

Large-Eddy Simulation of Supercritical Combustion: Model Validation Against Gaseous H₂–O₂ Injector

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Supercritical combustion has attracted significant interest due to its applications in high-pressure combustion devices. Validation of supercritical combustion modeling, however, has not been well reported because of the lack of experimental data with sufficient spatial and temporal resolution as well as the complexity associated with modeling and simulations. The present work begins to bridge this gap with a systematic examination of gaseous H₂–O₂ combustion of a shear coaxial injector at supercritical conditions, using both large-eddy simulation and detached-eddy simulation approaches. The formulation accommodates the full conservation laws and real-fluid thermodynamics and transport theories. Turbulence/chemistry interactions are treated by means of the flamelet and flamelet/progress-variable approaches. A nonpremixed jet flame (Sandia flame D) was first considered for code validation at ideal-gas conditions. The gaseous H₂–O₂ combustion at supercritical conditions was then studied systematically using different combinations of turbulence closure and combustion models. Special attention was given to comparison with measured wall heat flux. The large-eddy simulation/flamelet, detached-eddy simulation/flamelet, and large-eddy simulation/flamelet/progress-variable approaches produced qualitatively similar results in terms of flow and flame structures as well as wall heat flux. The present work was also compared with studies conducted by other research groups.

Nomenclature

b	=	parameter in the equation of state
C	=	progress variable
C_R, C_I	=	model constants for subgrid-scale models
D	=	mass diffusivity
d	=	wall distance
E	=	total internal energy
f	=	mixture fraction
f_b, f_d	=	blending function
h, H	=	enthalpy
k	=	kinetic energy
K_b	=	model constant for variance of mixture fraction
l	=	length scale in detached eddy simulation
P	=	probability
Pr_t	=	turbulent Prandtl number
p	=	pressure
q, Q	=	heat flux
S	=	strain
Sc_t	=	turbulent Schmidt number
t	=	time
u	=	velocity
x	=	spatial coordinate
Y	=	mass fraction
α	=	diffusivity of progress variable
β	=	model coefficient in the $k - \omega$ model
δ	=	Kronecker delta
μ	=	dynamic viscosity
ρ	=	density
σ^{SGS}	=	subgrid-scale viscous work
τ	=	viscous shear stress
Φ^{SGS}	=	subgrid flux of mixture fraction

Ψ^{SGS}	=	subgrid flux of progress variable
ω	=	reaction rate; vorticity in the $k - \omega$ model

Subscripts

i	=	species component
i, j, k	=	tensor index

Superscript

SGS	=	subgrid scale
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I. Introduction

MANY practical combustion devices operate at pressures and temperatures well above the critical points of injected liquid fuels and oxidizers, a situation commonly known as supercritical combustion [1]. Two different scenarios have been identified, depending on the propellant injection temperatures [2]. When both reactants are delivered at temperatures higher than their respective critical points, the reactants remain supercritical throughout their lifetimes. A notable example is the main combustion chamber of a full-flow staged-combustion-cycle rocket engine [3]. If one or both reactants are injected at temperatures lower than the critical values, the fluid will experience a continuous transition from a subcritical to a supercritical state. The physical processes associated with this scenario are intricate. The transition of the fluid state typically occurs in an extremely thin layer and is accompanied with rapid variations of thermophysical properties. In a typical first-stage or boost liquid rocket engine, the density ratio between the injected liquid propellant and gaseous combustion products is on the order of 100 with a temperature ratio of 30 [3,4]. The length scale for such rapid variations could be less than 0.01 mm. These conditions pose severe challenges for numerical simulation, in grid resolution, accuracy, robustness, and efficiency.

Experimental investigations of high-pressure combustion remain limited. The main obstacles lie in conducting diagnostics with sufficient spatial and temporal resolution. Mayer et al. [5,6] performed shadowgraph and OH-emission imaging studies to examine the injection, mixing, and combustion of liquid oxygen (LOX) and gaseous hydrogen (GH₂) in a single-element injector facility at a pressure range of 1.5–10 MPa. Both subcritical and supercritical cases were treated. Habiballah et al. [7] applied flow visualization and coherent anti-Stokes Raman scattering (CARS) techniques to

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explore fluid mixing and combustion of shear-coaxial injectors. Qualitative differences were observed between subcritical and supercritical flames, and the disappearance of liquid ligaments and droplets at supercritical conditions was noted. The CARS measurement of temperature was found to be inaccurate at high pressures. Singla et al. [8] investigated the flame structures of LOX with either gaseous or liquid methane (GCH_4 and LCH_4) downstream of a shear coaxial injector by examining OH^* and CH^* emissions in the pressure range of 4.5–6.0 MPa. The same problem was later studied using the planar laser-induced fluorescence (PLIF) technique [9]. As a consequence of laser absorption, high-quality PLIF images for LOX/ GCH_4 flames could only be obtained at pressures below 2.5 MPa. Smith et al. [10] conducted OH chemiluminescence and shadowgraph visualization of LOX/ GH_2 combustion at sub-, near-, and supercritical conditions. Recently, Lux and Haidn [11,12] investigated the ignition, flame anchoring, and combustion dynamics of LOX/ GCH_4 shear coaxial injectors at pressures of 4–6 MPa using OH and CH emission images. In spite of the encouraging progress made so far, quantitative information extracted from the imaging techniques appears to be limited. Most quantitative measurements of supercritical combustion lie in the distributions of pressure and temperature along the combustor wall [13,14].

Oefelein and Yang [2] conducted a pioneering study of supercritical combustion of a LOX/ GH_2 shear coaxial injector with laminar chemistry by means of large-eddy simulation (LES) and quasi-two-dimensional direct numerical simulation techniques. Emphasis was placed on the near-field flow evolution and flame stabilization. Zong and Yang [15] evaluated several different combustion models for supercritical combustion of LOX/ GCH_4 in a two-dimensional configuration. It was found that the flamelet model was appropriate for the chosen operating conditions [15,16]. Masquelet et al. [17] performed axisymmetric simulations of LOX/ GH_2 combustion in a subscale multi-injector chamber using a simple eddy breakup model. The predicted wall heat flux profile showed significant deviation from experimental measurements. Masquelet and Menon [18] later conducted both two-dimensional (2-D) axisymmetric simulations and three-dimensional (3-D) LES of supercritical GOX/ GH_2 combustion of a single-element shear coaxial injector with laminar chemistry. The 3-D prediction of the wall heat flux captured the trend of measured data fairly well. Schmitt et al. [19,20] performed 3-D LES studies of LOX/ GH_2 and LOX/ GCH_4 combustion at transcritical conditions using an infinitely fast single-step reaction with filtered reaction rate. The calculated flame structures showed reasonable agreement with experimental images. Recently, efforts have also been made to use flamelet-type tabulations for supercritical combustion modeling, along with real-gas equations of state as well as thermodynamic and transport properties. Cutrone et al. [21] used the flamelet/progress-variable approach within the context of Reynolds-averaged Navier–Stokes (RANS) to model a rocket combustor and achieved encouraging results. Lacaze and Oefelein [22] studied counterflow diffusion flames in a two-dimensional configuration. They then proposed a flamelet method to tabulate thermophysical properties, as well as density and mass fractions, as a function of the mixture fraction, pressure, and enthalpy of the mixture. Petit et al. [23] used tabulated species mass fractions and thermodynamic data to evaluate partial derivatives to achieve a self-consistent formulation.

Although considerable efforts have been made to study supercritical combustion, the current understanding is not sufficient to establish a quantitative knowledge base for design optimization of injectors and combustors. Numerical modeling has not yet played a predictive role in identifying key mechanisms and design attributes, for reasons that fall into two broad categories [24]. First, the development of high-fidelity and robust numerical tools that can accommodate all key physiochemical processes is a formidable task. Second, validation of such numerical tools at representative supercritical conditions still lags development because of the lack of detailed experimental data.

The modeling and simulation of supercritical combustion at conditions representative of realistic engine operating conditions pose an array of challenges [1,2]. First, a combustion system involves a broad range of length scales and Reynolds numbers. Turbulence modeling in different regions of the combustor requires different levels

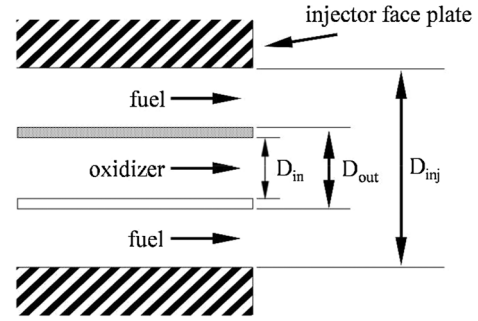


Fig. 1 Schematic diagram of a shear coaxial injector.

of grid resolution and modeling strategies. For example, typical turbulent pipe flows are encountered inside shear coaxial injectors with diameters less than several millimeters, as shown schematically in Fig. 1. Flow recirculation takes place immediately downstream of the injector lip, with a characteristic thickness in the submillimeter range. Mixing layers then develop between the two propellant streams to form a region within which chemical reactions occur and the flame spreads (typically 10–100 mm in length). The length scales of the flowfield vary dramatically in those regions and require different modeling approaches. Furthermore, numerical simulations of turbulent flows require realistic inlet boundary conditions and appropriate near-wall treatment. Turbulence/chemistry interaction also needs special consideration. In addition to all the traditional difficulties for turbulent reacting flows, unique problems arise at high-pressure conditions. Nonidealities in thermodynamic and transport properties impose extra numerical difficulties, especially in the transition from a subcritical to a supercritical state, which usually takes place in an extremely thin fluid layer and is characterized with steep gradients of those properties [1,2].

The present work extends a previously developed theoretical and numerical framework [25,26] to treat supercritical combustion using the compressible flamelet model at realistic engine operating conditions. The supercritical combustion of gaseous oxygen and hydrogen of a shear-coaxial injector is studied using the LES/flamelet, detached-eddy simulation (DES)/flamelet, and LES/flamelet/progress-variable approaches. Results are benchmarked with measured heat flux along the chamber wall and compared with simulations using different approaches. With the current wall resolution, LES is found to be preferable to DES, and the flamelet/progress-variable method is found to predict slightly shorter flames.

II. Theoretical Formulation

The theoretical formulation is based on a large-eddy simulation (LES) approach. Large-scale flow motions are resolved directly, whereas the effects of subgrid-scale (SGS) eddies on resolved flow motions are modeled. The model treats the Favre-filtered conservation equations of mass, momentum, and energy in the following conservative form [2].

Mass:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0 \quad (1)$$

Momentum:

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij})}{\partial x_j} = \frac{\partial (\tilde{\tau}_{ij} - \tau_{ij}^{\text{SGS}} + D_{ij}^{\text{SGS}})}{\partial x_j} \quad (2)$$

Energy:

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial ((\bar{\rho} \tilde{E} + \bar{p}) \tilde{u}_j)}{\partial x_j} = \frac{\partial (-\tilde{q}_j + \tilde{u}_i \tilde{\tau}_{ij} - Q_j^{\text{SGS}} - H_j^{\text{SGS}} + \sigma_j^{\text{SGS}})}{\partial x_j} \quad (3)$$

where the overbars and tildes denote the spatial and Favre filtering, respectively. ρ , u_j , p , E , τ_{ij} , and q_j represent the density and velocity components, pressure, specific total energy, viscous stress tensor, and heat flux, respectively. The nonlinearity of the viscous stress D_{ij}^{SGS} , heat flux Q_j^{SGS} , and viscous work σ_j^{SGS} terms are neglected because their contribution is small. The SGS stress term τ_{ij}^{SGS} is calculated with a compressible-flow version of the eddy-viscosity model [27,28].

A. Near-Wall Treatment

The computational cost of LES simulations increases rapidly with Reynolds number for wall-bounded flows. The grid number for wall-resolved LES of turbulent boundary layers scales with Re^n , where n is larger than 1.6 [29]. Calculations for practical geometries therefore present a formidable task. The situation becomes even more challenging for high pressures, due to the linear dependence of the Reynolds number on pressure. To alleviate computational difficulties and retain LES accuracy, various wall models have been developed [30,31], including the detached-eddy simulation (DES) method. In DES, the near-wall region is treated with traditional RANS modeling, and the outer flow region is resolved with LES, with a smooth transition between the two regions. The Spalart–Allmaras model is employed in the present numerical scheme [32,33], with subgrid length scales following the improved delayed DES (IDDES) formulation as described in [28].

B. Turbulent Combustion Models

Modeling of turbulence/chemistry interactions in a physically meaningful manner represents a critical challenge in numerical simulations of high-pressure combustion. In the present study, both the flamelet and the flamelet/progress-variable approaches are developed and implemented.

1. Flamelet Model

In turbulent combustion, if the local flame length scales are shorter than those of the Kolmogorov eddies, the flame falls in the flamelet regime. The inner structure of the flame remains the same as in a laminar flame, and the effect of turbulence can be seen as external strain imposed on the flame zone [34]. Taking advantage of the separation of scales, the inner structure of the flame can be handled separately from the turbulence. Instead of directly solving the transport equations for species concentration, which causes computational stiffness due to the small time scales of chemical reactions, the flamelet model solves the following conservation equation for the mixture fraction, in a coupled manner with the mass, momentum, and energy equations:

$$\frac{\partial \tilde{f}}{\partial t} + \frac{\partial(\tilde{\rho} \tilde{u}_j \tilde{f})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\tilde{\rho} \tilde{D} \frac{\partial \tilde{f}}{\partial x_j} + \Phi_j^{\text{SGS}} \right) \quad (4)$$

Because the mixture fraction f is a conserved scalar, the subgrid scalar flux Φ_j^{SGS} , can be easily modeled with an eddy viscosity model based on the gradient transport assumption. Local mass fractions can be obtained from a precalculated flamelet library using the mixture fraction, its subgrid variance, and the scalar dissipation rate as input parameters to determine the entry in the library [16]. The differential diffusion effect is not taken into account in Eq. (4). This may be a concern in laminar flow regions for fuels with nonunity Lewis numbers (such as hydrogen).

The subgrid filtered density function (FDF) is approximated with the β -function probability density function [34] because it provides a reasonable estimate of the SGS mixture fraction distribution for nonpremixed combustion [35]. The SGS variance of the mixture fraction, f'^2 , is modeled based on the scale similarity assumption [36],

$$\widetilde{f'^2} K_b = \overline{(\tilde{f} - \tilde{\bar{f}})^2} / \tilde{\bar{\rho}} \quad (5)$$

where K_b is a model constant chosen to be 3.

For convenience, the FDF of the scalar dissipation rate, $\tilde{P}(\chi_f)$, is modeled with a Dirac peak at the filtered scalar dissipation rate. The filtered rate of the scalar dissipation, $\tilde{\chi}$, is modeled based on an eddy viscosity approach [37]:

$$\tilde{\chi} = 2 \left(\frac{\nu}{Sc} + \frac{\nu_t}{Sc_t} \right) \left(\frac{\partial f}{\partial x_j} \frac{\partial f}{\partial x_j} \right) \quad (6)$$

The thermochemistry state relation can be established through a steady-state flamelet approach using any detailed chemical mechanism [38–41].

2. Flamelet/Progress-Variable Approach

Although the laminar flamelet method is relatively inexpensive and easy to implement, it suffers from a major deficiency: the mixture fraction does not carry any information about the chemical reaction state. The scalar dissipation rate is used to account for turbulence stretching and the quenching effect, but it does not provide a unique mapping from the mixture fraction to the corresponding chemical state [42]. The flamelet/progress-variable (FPV) method therefore uses a progress variable to replace the scalar dissipation rate. A progress variable can be defined as the sum of major combustion products. In the present work, in the present work, $C = Y_{\text{H}_2\text{O}} + Y_{\text{CO}} + Y_{\text{H}_2} + Y_{\text{CO}_2}$ for the Sandia flame D, and $C = Y_{\text{H}_2\text{O}}$ for the H_2 – O_2 flame. The transport equation for the progress variable can be derived from the species transport equations as follows [42]:

$$\frac{\partial \tilde{\rho} \tilde{C}}{\partial t} + \frac{\partial(\tilde{\rho} \tilde{u}_j \tilde{C})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\tilde{\rho} \alpha \frac{\partial \tilde{C}}{\partial x_j} + \Psi_j^{\text{SGS}} \right) + \tilde{\rho} \tilde{\omega}_C \quad (7)$$

where α is the diffusivity of the progress variable, $\tilde{\omega}_C$ is the reaction rate of the progress variable, and Ψ_j^{SGS} denotes the SGS flux of the progress variable. This model has been found to be able to account for extinction, ignition, and unsteady mixing [42].

In the FPV approach, as in the flamelet model, filtered combustion variables are obtained by convoluting the state relationships, $Y_i(f, C)$, with a joint filtered density function of the mixture fraction and progress variable, $\tilde{P}(f, C)$:

$$\tilde{Y}_i(x, t) = \int_0^1 \int_0^1 Y_i(f, C) \tilde{P}(f, C) dC df \quad (8)$$

Following [42], a delta function distribution for the FDF of the progress variable is assumed. The filtered mass fraction becomes

$$\tilde{Y}_i(x, t) = \int_0^1 \int_0^1 Y_i(f, C) \tilde{P}(f) \delta(C - \tilde{C}) dC df \quad (9)$$

where

$$\tilde{C} = \int_0^1 C(f, \chi_0) \tilde{P}(f) df \quad (10)$$

and χ_0 is a flame parameter, indicating that $\tilde{C}$ is calculated from a laminar flame with a characteristic scalar dissipation of χ_0 . The filtered reaction rate of the progress variable is obtained in a similar fashion:

$$\tilde{\omega}_C = \int_0^1 \int_0^1 \omega_C(f, C) \tilde{P}(f) \delta(C - \tilde{C}) dC df \quad (11)$$

3. Equation of State and Property Evaluation

The present numerical framework treats thermodynamic properties and numerical Jacobian matrices in a unified manner based on fundamental thermodynamics theories [1,26]. The scheme can accommodate any form of the equation of state, including the Soave–Redlich–Kwong and the ideal gas equations of state, as used in the

present study. The transport properties are obtained using extended corresponding-state principles as detailed in [1].

III. Numerical Method

The theoretical formulation outlined in the previous section requires a robust computational scheme to handle the numerical stiffness arising from steep variations of flow properties and disparities of characteristic time and length scales. A unified treatment of general fluid thermodynamics, based on the concepts of partial-mass and partial-density properties, is established and incorporated into a preconditioning scheme [26,43]. All the numerical properties, including the preconditioning matrix, Jacobian matrices, and eigenvalues, are derived directly from fundamental thermodynamics theories, rendering a self-consistent and robust algorithm. The details of the numerical framework are described in previous studies [25,26,43].

IV. Model Validation

The numerical accuracy of the present scheme within the context of LES has been carefully assessed based on the decay of the kinetic energy of isotropic turbulence, before further validation against the Sandia flame D [44] (shown in Fig. 2). The Sandia flame D has a moderate Reynolds number of 22,400 and a small probability of local extinction. A detailed database of measured temperature, species, and velocity profiles is available for validation [45,46]. The flamelet/progress-variable (FPV) approach was applied to this nonpremixed flame case. The GRI-Mech 3.0 [47] chemical kinetic mechanism was adopted to generate the flamelet library. Turbulence closure for the flowfield was achieved by a static Smagorinsky model. The turbulence at the inlet was generated by mapping its counterpart at a downstream location to the inlet, as described in [48], to ensure a fully turbulent pipe flow in the fuel nozzle.

The computational domain consists of a total of 2.7 million cells, with $310 \times 130 \times 64$ cells in the axial, radial, and azimuthal directions, respectively. Special attention was given to the grid arrangement in the center region to avoid the singularity problem. The grid is clustered near the wall, and 26 cells are employed to cover the nozzle rim with a thickness of 0.25 mm. The computational domain is about the same as that of the LES study by Pitsch and Steiner [49], but the grid was made finer than that used in [49] to ensure appropriate grid resolution. Calculations were run for more than three flow-through times before data were collected for analysis.

Figure 2a shows good agreement between the experimental flame image and the calculated temperature contour. Figure 2b shows the instantaneous temperature distribution of the flame after the flowfield reaches its stationary state. The color scale is cut off at 400 K for better illustration of the flame evolution. A bright flame zone is observed in a region with $20 \leq x/D_i \leq 40$, where the mixing and reaction of the fuel and oxidizer have completed. The flame tip is located around $x/D = 65$, which is very close to the visible flame length of 67 jet diameters measured in the experiment. In the vicinity of the fuel nozzle exit, as observed by Pitsch and Steiner [49], the flow structures resemble those of a laminar flow.

Figure 3 shows the calculated profiles of time-mean and rms temperatures as well as mass fractions of major species along the jet centerline. The results show excellent agreement with experimental measurements. The local minima and maxima are well captured. The flame evolution is dictated by both turbulent mixing and reactions. To separate out the effect of turbulent mixing on combustion, conditionally averaged quantities are calculated, as presented in Fig. 4. Good comparison with experimental data was achieved; the experimental uncertainties are 3% for the temperature, 4% for the mass fractions of water and CO_2 , 10% for OH, and 10–20% for CO [45]. These uncertainties suggest that the present model and numerical treatment function effectively in predicting turbulent nonpremixed flames.

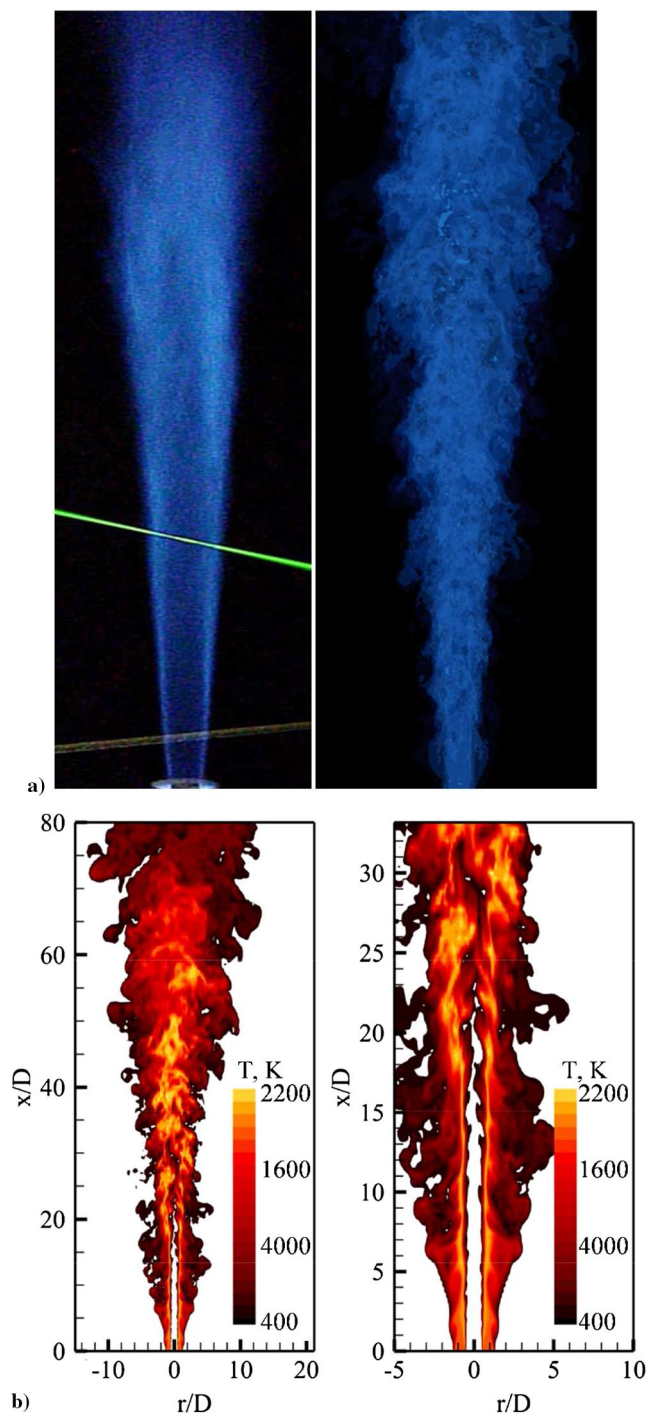


Fig. 2 Flame images: a) experimental (left) [45] and numerical (right); and b) global and close-up views, numerical.

V. Supercritical Combustion of GO_2 and GH_2 of Shear Coaxial Injector

The numerical framework described previously is applied to simulate the supercritical combustion of gaseous oxygen and hydrogen of a shear-coaxial injector as described in the experiment work in [13]. The dimensions of the injector, the combustion chamber, and the nozzle are given in Table 1. Table 2 summarizes the flow conditions of the two propellant streams. The operating pressure is 5.2 MPa. In the experiment [13], coaxial thermocouples are embedded in the chamber wall for temperature and heat flux measurements. Each thermocouple measures the temperature at two radial locations. The measured data are used as boundary condition in the numerical study. The wall heat flux is determined from the measured temperatures by solving a one-dimensional unsteady heat conduction equation.

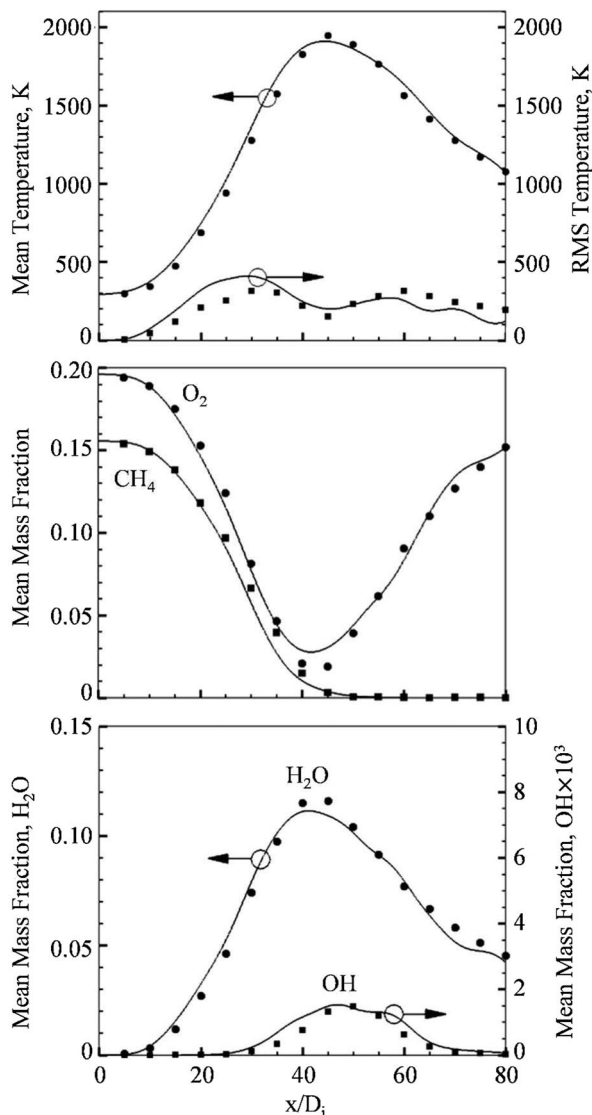


Fig. 3 Axial profiles of temperature and major species concentrations. Lines: simulation, symbols: experiment [45].

In the present study, the computational domain covers a flow region 5 mm upstream of the injector exit, the combustion chamber, and the exhaust nozzle. The grid consists of a total of 6.8 million numerical cells, with a distribution of $500 \times 212 \times 64$ in the axial, radial, and azimuthal directions in the chamber, respectively. Special attention is paid to the grid resolution close to the chamber wall, to ensure an accurate prediction of the wall heat flux. A minimum of $5 \mu\text{m}$ is used for the first grid spacing next to the wall, which corresponds to $y^+ < 1$. The grid stretching factor is less than 1.1. Grids are also clustered in the near field of the injector to resolve the local flow dynamics involving the interactions of turbulent shear and recirculating flows originating from the injector exit. There are 20 cells across the injector lip. The computational domain is divided into 297 blocks, with each calculated on a 2.4 GHz Opteron processor of a distributed-memory computing cluster.

The measured temperature distribution is applied to the combustor wall [13], whereas an adiabatic boundary condition is assumed at the injector interior wall. At the injector inlet, the bulk axial velocities of the oxidizer and fuel streams are selected to match the mean mass flow rates. The temperatures of both streams are fixed, and the pressure is obtained through a one-dimensional approximation to the axial momentum equation. A uniform temperature of 755 K is assumed at the oxidizer post and the head end of the combustion chamber. The nonslip condition is enforced along the solid wall. A supersonic outlet boundary is employed at the exit of the exhaust nozzle.

The thermochemistry state relation is established through a steady-state flamelet approach featuring a detailed H_2/O_2 reaction mechanism that includes eight species (H_2 , O_2 , H , O , OH , H_2O , and H_2O_2) and 19 reversible reactions [50]. This mechanism has been validated against experimental data over a pressure range of 0.03–8.8 MPa. To build the flamelet library, calculations were performed for counterflow diffusion flames, with the inlet conditions specified according to the fluid states listed in Table 2. The strain rate varies from 10 s^{-1} to the extinction point and decreases until the maximum flame temperature is reached [40]. A total of 200 different strain rates are considered.

The flowfield is initialized with a steady-state RANS solution. Calculation is first conducted for three flow-through times (27 ms) to wash out initial transients. Flow statistics are then collected for five flow-through times. The kinetic energy spectra in the near field of the injector are shown in Fig. 5. The slope of the turbulent kinetic energy (TKE) spectrum is consistent with the Kolmogorov–Obukhov ($-5/3$) law in the high-wave-number regime, which demonstrates that the grid size falls in the inertial subrange. The effect of grid resolution on the results is discussed further in Sec. VI.

VI. Results and Discussion

To assess the effects of turbulence and combustion modeling on the results, three different approaches are used in the present study. The baseline case employs LES and the flamelet model; the second case is based on DES along with the flamelet model; and the third case combines LES with the flamelet/progress-variable approach. For comparison, the same boundary conditions, grid system, and numerical parameters (such as Courant–Friedrichs–Lewy number and numerical dissipation coefficients) are used for all three cases.

A. Large-Eddy Simulation/Flamelet Approach

Calculations were first carried out for three flow-through times to allow the completion of flow transients. Once a stationary state is reached, the flow properties are collected for an extended time period to facilitate the extraction of statistically meaningful information. Figure 6 shows snapshots of the distributions of the temperature and mass fractions of hydrogen, oxygen, water vapor, and OH radicals. Immediately upon injection of reactants into the combustion chamber, strong shear layers occur as a consequence of the difference in momentum between the two reactant streams. The oxygen jet breaks up within a short distance from the injector exit. Large-scale flow structures arise and are convected downstream, promoting the mixing between reactants and ensuing flame development. As the flow further evolves, intensive turbulent mixing smears out flow nonuniformity and renders a well-developed cylinder flow. The most dynamic region appears before the end of the oxygen jet ($x \approx 0.05 \text{ m}$). This region is characterized by strong fluctuations of temperature and species concentrations, although the flame is anchored at the injector exit in the wake of the oxygen post. A thermal boundary layer is formed around the inner wall of the combustion chamber.

The time-averaged contour plots shown in Fig. 7 clearly indicate an upstream region that features a potential core flow surrounded by mixing layers and flame zones as well as a uniform downstream region. The hydrogen stream penetrates only a small distance into the combustion chamber before it mixes with the oxidizer and burns. The stream expands slightly in the radial direction due to the volume dilatation caused by the heat release. The flame length is dictated by the behavior of the oxidizer potential core, which in turn depends on the development of the surrounding turbulent mixing layers. Immediately downstream of the flame tip, the temperature achieves its maximum value and is uniformly distributed in the radial direction. The OH mass fraction is relatively small in the upstream region, compared to its equilibrium value of 0.08 in the downstream region.

Figure 8 shows the mean streamlines overlaid on the temperature contour. A large recirculation zone is observed between the flame and the chamber wall, and a smaller recirculation bubble appears in the corner of the combustor. The recirculation zones resemble that of a backward-facing step flow. The slope of the inner side of the bigger bubble is strongly correlated with the hydrogen flow, which expands

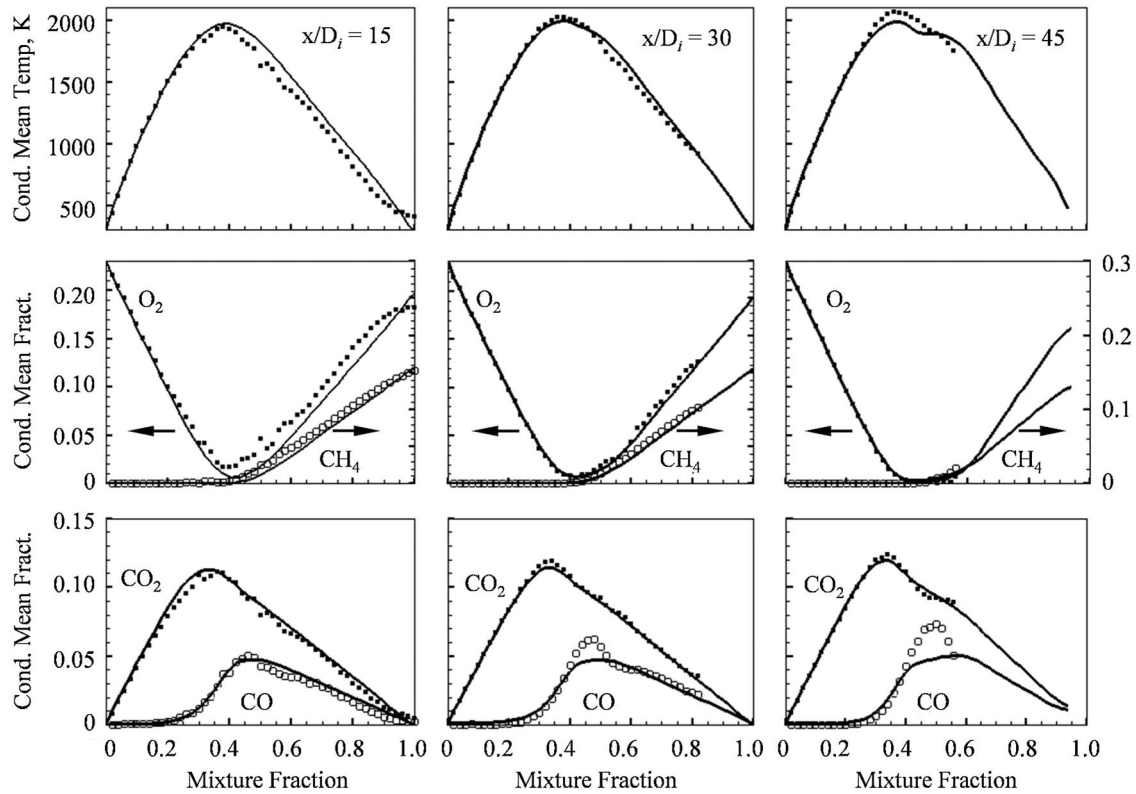


Fig. 4 Conditional average of temperature and major species concentration. Lines: simulation, symbols: experiment [45].

toward the wall due to the heat release from combustion. The recirculation zones are characterized by relatively small velocity and long residence time. It takes a very long time (more than 27 ms) for the disturbances in the recirculation zones to propagate out of the computational domain. The numerical convergence is slow, and thus the computational time required is significant, on the order of 0.1 s.

Figure 9 shows the measured temperature and heat flux along the chamber wall. The calculated heat flux is also included. The wall temperature profile shows a small peak close to the injector exit, and then a trough, before a rapid increase to the maximum, followed by a

slow and consistent decrease with downstream distance. The calculated heat flux shows exactly the same trend as the temperature. Figure 10 shows the distributions of the heat flux and near-wall ($y = 0.019$ m) axial velocity magnitude. The flow velocity is quite small at the corner of the combustion chamber, thereby minimizing heat flux through diminished heat convection. As the flow enters the small recirculation zone, the increased velocity enhances heat transfer and results in a small peak in the heat flux and wall temperature profiles next to the head end of the combustor. Moving farther downstream, the velocity reaches its minimum at the reattachment of the corner recirculation bubble (see Fig. 8). The corresponding decrease in the convective heat transfer produces local minima of the wall temperature and heat flux. As the recirculation bubble expands toward the wall, the heat transfer is enhanced by the increasing velocity magnitude and the presence of hot combustion products carried from the flame zone. A rapid increase thus occurs in the near-wall velocity and heat flux. The axial velocity magnitude and heat flux achieve their maximum values at approximately the same axial location ($x = 0.05$ m). A decrease in the axial velocity follows, and the increase in the flow temperature continues as combustion proceeds, resulting in a slow decrease in heat flux. At $x = 0.1$ m, combustion is complete, and a turbulent boundary layer starts to grow along the chamber wall, leading to the slow decrease of the wall temperature and heat flux.

Overall, the present numerical simulation correctly predicts the heat flux profile, especially in the downstream region, with an uncertainty of less than 10%. Although the magnitude of the calculated heat flux is higher than the experimental value in the upstream region ($x < 0.1$ m), the simulation captures the two local maxima in the wall temperature profile, as indicated by the heat transfer analysis. The uncertainties in the experimental results should also be noted. Both the measurement uncertainties and the uncertainties in calculating the heat flux from the data contribute to the error of the reported experimental data. The uncertainty of the heat flux measurement is reported to be about $0.2 \text{ MW}/(\text{m}^2 \cdot \text{s})$ [13], which is less than 2% of the mean value.

The heat transfer calculation from the experimental data also merits closer examination. In the experiment, each coaxial thermocouple measured temperature at two radial locations. The first sensor was

Table 1 Dimensions of shear coaxial injector and combustion chamber [13]

Parameter	Value
Oxygen post inner diameter D_{in}	5.26 mm
Fuel annulus inner diameter D_{out}	6.3 mm
Fuel annulus outer diameter D_{inj}	7.49 mm
Oxygen post recess length L_r	0.43 mm
Combustion chamber length L_c	337 mm
Combustion chamber diameter D_c	38.1 mm
Nozzle throat diameter D_n	8.17 mm

Table 2 Flow conditions and thermodynamic properties of propellants [13]

Parameter	Oxidizer stream	Fuel stream
p , MPa	5.2	5.2
Composition by mass	$0.945(\text{O}_2)/0.055(\text{H}_2\text{O})$	$0.402(\text{H}_2)/0.598(\text{H}_2\text{O})$
T , K	711	800
u , m/s	150	750
ρ , kg/m ³	26.8	3.3
$\dot{m}$, kg/s	0.09	0.032
$(\rho u^2)_F/(\rho u^2)_O$	2.92	2.92
M	0.31	0.51
Re^a	6.0×10^5	1.6×10^5
ν , m ² /s	1.35×10^{-6}	5.44×10^{-6}

^a $Re_{O_2} = u_0 D_{out}/\nu_0$, $Re_f = u_f(D_{inj} - D_{out})/\nu_f$.

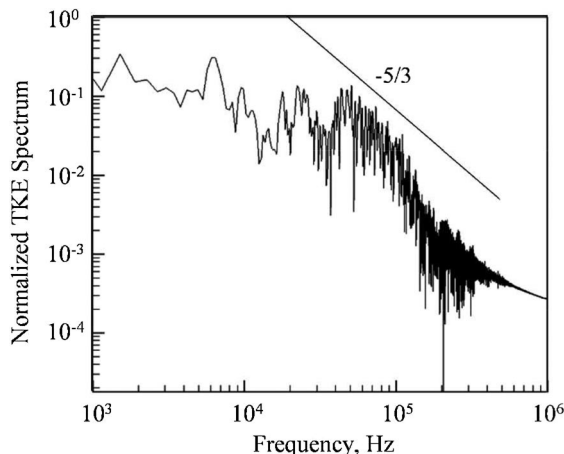


Fig. 5 TKE spectrum in the near field of the injector.

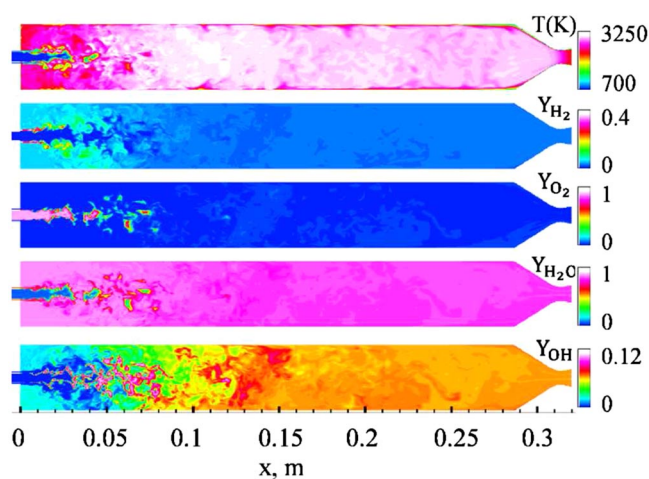


Fig. 6 Snapshots of temperature and mass-fraction fields of H_2 , O_2 , H_2O , and OH . LES/flamelet case.

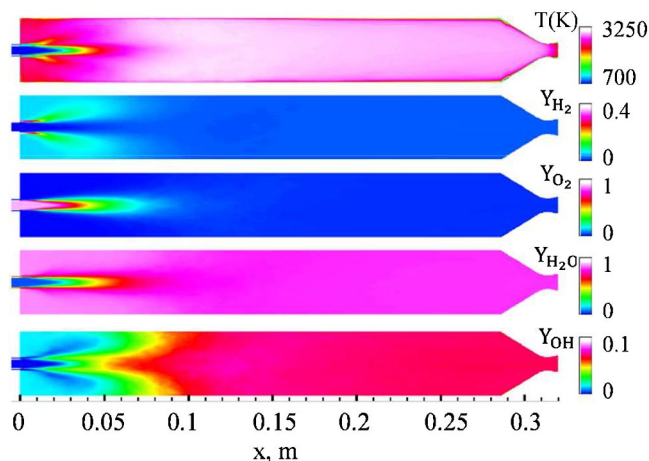


Fig. 7 Time-averaged fields of temperature and mass fractions of H_2 , O_2 , H_2O , and OH . LES/flamelet case.

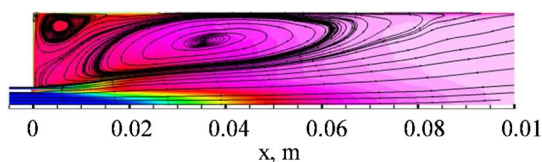


Fig. 8 Time-averaged streamlines overlaid on temperature distribution. LES/flamelet case.

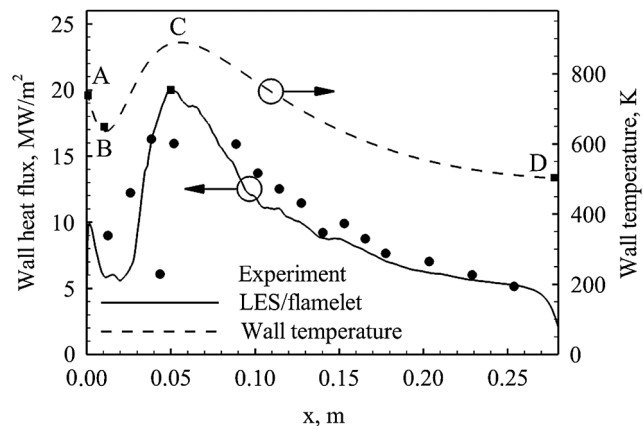


Fig. 9 Distributions of temperature and heat flux along combustor wall [13].

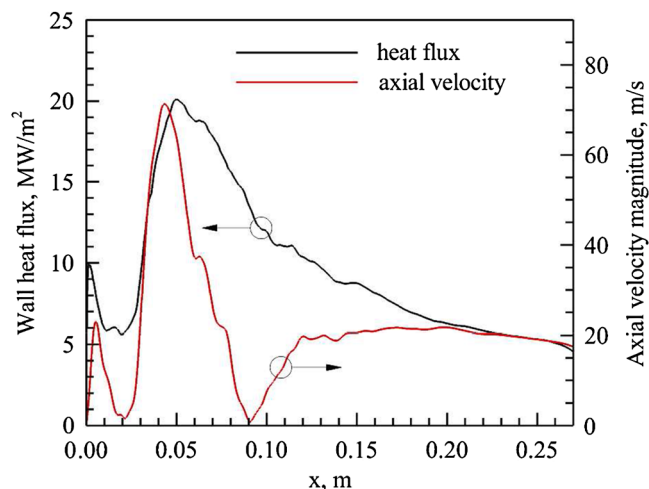


Fig. 10 Distributions of calculated wall heat flux and near-wall ($y = 0.019$ m) axial velocity magnitude. LES/flamelet case.

located at the surface of the chamber wall, was contoured to fit the chamber curvature, and measured the temperature at the surface of the combustion chamber. The second sensor was recessed by a quarter inch into the chamber wall. The wall heat flux was calculated from the temperature measurements with a one-dimensional transient heat conduction equation. Heat conduction in the axial direction was neglected, based on the argument that it is much smaller than in the radial direction. The assumption, however, is not always valid, especially in the upstream region (see Table 3). For example, at $x = 0.05$ m, the axial temperature gradient is about 25% of its radial counterpart. The present study as presented sheds some light on the role of axial heat transfer.

Standalone unsteady one- and two-dimensional simulations of the heat transfer in the chamber wall were performed using the measured surface temperature as boundary conditions. Figure 11 shows the predicted distributions of wall heat flux in the radial direction. Note that $t = 0$ corresponds to the time when steady combustion is just established in the chamber. The heat flux decreases with time due to the heat-sink nature of the combustor hardware. At $t = 0.8$ s, the one-dimensional (1-D) prediction closely matches the measurement. The 2-D calculation, however, predicts a slightly higher maximum and a lower minimum. The difference between the 1-D and 2-D models increases with time. At $t = 2$ s, the difference is about 50% of the 2-D result in the upstream region. Axial heat conduction plays a significant role, especially in the later stages of the flow evolution. The measured heat flux (based on the temperature gradient in the radial direction) appears to overshoot the minimum and underpredict the maximum values. The current calculations are believed to reflect the physical processes more closely than do the heat transfer values calculated from the experimental data.

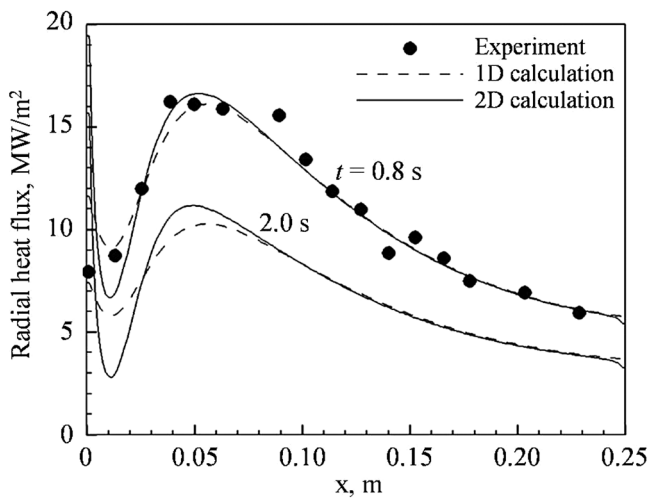
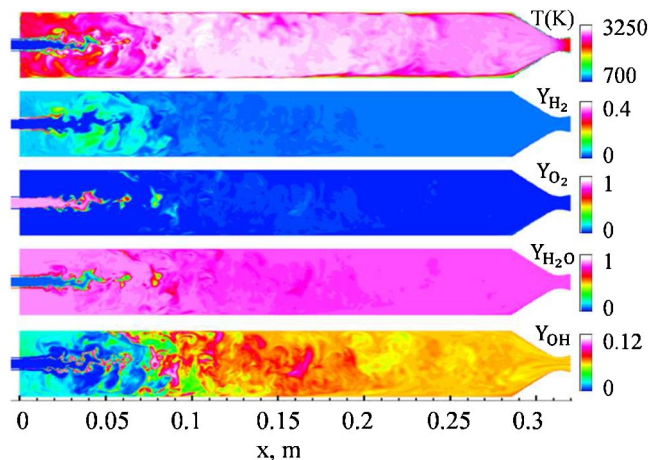
Table 3 Mean temperature gradients at different locations

Ranges considered	A-B	B-C	C-D	B-D
Axial direction, K/m	5730	2650	1050	1720
Points	A	B	C	D
Radial direction, K/m	18,600	33,000	18,600	12,000
Ratio, %	26	12	26	7

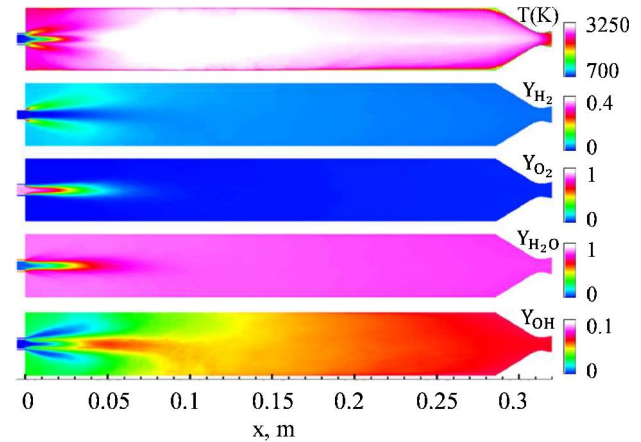
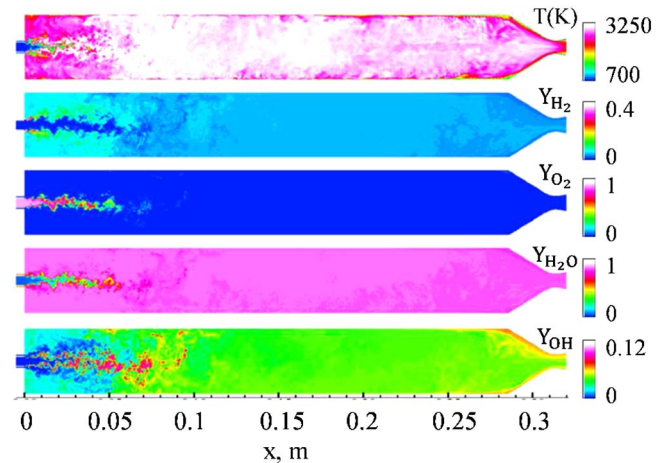
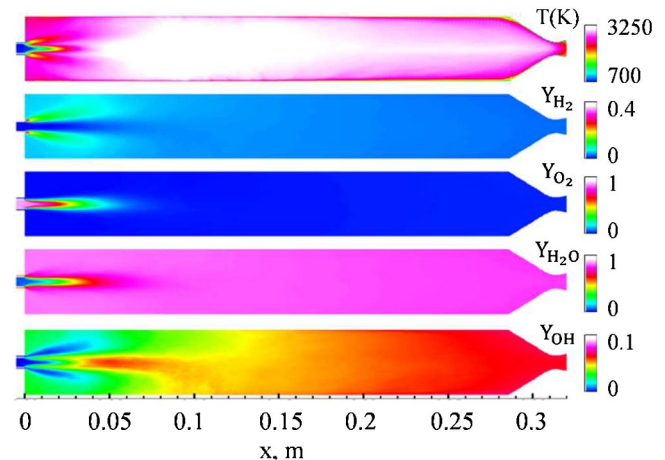
B. Detached-Eddy Simulation/Flamelet Approach

Near-wall turbulence modeling is important for accurate prediction of wall heat transfer. To assess the effect of wall treatment on heat-flux prediction, the IDDES methodology is adopted in the current work. The IDDES formulation works as traditional RANS in the near-wall layers and recovers to LES in the core flow. The turbulent viscosity near the injector exit is overshoot in the IDDES simulation, however, because of the slow LES development in mixing layers (discussed by Spalart [31]). A zonal approach that enforces LES in the mixing layers is employed to avoid this problem.

Figures 12 and 13 show the instantaneous and mean flowfields of temperature and mass fractions of hydrogen, oxygen, water, and OH radicals, respectively. (The asymmetric flow structures that appear in the mean contours, as also seen in the LES/FPV case, are due to the limited physical time of simulation). Because the major difference between the baseline and DES case lies in the treatment of the wall boundary layer, it is reasonable that the flame behavior, hydrogen stream penetration, and flow structure remain the same as in the baseline case. The thermal boundary layer along the wall, on the other hand, is different, in that it grows faster after reattachment.

**Fig. 11** Distributions of radial heat flux at two different time instants.**Fig. 12** Instantaneous fields of temperature and mass fractions of H_2 , O_2 , H_2O , and OH. DES/flamelet case.**C. Large-Eddy Simulation/Flame and Progress-Variable Approach**

Figures 14 and 15 show the results for the flamelet/progress-variable (FPV) case. Compared to the other two cases, the FPV approach leads to a shorter potential core and flame length. More dynamic structures are produced in the mixing layer. In addition, the FPV model predicts a higher OH level in the flame region and a lower OH level in the downstream region.

**Fig. 13** Time-averaged fields of temperature and mass fractions of H_2 , O_2 , H_2O , and OH. DES/flamelet case.**Fig. 14** Instantaneous fields of temperature and mass fractions of H_2 , O_2 , H_2O , and OH. LES/FPV case.**Fig. 15** Time-averaged fields of temperature and mass fractions of H_2 , O_2 , H_2O , and OH. LES/FPV case.

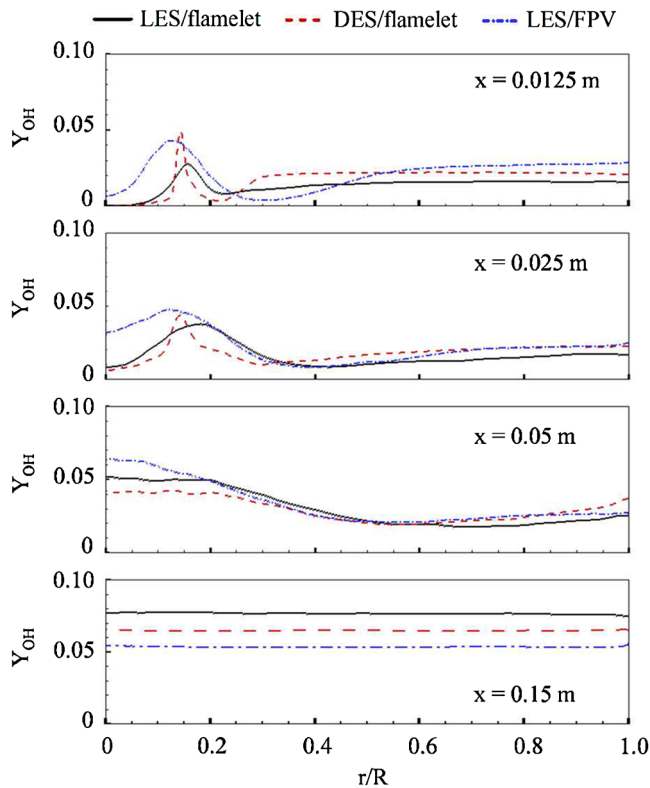


Fig. 16 Radial distributions of OH mass fraction at different axial locations.

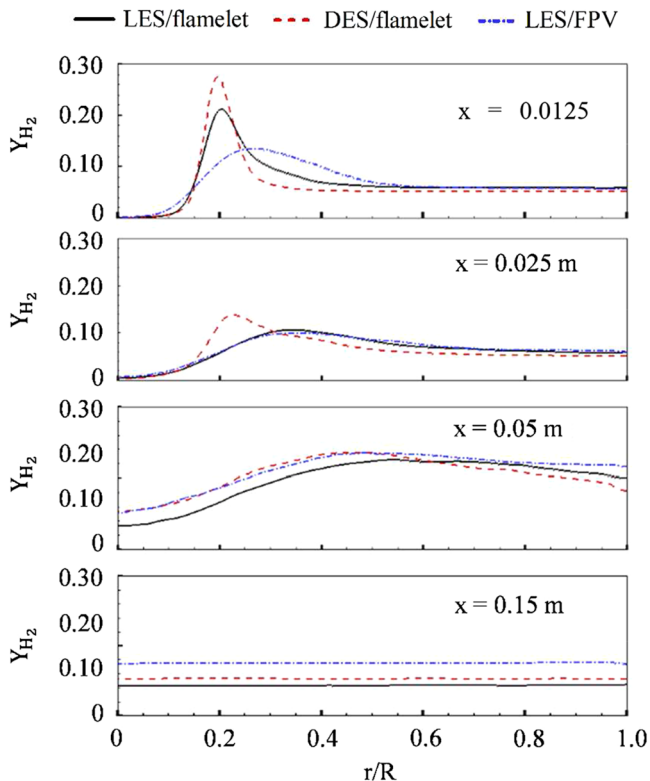


Fig. 17 Radial distributions of H_2 mass fraction at different axial locations.

D. Comparison of the Three Approaches

Figures 16 and 17 show the radial distributions of mass fractions of OH and H_2 at four different axial locations. In the vicinity of the injector faceplate ($x = 0.0125$ m), the baseline and DES cases show similar results. The LES/FPV approach leads to a higher OH

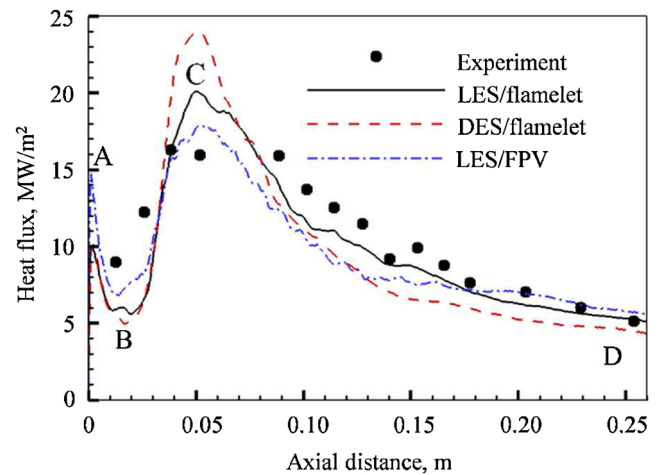


Fig. 18 Present numerical predictions of heat flux profiles compared to experimental data [13].

concentration near the centerline, corresponding to a shorter flame length, as also shown in Figs. 7, 13, and 15. The LES/FPV case features a wider flame region as compared to the other two cases.

At $x = 0.025$ m, the DES case shows slower development of the mixing layer and a thinner flame. For the FPV case, the combustion is half complete and exhibits a much higher and more uniform temperature profile.

At $x = 0.05$ m, the three cases show very similar results, except near the centerline, where the OH radical concentration indicates that more intensive combustion takes place in the FPV case, as reflected in the higher centerline temperature.

Moving farther downstream, at $x = 0.15$ m, a uniform flowfield has been established in all three cases. The temperature profiles are essentially identical, but the H_2 and OH mass fractions are slightly different. The larger value of H_2 mass fraction and small level of OH in the LES/FPV case indicate that combustion is yet to complete at this location and continues downstream.

Figure 18 presents the heat flux profiles for the three cases. The overall trends are very similar. In the near field of the injection, the velocity magnitude is small. The baseline and DES results are almost the same, suggesting that the LES and DES are equivalent in turbulence modeling with the present grid resolution. The peak heat flux for the baseline and DES case, however, deviates significantly at approximately $x = 0.05$ m, where the near-wall axial velocity approaches its local maximum. The difference in wall treatment between the baseline LES and DES cases causes significant difference in turbulent viscosity near the wall in the high-speed region and in the subsequent boundary-layer development. The mismatch of the two cases starting from the location of maximum heat flux indicates that the effect of wall treatment on heat flux is large. Given the small mesh size distribution along the combustor wall, the turbulent boundary layers are well resolved in the LES. The DES approach that blends the RANS model near the wall and LES in separated flow regions is believed to be less accurate than LES. The FPV case has a much shorter flame and different recirculation flows, which give rise to larger heat flux in the near-field region but smaller heat flux in the downstream region, where combustion is complete and a thermal boundary layer is established along the combustor.

It is clear from the preceding studies that both the combustion model and the near-wall turbulence treatment play an important role in determining the heat transfer characteristics. The wall treatment directly affects the boundary layer and the ensuing heat-transfer behaviors but does not change the locations of extreme values. The combustion model, on the other hand, has a direct impact on the flame and recirculating flow evolution. All the cases are qualitatively consistent in terms of the flame and flow structures as well as the heat flux profile, and so the baseline results will be used for discussion in the rest of the paper.

Table 4 Grid distribution in combustion chamber

Numerical studies	Axial direction	Radial direction	Azimuthal direction	Total grid number (million)
Current study	500	212	64	6.8
3-D LES, Masquelet and Menon [18]	611	87	65	3.5
3-D LES, Tucker et al. [51]	1536	368	256	225
2-D URANS, Lian et al. [52]	—	—	—	0.25
2-D RANS, Tucker et al. [51]	98	98	—	0.01

E. Comparison with Other Numerical Studies

The baseline case was benchmarked with computational simulations conducted by several different research groups [24,51]. Table 4 lists the numerical grid distributions employed in these studies. Compared to the present work, Oefelein's grid is 3, 4.0, and 1.7 times finer in the axial, azimuthal, and radial directions, respectively. Masquelet and Menon's grid [18] is on par with the present work in the axial and azimuthal directions but much coarser near the wall due to the use of near-wall treatment. It should be noted that the Pennsylvania State University LES in [51] was a 2-D axisymmetric simulation, which has been updated to the present 3-D LES. The unsteady Reynolds-averaged Navier–Stokes (URANS) case by Lian et al. was further refined in [52].

Figure 19 shows the distributions of the wall temperature and heat flux profiles along the combustion chamber for all the numerical studies and experimental data. In the downstream region ($x > 0.1$ m), all the numerical studies capture the trend of the heat flux rate accurately, except for the RANS case. The heat flux profiles differ mainly in the upstream region ($x \leq 0.1$ m). The present study, Menon's LES, and Merkle's URANS all predict the spike in the vicinity of the head end and the local minimum, but the magnitudes are quite different. Oefelein's 3-D LES result agrees quite well with experimental data, though it misses the local minimum in the wall temperature profile. Considering the effect of axial heat conduction in the chamber wall discussed previously, this result appears to overpredict the actual heat flux (in the region between $x = 0.04$ and 0.1 m). The maximum heat flux takes place at approximately the same axial location for all the results, but the shapes and magnitudes of the maxima are noticeably different.

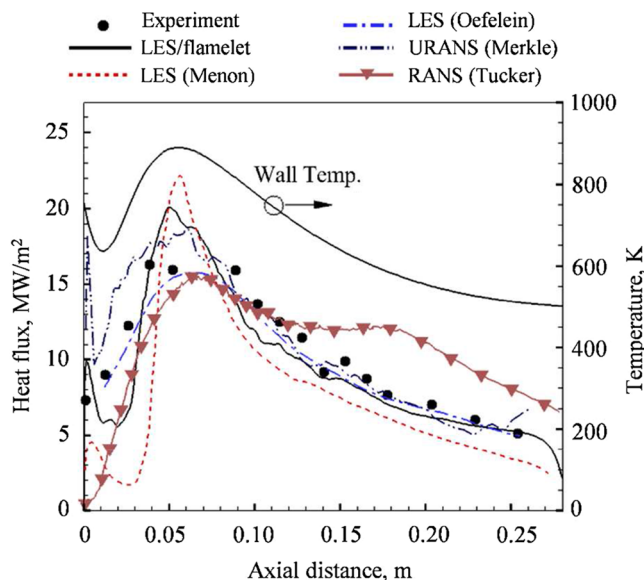
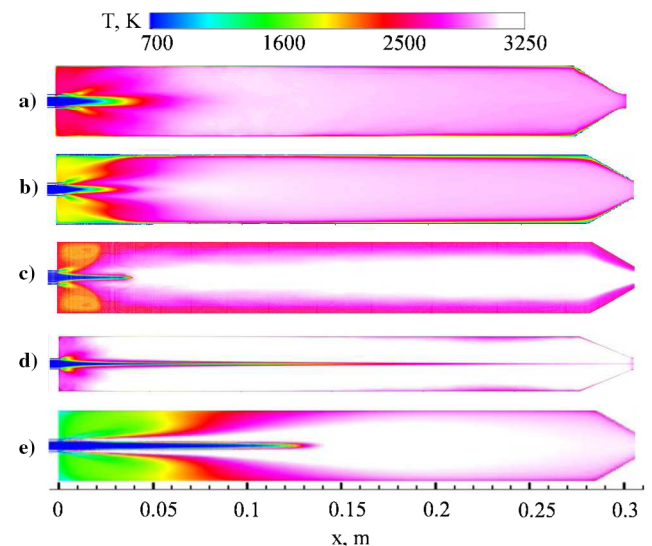
Figure 20 shows the calculated mean temperature distributions. All the cases exhibit uniform temperature distributions in the downstream region, except for Oefelein's case (Fig. 20c), which is characterized by a hot core region and a thick thermal boundary layer with much lower temperature. Menon's result (Fig. 20b) also indicates the existence of a thermal boundary layer, a phenomenon responsible for

the underprediction of heat flux. This may be attributable to the coarse grid resolution in the boundary layer. In the upstream region, the temperature and ensuing heat flux distributions differ considerably.

Figure 21 shows the mean streamlines overlaid on the temperature field in the near field of the injector. Except for Oefelein's case, they all feature two recirculation zones: a small clock-wise rotating zone in the corner and a larger, stronger, counterclockwise rotating zone next to it. Oefelein's case shows three zones, with the first two rotating in opposite directions. The difference may be attributable to grid resolution, turbulence modeling, combustion models, or numerical algorithm. The grid resolution in the present work is slightly coarser in the radial direction than Oefelein's, but the predicted flow speed in the recirculation zone is quite low. Menon's grid is much coarser in the radial direction, but it predicts flow structures very similar to the present study. This suggests that the disparity in the calculated recirculation flow is not caused by grid resolution alone, but by the combustion and turbulence modeling, coupled with grid resolution.

The correlation between heat flux and near-wall velocity (see Fig. 10) suggests that, in Oefelein's case, the near-wall velocity increases from zero at the corner to its first peak in the center of the big recirculation bubble and then decreases to a local minimum between the two bubbles at $x = 0.025$ m. The heat flux, however, does not show a decrease at $x = 0.025$ m, probably due to the hot combustion products brought to this region. In the other cases, no hot gas comes directly to the region between the two bubbles. Farther downstream, the elongated bubble acts as a mixing layer, through which heat is exchanged between the hot core region and the cold chamber wall. This observation suggests that the underlying physics of the heat flux profile in Oefelein's case is quite different from all other cases. Further analysis is required to illuminate the physical processes involved.

To further illuminate the flame structure, the time-mean distributions of OH mass fraction are shown in Fig. 22. The 2-D RANS case, with neither the large-scale mixing nor the subgrid-scale turbulence chemistry interactions included, results in a long, thin flame in the mixing layer before the oxidizer jet breakup at the flame tip, where

**Fig. 19** Comparison of predicted wall heat flux with experimental data.**Fig. 20** Time-averaged temperature: a) present study, b) Menon [18], c) Oefelein [51], d) Merkle [52], and e) Tucker [51].

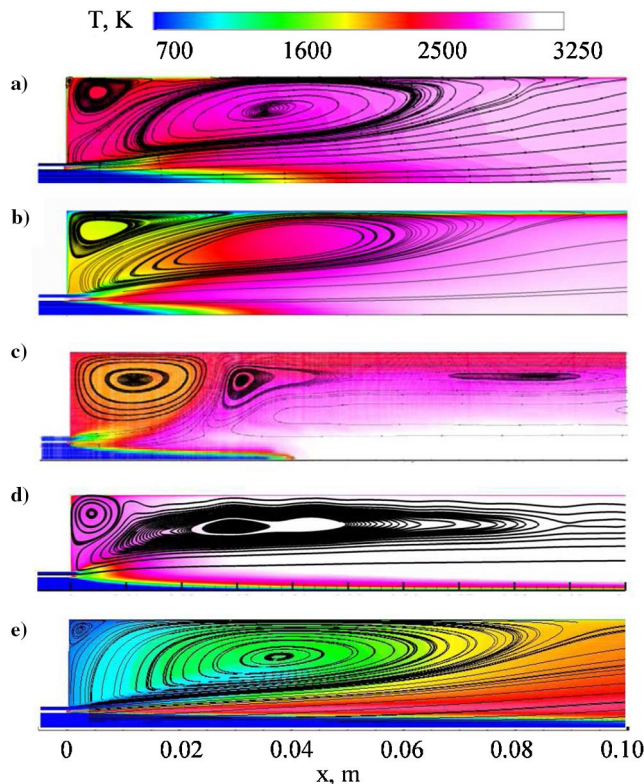


Fig. 21 Time-averaged streamlines overlaid on temperature: a) present study, b) Menon [18], c) Oefelein [51], d) Merkle [52], and e) Tucker [51].

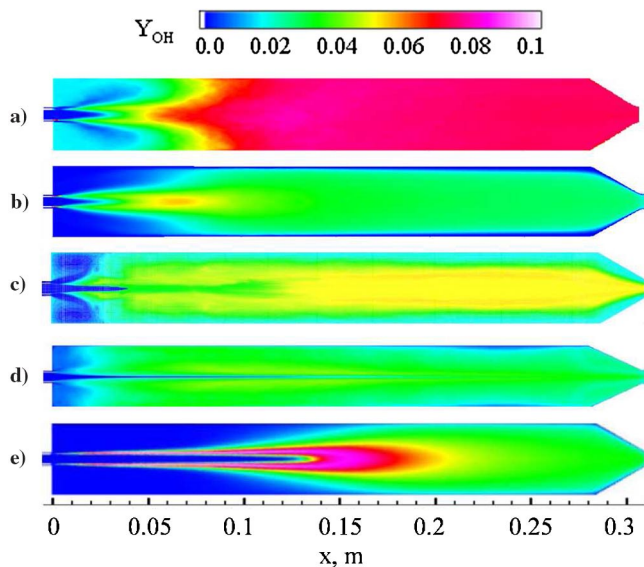


Fig. 22 Time-averaged fields of OH mass fraction: a) present study, b) Menon [18], c) Oefelein [51], d) Merkle [52], and e) Tucker [51].

intense chemical reaction takes place in a small region. The 2-D RANS result is questionable and thus is omitted from further discussion here.

The OH mass fractions show significant differences among the LES cases. The differences in the upstream region indicate different flame structures. In the downstream region, the OH mass fraction in Oefelein's case is consistent with its temperature profiles. There is not much combustion product between the radial location of 10 mm and the chamber wall, a region that occupies 75% of the combustion volume. On the other hand, the results from the present study and Menon and Merkle's cases are radically uniform. The combustion is complete, and hot products fill the entire chamber.

Figure 23 shows the time-mean field of hydrogen mass fraction. The hydrogen flow along the wall in Oefelein's case is visible

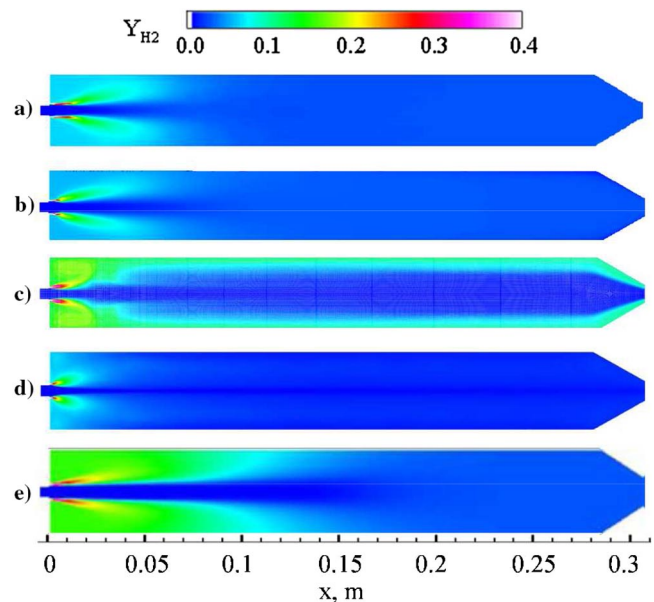


Fig. 23 Time-averaged distributions of H_2 mass fraction: a) present study, b) Menon [18], c) Oefelein [51], d) Merkle [52], and e) Tucker [51].

throughout the chamber. All other cases show uniform profiles in the downstream region. The near-field mixing rates are significantly different and demand careful examination. The RANS case dramatically underpredicts the mixing between the two propellant streams, due to the lack of resolution of flow motions. All of the other cases feature much shorter fuel streams. The URANS case has the shortest hydrogen potential core; Oefelein's hydrogen stream is the second shortest and is the shortest among the three LES studies. In Oefelein's case, the hydrogen jet breaks up immediately after being injected into the chamber, especially on the outer side of the fuel stream. Similar breakup is not observed in Menon's case or the present study. If the hydrogen stream is not entrained into the corner region, more intensive reactions are expected to release thermal energy and accelerate the flow to form an expanded recirculation zone, as in the other cases. It is the entrainment of hydrogen into the corner recirculation flow that hinders the mixing with oxygen and subsequently modifies the flow structure and wall heat flux.

It is noted that the LES/FPV case also has very short oxidizer and fuel streams, due to early breakup, but no hydrogen is entrained into the corner, as in Oefelein's case. The LES/FPV approach has finite rate chemistry built into the model and thus has the ability to capture unsteady combustion behaviors. Menon's case uses detailed finite rate chemistry to calculate chemical reaction rates. Neither case produces a fuel-rich recirculation bubble in the corner.

The significant differences in the near-field flame structure and wall heat flux seen in these five cases are attributed to the effect of turbulent combustion modeling. Two possible scenarios exist. First, Oefelein's approach reproduces the physics the best. Second, the present study accurately predicts the major physics in the chamber and the heat flux along the wall. If the former is the case, the divergence in the results is most likely caused by the effects of grid resolution on combustion modeling. In Oefelein's case, the grid resolution is so fine that the local mixing and flame structures can be largely resolved. In the other studies, similar turbulence modeling does not lead to the same flame structures because the grids are much coarser, and the subgrid-scale combustion modeling strategies do not predict the subgrid-scale mixing and combustion properly. The current turbulence models are not capable of reproducing the physics correctly with relatively affordable computational resources. Further development of combustion models is crucial.

Heat flux is the result of a series of processes taking place in the chamber. After the propellants are delivered into the chamber, mixing is achieved through the shear layers between the fuel and oxidizer stream. The flame is anchored in the near field of the injector and rapidly spreads to the whole chamber due to propellant jet breakup and rapid mixing. Heat is released in the flame region, and combustion products

are convected with large-scale turbulent motions to the combustor wall, where heat transfer from the hot gases to the chamber wall occurs. Temperature nonuniformity in the axial direction causes axial heat conduction within the copper heat-sink wall, where the temperature is measured for calculation of heat flux at the inner surface of the wall.

In modeling these physical processes, various uncertainties arise. The grid resolution, turbulence modeling, turbulence/chemistry interactions, and treatment of the wall boundary layer all have significant effects on the final prediction of heat flux. A careful analysis of the results identifies the underlying processes and suggests that close attention be paid to the modeling characteristics to produce physically correct results.

More experimental data always help verify the analysis and simplify the model validation process. Specifically, if flowfield images, such as shadowgraphs and OH emission images, could be obtained with simultaneous heat flux data, it would be much easier to assess the accuracy of numerical schemes. If both heat flux profiles and flow/flame structures can be simulated correctly, the reliability of computational-fluid-dynamics codes can be dramatically improved, and numerical analysis tools would offer the possibility of cost-effective design optimization.

VII. Conclusions

A comprehensive theoretical/numerical framework has been established for supercritical combustion modeling. The accuracy of the entire scheme was first assessed for the spectrum of turbulence kinetic energy in decaying isotropic turbulence. The numerical framework was then validated against a nonpremixed turbulent flame (Sandia flame D). The calculated flame shape was found to resemble the experimentally determined image. The axial distributions of time-mean and rms temperatures, as well as mass fractions of major species, are in excellent agreement with the measurements. The conditional averages of temperature and mass fractions of major species at different axial locations further demonstrate the accuracy of the current modeling approach.

The gaseous H_2 - O_2 combustion of a shear coaxial injector at supercritical conditions was studied with several turbulence and combustion models. The large-eddy simulation (LES)/flamelet model combination shows the best results in terms of heat flux prediction. The detached-eddy simulation (DES)/flamelet model gives similar flame and flow structures in the separated flow region, where DES essentially works as LES. The major difference lies in the development of the thermal boundary layer, especially in the high-speed region, because DES models the boundary layer in a RANS regime. The LES/flamelet and LES/flamelet/progress-variable models show considerable differences in the near-field flame structures. The LES/FPV approach leads to earlier jet breakup and a shorter flame as compared to the baseline LES/flamelet case, and the higher temperature in the near-field region leads to a slightly higher calculated near-field heat flux. Downstream of the flame tip, the time-mean temperature in these two cases is very close, although the difference in the upstream region causes an offset in the heat flux profile in the downstream region. All three cases show that both turbulence and combustion models have a strong effect on the wall heat flux prediction.

The results were carefully compared with numerical predictions from other studies, including different types of LES and URANS. The near-field flame structures in the LES cases show huge differences in terms of jet lengths, temperature and species distributions, and flow structures (such as recirculation zones). The analysis with the finest grid resolution (Oefelein's LES case) best predicts the measured heat flux profile, although the recirculation zones in the near field and species concentrations in the downstream regions are significantly different from the predictions of all other studies. The URANS, Menon's LES, and the current study, on the other hand, show qualitatively similar flow structures and species distributions. The existing experimental measurements of wall heat flux are insufficient for code validation. Further experimental information such as near-field flame images are required to validate calculated flame structures.

Acknowledgments

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