f \times 2\pi$. Case ID: $C_0$ (top) and $C_1$ (bottom).

The role that the differences in Lewis numbers play in numerically capturing auto-ignition and flame stabilization is then described. Time sequences of heat release rate fields, i.e., $\dot{\omega}_T$, on the symmetry plane in the central region of $(20 - 50)D_f \times 5D_f \times 2\pi$ for cases $C_0$ and $C_1$ are depicted in Figs. 7(a)–7(k). These frames cover the statistics collection period of 0.25 ms with an interval of 0.025 ms. Both numerical predictions report temporal variations of flame position subject to occasional prolonged and compact flames, similar to the work of Bouheraoua et al. This phenomenon is anticipated as a characteristic of turbulent lifted flames in supersonic or subsonic jets, see Refs. 61 and 62. Using either diffusion model, isolated auto-ignition spots, e.g., $AI_0$ and $AI_1$, with spotty high values of $\dot{\omega}_T$ in Figs. 7(b1) and 7(d2), periodically occur upstream of the main burning zones. The auto-ignition spots are mostly captured in the shear layers of fuel and coflow jets by the mixture-averaged diffusion model and are generally weak.
recurrently form near the jet symmetry. They always accumulate into continuous reacting regions downstream and strengthen the main flame subsequently. The differences are distinguishable between Figs. 7(k1) and 7(k2) in the two dashed boxes. Note that the unity-Lewis number assumption underestimates the mass diffusion of light species, e.g., H$_2$ in the central fuel jet, while overestimates that of heavy species, e.g., O$_2$ in the surrounding annular air stream, discussed later in Fig. 10. Premixed unburned H$_2$-O$_2$ pockets as favorable locations for auto-ignition tend to build relatively away from the jet symmetry and each other using the mixture-averaged diffusion model, as more H$_2$ diffuses outwards but less O$_2$ diffuses inwards. These auto-ignition spots cannot co-strengthen effectively and, thus, own lower strengths.
The underlying stabilization mechanism of the flame is that the intricate coupling of auto-ignition and upstream diamond-shaped shocks controls its dynamics and position oscillations, which has been specified in Refs. 8 and 10. The different predictions of auto-ignition and upstream diamond-shaped shocks have been studied in detail.
locations and strengths contribute to different flame structures solved using the two diffusion models. In Fig. 7, the main flames demonstrated in the top frames further distribute on two sides of the jet symmetry and stabilize at higher streamwise positions compared to those in the bottom frames.

Figures 8(a) and 8(b) provide quantitative comparisons on temporal evolutions of flame base location and maximum $\bar{\omega}_T$ between cases $C_0$ and $C_r$, respectively. The flame base is identified where $\bar{\omega}_T$ peaks instantaneously as in Ref. 10. It irregularly oscillates in a range of $x/D_f = 32.9 – 49.1$ using the mixture-averaged diffusion model, generally higher than $x/D_f = 18.1 – 40.7$ using the unity-Levis number assumption. In contrast, the two corresponding ranges of maximum $\bar{\omega}_T$, i.e., $4.4 \times 10^{10} – 7.4 \times 10^{10}$ and $4.9 \times 10^{10} – 7.9 \times 10^{10}$ $\text{m}^3$/s, respectively, are close.

A signed flame index conditioning on localized $\bar{\omega}_T$, i.e., $\bar{\xi}_{SFI-\bar{\omega}_T}$, is used to analyze differences in mixed combustion modes attached to flame stabilization predicted by the two diffusion models. It is defined as

$$\bar{\xi}_{SFI-\bar{\omega}_T} = \bar{\xi}_{pre-\bar{\omega}_T} + \bar{\xi}_{diff-\bar{\omega}_T},$$

(12)

where $\bar{\xi}_{pre-\bar{\omega}_T}$ and $\bar{\xi}_{diff-\bar{\omega}_T}$ are, respectively, computed by

$$\begin{align*}
\bar{\xi}_{pre-\bar{\omega}_T} &= \max[\text{sign} (\nabla \bar{Y}_{H_2} \cdot \nabla \bar{Y}_{O_2} - \varepsilon), 0]\max[\text{sign} (\bar{\omega}_T - \bar{\xi}_{SFI-\bar{\omega}_T})] \\
\bar{\xi}_{diff-\bar{\omega}_T} &= \min[\text{sign} (\nabla \bar{Y}_{H_2} \cdot \nabla \bar{Y}_{O_2} + \varepsilon), 0]\max[\text{sign} (\bar{\omega}_T - \bar{\xi}_{SFI-\bar{\omega}_T})],
\end{align*}$$

(13)

Here, $\max(x, y)$ and $\min(x, y)$ functions return the larger and smaller one between $x$ and $y$, respectively; the sign($x$) function returns 1 if $x \geq 0$ and $-1$ if $x < 0$. $\nabla \bar{Y}_{H_2}$ and $\nabla \bar{Y}_{O_2}$ denote the mass fractions of $H_2$ and $O_2$, respectively. Non-negligible positive dot products of their gradients are distinguished from the rest with $\varepsilon$ being a small positive constant, say $10^{-9}$ here. $\bar{\omega}_T$ is the volume average of $\bar{\omega}_T$ over the whole computational domain, and $\gamma \bar{\omega}_T$ provides a threshold to identify non-negligible $\bar{\omega}_T$ with $\gamma$ being a small fraction, say 1% here.

Three combinations of $\bar{\xi}_{pre-\bar{\omega}_T}$ and $\bar{\xi}_{diff-\bar{\omega}_T}$ read

$$\begin{align*}
\bar{\xi}_{pre-\bar{\omega}_T} &= 1, \bar{\xi}_{diff-\bar{\omega}_T} = 0, \text{if}\ \nabla \bar{Y}_{H_2} \cdot \nabla \bar{Y}_{O_2} \geq \varepsilon \text{ and } \bar{\omega}_T \geq \bar{\xi}_{SFI-\bar{\omega}_T} \\
\bar{\xi}_{pre-\bar{\omega}_T} &= 0, \bar{\xi}_{diff-\bar{\omega}_T} = -1, \text{if}\ \nabla \bar{Y}_{H_2} \cdot \nabla \bar{Y}_{O_2} < -\varepsilon \text{ and } \bar{\omega}_T \geq \bar{\xi}_{SFI-\bar{\omega}_T} \\
\bar{\xi}_{pre-\bar{\omega}_T} &= 0, \bar{\xi}_{diff-\bar{\omega}_T} = 0, \text{if}\ \varepsilon \leq \nabla \bar{Y}_{H_2} \cdot \nabla \bar{Y}_{O_2} < \varepsilon \text{ or } \bar{\omega}_T < \bar{\xi}_{SFI-\bar{\omega}_T},
\end{align*}$$

(14)

which correspond to three values of $\bar{\xi}_{SFI-\bar{\omega}_T}$ differentiating three regimes of flow fields: premixed combustion zones with $\bar{\xi}_{SFI-\bar{\omega}_T} = 1$ (non-negligible co-gradient variations of $H_2$ and $O_2$ with non-negligible $\bar{\omega}_T$), diffusion combustion zones with $\bar{\xi}_{SFI-\bar{\omega}_T} = -1$ (non-negligible counter-gradient variations of $H_2$ and $O_2$ with non-negligible $\bar{\omega}_T$), and non-reacting zones with $\bar{\xi}_{SFI-\bar{\omega}_T} = 0$ (negligible co- and counter-gradient variations of $H_2$ and $O_2$ or negligible $\bar{\omega}_T$).

Figures 9(a) and 9(b) depict instantaneous contours of $\bar{\xi}_{SFI-\bar{\omega}_T}$ on the symmetry plane in the central region of
$70D_f \times 10D_f \times 2\pi$ for cases $C_0$ and $C_1$, respectively. Closely downstream of the fuel and coflow inlets, it is filled with a flameless region, i.e., Zone I, using the mixture-averaged diffusion model but two thin diffusion flame stripes, i.e., Zone II, using the unity-Lewis number assumption. Zone III with ribbon-like diffusion flames and two premixed combustion spots inside follows Zone I. Zone IV with spatially more continuous diffusion combustion enclosing more premixed combustion spots follows Zone II. These remarkable differences in distributions of both diffusion and premixed combustion zones are triggered by different predictions of the fuel ($H_2$) and oxidizer ($O_2$) mass diffusion in their shear layers. They affect flame structures and stabilization further downstream.

The choice of diffusion models directly changes the filtered mass and thermal diffusivities, i.e., $D_i$ and $\kappa$. The mass and thermal diffusion terms, i.e., $[-\nabla \cdot J_i]$ and $[-\nabla \cdot J_h]$, respectively, determined by $D_i$ and $\kappa$ in Eqs. (7) and (8), are consequently changed. Their different predictions co-contribute to the numerical results demonstrated in Figs. 2–9 and are, thus, analyzed and compared between cases $C_0$ and $C_1$.

Instantaneous scatter plots of $[-\nabla \cdot J_i]$ for some species against their corresponding mole fractions, i.e., $\bar{X}_i$, on the symmetry plane in the central region of $70D_f \times 5D_f \times 2\pi$ are presented in Figs. 10(a)–10(f). The evolutionary tendencies of $[-\nabla \cdot J_i]$ with respect to $\bar{X}_i$ predicted by the two diffusion models are alike. The species mass diffusion primarily occurs at fuel and coflow mixing layers where higher $\bar{X}_{H_2}$ but lower $\bar{X}_{O_2}$ and $\bar{X}_{N_2}$ are numerically observed [see Figs. 2(a)–2(d)]. Over the entire ranges of corresponding species mole fractions, $[-\nabla \cdot J_{O_2}]$ and $[-\nabla \cdot J_{N_2}]$ for heavy species are overestimated, while $[-\nabla \cdot J_{H_2}]$ and $[-\nabla \cdot J_{H}]$ for light species are highly underestimated using the unity-Lewis number assumption, compared to the mixture-averaged diffusion model. The two predictions of $[-\nabla \cdot J_{OH}]$ and $[-\nabla \cdot J_{H_2O}]$ for medium-weight species are equally matched. The most different numerical results of the mass diffusion for $H_2$ and $H$ may play a considerable part in triggering those of auto-ignition locations and strengths, and thus, flame structures and stabilization.

Figures 11(a) and 11(c1)–(c3) quantitatively show centerline and radial profiles of instantaneous $[-\nabla \cdot J_h]$ at three streamwise distances, respectively. Instantaneous contours of $[-\nabla \cdot J_h]$ on the symmetry plane in the central region of $70D_f \times 10D_f \times 2\pi$ are qualitatively depicted in Figs. 11(b1) and 11(b2). The thermal diffusion sees positive and negative peaks around the fuel and coflow inlets using both diffusion models in Fig. 11(a). Along the centerline, its absolute value overall shrinks with fluctuations and localized growths inside the two premixed combustion zones downstream of Zones III and IV, see Figs. 9(a) and 9(b). In Fig. 11(b1), the mixture-averaged diffusion model numerically reports large values of $[-\nabla \cdot J_h]$ near both the coflow center and circumference where it mixes with the fuel and the ambient air, respectively. The unity-Lewis number assumption, whereas, predicts noticeable thermal diffusion only at the fuel and coflow mixing layers in Fig. 11(b2). Figure 11(c1)–11(c3) support this. The former profiles have ups and downs of $[-\nabla \cdot J_h]$ at four spanwise locations, while only the two near the jet symmetry are noticeably displayed by the latter ones. More heat diffuses outwards at the coflow circumference where $[-\nabla \cdot J_h]$ acts as sink terms with its negative parts dominating positive parts using the mixture-averaged diffusion model, compared to the unity-Lewis number assumption.
The aforementioned differences in behaviors of the two diffusion models specify the impacts of Lewis number on the LES of Cheng supersonic flame. These findings are further validated by a scale analysis of the diffusion and convection terms in Eqs. (7) and (8). The absolute values of ratios between mass diffusion and convection terms, i.e., \( \frac{\nabla \cdot \mathbf{J}_i}{\nabla \cdot (\bar{\mathbf{u}} \rho Y_i)} \), for some species, and thermal diffusion and convection terms, i.e., \( \frac{\nabla \cdot \mathbf{J}_h}{\nabla \cdot (\bar{\mathbf{u}} \rho h_s)} \), are examined. They are hereafter termed as \( R_{1,i} \) and \( R_{1,h} \), respectively, whose instantaneous percentages in the central region of 70\( D_f / C_2 \) are presented in Figs. 12(a)–12(f) and 12(g). \( R_{1,H_2} \) and \( R_{1,H} \) for light species exhibit similar proportional distributions. Their values are mostly between 0.01 and 0.1, accounting for 45.2% and 42.6%, respectively; next are the 0–0.01 and 0.1–1 groups; those over 1 are the least. The percentages of \( R_{1,OH} \) and \( R_{1,H_2O} \) for medium-weight species and \( R_{1,H} \) are inversely related to magnitudes of these ranges. Those representing diffusion over one-tenth of convection, i.e., 18%, 13.6%, and 8.3%, still matter. The mass diffusion of heavy species plays a secondary role in comparison with their convection with the percentages of \( R_{1,O_2} \leq 0.01 \) and \( R_{1,N_2} \leq 0.01 \) equal to 89.3% and 85.1%, respectively. In general, both the mass and thermal diffusions are less than convection but non-negligible, especially for \( H_2 \) and \( H \), which explains the phenomena that the differences in Lewis numbers trigger those in the numerical results.

B. Impacts of turbulent Schmidt and Prandtl numbers

The impacts of turbulent Schmidt and Prandtl numbers on the LES of Cheng supersonic flame are assessed by comparing numerical results solved using different combinations of the two parameters, i.e., Cases \( C_0 \) and \( C_2 \)–\( C_4 \). Figures 13(a) and 13(b) depict mean and instantaneous distributions of temperature, i.e., \( \bar{T} \) and \( T \), and axial velocity, i.e., \( \bar{u}_x \) and \( u_x \), respectively. The left and right sides of each frame on the symmetry plane in the central region of 70\( D_f \times 10D_f \times 2\pi \) correspond to \( \bar{T} \) and \( T \), respectively. The four sets of turbulent Schmidt and Prandtl numbers with \( Sct \) and \( Prt \) equal to 0.5 or 1.0 agree relatively well in predicting the lower halves where \( x / D_f \leq 30 \) in both the instantaneous and mean contours. The upper halves of the instantaneous temperature fields, especially the flame regions with pronounced rises of \( T \), see noticeable localized differences. Those of \( u_x \) accordingly demonstrate differences in flow patterns subject to turbulent eddies. Note that although the turbulent transfer of energy is calculated from that of momentum by \( Pr_t \), the former affects the latter in turn as they are coupled. The interplay of instantaneous flame and flow structures is likewise anticipated. The time-averaged flame lengths and widths along the streamwise and spanwise directions, respectively, are qualitatively identified from the predictions of \( \bar{T} \). They significantly vary against \( Sct \) but are less dependent on \( Pr_t \); longer and narrower flames are numerically captured with \( Sct = 1.0 \) for cases \( C_0 \) and...
Similarities among the four mean flame liftoff heights, i.e., \( l_f^0 \) at 38.9\( D_f \), \( l_f^2 \) at 38.9\( D_f \), and \( l_f^3 \) at 39.3\( D_f \) marked in Figs. 13(a1)–13(a4), respectively, are predicted. These results indicate that both \( Sc_t \) and \( Pr_t \) impose minor influences on the mean flame liftoff height, compared to the choice of diffusion models with the inconsistency between \( l_f^0 \) and \( l_f^1 \). The contours of \( \langle u_x \rangle \) are comparatively less sensitive to different \( Sc_t \) and \( Pr_t \) than those of \( \langle T \rangle \), which has been reported by Zheng and Yan.29 When \( Sc_t = 1.0 \), the two central zones...
with large values of \( \langle u_e \rangle \), roughly representing run-up distances of fuel and coflow jets, almost cover the whole computational domain. Their counterparts with \( Sc_t = 0.5 \) for cases \( C_2 \) and \( C_6 \), whereas, are moderately shortened.

The radial profiles of \( \langle u_e \rangle \) at \( x/D_f = 32.3 \) and \( x/D_f = 43.1 \) for cases \( C_0 \) and \( C_2 - C_4 \) are presented in Figs. 14(a1) and 14(a2), respectively, along with the corresponding experimental data from Ref. 14. At both streamwise distances, all of them display overestimations of \( \langle u_e \rangle \) in the central jet but underestimations of radial coflow spreading into the ambient air. The experimental and numerical differences are likely caused by insufficient mesh resolution in the outer shear layers near the coflow circumference. The fact that inflow velocity fluctuations in the experiments cannot be perfectly mimicked by the synthetic ones used in the present simulations may co-contribute to them.5,23,13

The variations of \( \langle u_e \rangle \) along the spanwise direction perfectly keep in step using either \( Sc_t/Pr_t \). The quantitative results agree with the qualitative ones of mean axial velocity fields in Figs. 13(b1)–13(b4). Differences in \( Sc_t \) and \( Pr_t \) barely trigger those in the predictions of \( \langle u_e \rangle \).

Figures 14(b1)–14(b3) show three groups of radial profiles for \( \langle T \rangle \). At \( x/D_f = 32.3 \) and \( x/D_f = 43.1 \), the numerical predictions of \( \langle T \rangle \) are in good agreement among Cases \( C_0 \) and \( C_2 - C_4 \); \( \langle T \rangle \) is highly underestimated at \( x/D_f = 32.3 \) by all the combinations of \( Sc_t \) and \( Pr_t \), as the streamwise location is upstream of \( l_f 0 \) and \( l_f 1 \), but downstream of the experimentally measured mean flame liftoff height, i.e., \( 25D_f \). The local minima of its numerical profiles near the jet symmetry are consistent with that of \( \langle X_{H_2O} \rangle \) in Fig. 3(c) attached to little product generation. Improvements regarding the underestimations of \( \langle T \rangle \) are observed at \( x/D_f = 43.1 \) in the flame regions. The numerical radial profiles of \( \langle T \rangle \) at \( x/D_f = 64.7 \) are closer to their experimental counterparts but see differences among themselves in the central jet. The one predicted by \( Sc_t = Pr_t = 1.0 \) achieves the best accuracy against the experimental data. The set of \( Sc_t = 1.0 \) and \( Pr_t = 0.5 \) comes the second, followed by the rest with \( Sc_t = 0.5 \).

The profiles of \( \langle T \rangle \) along the centerline are compared among Cases \( C_0 \) and \( C_2 - C_4 \) in Fig. 15. The four numerical predictions deviate from the experimental data since about \( x/D_f = 10 \) due to the occurrence of combustion far upstream in the experiments. Their centerline profiles continue to closely overlap downstream until over \( x/D_f = 50 \) where differences start to be triggered by those in \( Sc_t \) and \( Pr_t \). The influences of \( Sc_t \) on \( \langle T \rangle \) in the flame regions are more significant than those of \( Pr_t \) but still quite limited.

Figures 14(a1)–16(d) depict instantaneous contours of \( \xi_{SFI} \) on the symmetry plane in the central region of \( 70D_f \times 10D_f \times 2H \) for cases \( C_0 \) and \( C_2 - C_4 \), respectively. Predicted by either \( Sc_t/Pr_t \), upstream areas where \( x/D_f \leq 30 \) consist of a flameless region followed by ribbon-like diffusion flames. Zones I–IV with some discretized bubbles of premixed combustion in an extensive background of diffusion flame follow them. Further downstream areas demonstrate a feature of premixed combustion blocks/stripes embedded on the left and right sides of spatially continuous diffusion combustion. When \( Pr_t = 1.0 \), the two distributions of premixed combustion zones located downstream of zones I and II are less expansive in the spanwise direction. The comparatively high turbulent transfer of energy with \( Pr_t = 0.5 \) promotes outward expansions of their counterparts. Differences in the turbulent transfer of species dependent on \( Sc_t \) also lead to such different predictions but play secondary roles. The premixed combustion blocks downstream of zone IV are marginally more widespread than those downstream of Zone III.

The aforementioned differences in behaviors of the different combinations of \( Sc_t \) and \( Pr_t \) specify their impacts on the LES of Cheng supersonic flame. Both \( Sc_t \) and \( Pr_t \) affect flame structures and stabilization, to which the degree, whereas, is less remarkable in comparison with Lewis number. These findings are further validated by a scale analysis of the SGS and filtered diffusion terms in Eqs. (7) and (8). The absolute values of ratios between SGS and filtered mass diffusion...
terms, i.e., \(|\nabla \cdot (\hat{\rho}D_{\text{gs}}\nabla \hat{Y}_i)\nabla \cdot (\hat{\rho}D_{\text{gs}}\nabla \hat{Y}_i)|\), for some species, and thermal diffusion terms, i.e., \(|\nabla \cdot (\hat{\rho}\alpha_{\text{gs}}\nabla h_i)\nabla \cdot (\hat{\rho} \xi \nabla h_i)|\), are examined. They are hereafter termed as \(R_{2,i}\) and \(R_{2,h}\), respectively, whose instantaneous percentages in the central region of \(70D_f \times 5D_f \times 2\pi\) located in several ranges for case \(C_4\) are presented in Figs. 17(a)–17(f) and 17(g). The majorities of \(R_{2,\text{H}_2O}\) and \(R_{2,\text{H}_2}\) for light species represent their SGS mass diffusion lower than filtered one. The sums of their percentages in the 0–0.01 and 0.1–1 groups are 68.4% and 76.3%, respectively. \(R_{2,\text{H}_2O}\) and \(R_{2,\text{H}_2}\) for medium-weight species fall largely in the two middle ranges. Those between 0.1 and 1, accounting for 43.5% and 40.9%, respectively, are the most. The magnitudes of SGS and filtered thermal diffusions are comparable as the percentages of \(R_{2,b}\) between 1 and 10 and over 10 almost counterbalance with those in the 0–0.1 and 0.1–1 groups, respectively. The proportionate distributions of \(R_{2,\text{O}_2}\) and \(R_{2,\text{N}_2}\) are alike. Their values over 1 occupying 57.4% and 59%, respectively, are more than the rest, indicating that SGS mass diffusion of heavy species matters. In general, with both maximum SGS mass and thermal diffusions when \(Sc = Pr = 0.5\) among all the tests, filtered diffusion still slightly dominates, except for \(O_2\) and \(N_2\), which explains the phenomena that the impacts of \(Sc\) and \(Pr\) on the numerical results are subordinate to those of Lewis number.

V. CONCLUSIONS

The impacts of Lewis (\(Le_i\), of the ith species), turbulent Schmidt, and Prandtl numbers (\(Sc\) and \(Pr_i\)) on the LES of supersonic turbulent flames are the focus of this work. For this purpose, the parametric LES studies on Cheng supersonic flame are performed. The present LES quality and reliability are validated via a posteriori analysis of mesh resolution for case \(C_0\) (species-specific \(Le_o\), \(Sc = 0.5\), \(Pr_i = 1.0\)). They are consolidated by the good agreement between the numerical solutions and the corresponding experimental measurements on statistics of scalars and velocity.

The differences in numerical results of instantaneous and/or time-averaged species mole fractions, mixture fraction, heat release rate, flame base location, and mixed modes of premixed and diffusion combustion between cases \(C_0\) and \(C_1\) (unity \(Le_o\), \(Sc = Pr_i = 1.0\)) describe the impacts of Lewis number. The major findings are summarized on the following points:

- Cases \(C_0\) and \(C_1\) see instantaneous localized differences in both the fuel-oxidizer mixing layers and the reacting regions and report different time-averaged flame liftoff heights.
- The auto-ignition spots are weaker and distribute relatively away from the jet symmetry and the main flames stabilize at higher streamwise positions in case \(C_0\) than case \(C_1\).
- The reason for the different numerical results is that the mass diffusion for light species and the thermal diffusion at the outer coflow-ambient air mixing layers are underestimated but the mass diffusion for heavy species is overestimated in case \(C_1\) than case \(C_0\).
- The impacts of Lewis number are explained by that both the mass and thermal diffusions are lower than convection in magnitude but remain non-negligible according to their scale analysis for case \(C_0\).

The differences in numerical results of instantaneous and/or time-averaged temperature, velocity, and mixed combustion modes among cases \(C_0\) and \(C_2\) (species-specific \(Le_o\), \(Sc = 0.5\), \(Pr_i = 1.0\)), \(C_3\) (species-specific \(Le_o\), \(Sc = Pr_i = 1.0\)), and \(C_4\) (species-specific \(Le_o\), \(Sc = Pr_i = 0.5\)) describe the impacts of \(Sc\) and \(Pr_i\), to which the
degree is less remarkable in comparison with Lewis number. The major findings are summarized on the following points:

- Cases $C_0$, $C_2$–$C_4$ see instantaneous localized differences mostly in the reacting regions and report similar time-averaged flame liftoff heights.
- The relatively minor impacts of $Sct$ and $Prt$ than Lewis number are rationalized by that both the sub-grid scale mass and thermal diffusions are subordinate to filtered diffusion in magnitude according to their scale analysis for case $C_4$.

While the impacts of Lewis number on the LES of supersonic turbulent flames are only assessed by comparing the numerical solutions using the mixture-averaged diffusion model and the unity-Lewis number assumption, the multi-component diffusion model is expected to further improve the numerical accuracy, which will be the focus of future study.

SUPPLEMENTARY MATERIAL

See the supplementary material for the quality and reliability of the LES studies on Cheng supersonic flame in this work evaluated via a posteriori analysis of mesh resolution.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Ruixuan Zhu: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

Zhiwei Huang: Formal analysis (equal); Methodology (equal); Software (equal); Validation (equal); Writing – review & editing (equal).

Chao Xu: Methodology (equal); Software (equal); Validation (supporting); Writing – review & editing (equal).

XiaoHang Fang: Methodology
DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES


