

Nonadiabatic Flamelet Formulation for Predicting Wall Heat Transfer in Rocket Engines

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A flamelet-based combustion model is proposed for the prediction of wall heat transfer in rocket engines and confined combustion systems. To account for convective heat loss due to the interaction of the flame with the wall, a permeable thermal boundary condition is introduced in the counterflow diffusion flame configuration. The solution of the resulting nonadiabatic flame structure forms a three-dimensional manifold, which is parameterized in terms of mixture fraction, progress variable, and temperature. The performance of the model is first evaluated through a direct numerical simulation analysis of an H_2/O_2 diffusion flame that is stabilized at an inert isothermal wall. The developed nonadiabatic flamelet model is shown to accurately predict the temperature, chemical composition, and wall heat transfer. Combined with a presumed probability density function closure, the model is then applied to large-eddy simulation of a single-injector rocket combustor to examine effects of heat transfer on the turbulent flame structure in rocket engines.

Nomenclature

C	=	progress variable
c_p	=	specific heat capacity at constant pressure
D	=	diffusion coefficient or diameter
Da	=	Damköhler number
E	=	specific total energy
e	=	specific internal energy
I	=	identity matrix
j	=	diffusion flux vector
L	=	characteristic device length scale
Nu	=	Nusselt number
Pr	=	Prandtl number
p	=	pressure
Q	=	heat release rate
q	=	heat flux vector
R	=	gas constant
r	=	radial direction
Sc	=	Schmidt number
T	=	temperature
t	=	time
u	=	velocity vector
u	=	axial velocity
x	=	streamwise or axial direction
Y	=	species mass fraction vector
Y_α	=	mass fraction of species α
y	=	wall-normal direction

Z	=	mixture fraction
δ_f	=	characteristic flame length scale
δ	=	boundary-layer thickness
μ	=	dynamic viscosity
ρ	=	density
τ	=	time scale
τ	=	viscous stress tensor
χ	=	scalar dissipation rate
ϕ	=	transported scalar
ψ	=	generic scalar vector
$\dot{\omega}$	=	source term vector
$\dot{\omega}_\alpha$	=	source term of species α

Subscripts

F	=	fuel
O	=	oxidizer
st	=	stoichiometric value
t	=	turbulent quantity
wall	=	quantity at the wall

Superscripts

-	=	Reynolds average
~	=	Favre average
//	=	fluctuations around mean
+	=	wall units

I. Introduction

TURBULENT combustion processes in technical systems, such as furnaces, internal combustion engines, gas turbines, and rocket motors, require the consideration of heat transfer and flame-wall interactions [1–3]. In particular, a major source for failures in the early design of rocket engines has been attributed to the inadequate characterization of heat transfer to the injector face plate, the combustion chamber, and the rocket skirt [4,5]. Therefore, the capability of accurately predicting the thermal loading is crucial for reducing uncertainties during the early development of rocket engines. The convective heat transfer rate from the hot gas to the solid surface is essential to the cooling of the combustion and thrust chamber walls, which has a direct impact on their lifetime [6].

Several challenges arise in the modeling of turbulent combustion processes that are characterized by significant heat losses.

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Specifically, strong heat losses can lead to flame quenching, enhanced emissions, and combustion instabilities [7–14]. Another issue is that the heat flux introduces a dependence on the alignment between flame and wall, spanning the limiting cases of head-on quenching and side-wall quenching [2]. Finally, the description of the thermoviscous boundary-layer structure introduces substantial resolution requirements, and wall-modeled large-eddy simulation (LES) for the accurate prediction of wall heat transfer is still an ongoing research topic [15–19].

Despite the remarkable progress in the development of computational methods for the prediction of rocket motors [20–24], the issue of modeling heat transfer has only recently found some attention. Most notable is the coordinated effort by Tucker et al. [25] on assessing current modeling capabilities in predicting wall heat transfer in a uni-element rocket injector. Although various modeling approaches (LES, (unsteady) Reynolds-averaged Navier–Stokes), combustion models (finite rate chemistry, flamelet formulations), algorithms, and grid arrangements (two- and three-dimensional computational domains) as well as different turbulence and subgrid closure models were employed, the outcome of this work represents an important step in establishing a benchmark for assessing the predictive capability of currently employed rocket engine modeling tools.

The objective of this work is to develop a flamelet-based combustion model for the prediction of wall heat transfer in rocket engines. Commonly employed flamelet models that are based on steady flamelet formulations rely on the underlying assumption that the flame state of a particular flamelet relaxes to the steady-state solution on a sufficiently fast time scale [26–29]. However, heat-loss processes that are associated with radiative and convective heat transfer evolve on time scales that are slow compared to chemical processes in typical combustion applications. To incorporate these nonadiabatic processes into the steady-state flamelet formulation, extensions have been proposed [30–40]. These extensions considered the modeling of radiative and convective heat losses, which were achieved by introducing enthalpy defect variables, including sink terms in the energy equation, or by rescaling the heat-release rate. Although these models provided improved predictions for temperature, they introduce assumptions about excess enthalpy, locality of the heat loss, and boundary conditions that limit their extension to turbulent diffusion flames.

The present work considers the modeling of wall heat transfer in the context of diffusion flames. To this end, convective heat-loss effects are introduced into the flamelet formulation locally to represent side-wall quenching in a physically consistent representation. The mathematical formulation of the model is described in Sec. II. After presenting the numerical approaches employed in Sec. III, the accuracy of the nonadiabatic flamelet model is examined through direct numerical simulation (DNS) in Sec. IV. The model is subsequently applied in LES of a uni-element rocket injector in Sec. V. The paper finishes with conclusions.

II. Nonadiabatic Flamelet Formulation

A. Model Formulation

The present work is concerned with the modeling of wall heat-loss effects and flame–wall interaction in the context of the laminar flamelet formulation [41]. In this formulation, the direction of heat flux is assumed to be primarily aligned with the gradient of mixture fraction (i.e., normal to the flame surface). As a result, heat losses can be introduced by an additional thermal boundary condition, whose location in mixture fraction coordinate is denoted by Z_{wall} . This is illustrated in Fig. 1, showing the schematic of the counterflow diffusion flame.

This configuration is modified by introducing a permeable wall that is isothermal and chemically inert. Without loss of generality, we assume in this study that the wall approaches the flame from the fuel-rich side, and corresponding boundary conditions in physical space are

$$x = x_{\text{wall}}; T = T_{\text{wall}}; \partial_x Y|_{x_{\text{wall}}^+} = \partial_x Y|_{x_{\text{wall}}^-}; \partial_x Z = 0 \quad (1)$$

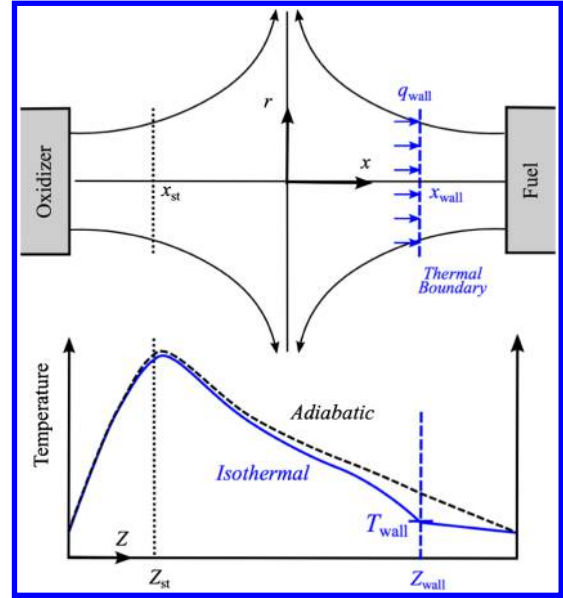


Fig. 1 Schematic of counterflow diffusion flame with flame-normal heat transfer in which the heat flux vector is aligned with the mixture fraction gradient.

where x_{wall} identifies the wall location, and the superscripts $+/-$ denote the two sides of the wall. The last condition ensures continuity of species flux, and ∂_x denotes the partial derivative with respect to the axial coordinate x . In this context, it is noted that this model can be extended by considering more general boundary conditions, for instance by including surface-catalytic effects, heat flux conditions, or wall-recombination reactions.

To illustrate the model formulation, we consider flamelet equations with unity Lewis number assumption, and the model can be directly extended to account for preferential diffusion [42]. After applying the flamelet transformation to the conservation equations for species and energy under consideration of boundary conditions, given in Eq. (1), the nonadiabatic flamelet equations take the following form:

$$\partial_t Y - \frac{\chi}{2} \frac{\partial^2 Y}{\partial Z^2} = \dot{\omega} \quad (2a)$$

$$\partial_t T - \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \frac{\chi}{2} \frac{\partial \ln(c_p)}{\partial Z} \frac{\partial T}{\partial Z} = \frac{Q}{c_p} \quad (2b)$$

for $Z \in (0, Z_{\text{wall}})$, and

$$\partial_t Y - \frac{\chi}{2} \frac{\partial^2 Y}{\partial Z^2} = 0 \quad (3a)$$

$$\partial_t T - \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \frac{\chi}{2} \frac{\partial \ln(c_p)}{\partial Z} \frac{\partial T}{\partial Z} = 0 \quad (3b)$$

for $Z \in (Z_{\text{wall}}, 1)$. These equations are solved subject to the following boundary conditions:

$$Z = 0: T = T_O; \quad Y = Y_O \quad (4a)$$

$$Z = Z_{\text{wall}}: T = T_{\text{wall}}; Y|_{Z_{\text{wall}}^-} = Y|_{Z_{\text{wall}}^+}; \partial_Z Y|_{Z_{\text{wall}}^-} = \partial_Z Y|_{Z_{\text{wall}}^+} \quad (4b)$$

$$Z = 1: T = T_F; \quad Y = Y_F \quad (4c)$$

where Z_{wall} is a model parameter representing the location of the thermal boundary condition transformed into the mixture fraction coordinate. The subscripts “F” and “O” refer to conditions in the fuel and oxidizer stream, respectively. Because of the Neumann boundary

condition of the mixture fraction at the wall, the scalar dissipation rate is thus modified to be

$$\chi = \chi_{st} \exp \left\{ -2 \left(\operatorname{erfc}^{-1} (2Z/Z_{wall}) \right)^2 + 2 \left(\operatorname{erfc}^{-1} (2Z_{st}/Z_{wall}) \right)^2 \right\} \quad (5)$$

The location and the temperature of the wall condition, namely Z_{wall} and T_{wall} , can be modified to span the entire gamut of possible conditions of flame–wall interaction. The specification of the wall conditions can also be acquired through measurements of mixture fraction and temperature in the near wall region. Thermal quenching will occur as the wall approaches the flame and heat loss is amplified.

The nonadiabatic flamelet model proposed introduces three different time scales, representing the characteristic diffusion time scale τ_{diff} , the convective heat transfer time scale τ_{conv} , and the characteristic chemical time scale τ_{chem} . The convective time scale is not explicitly specified but embedded in the time scale for the change of Z_{wall} . The ratio between these scales can be written as [37,43]

$$\tau_{diff} : \tau_{conv} : \tau_{chem} = Da : \frac{Da Pr L^2}{Nu_L \delta_f^2} : 1 \quad (6)$$

where Da is the Damköhler number, Pr is the Prandtl number, Nu_L is the Nusselt number associated with the device length scale L , and δ_f is the characteristic flame length scale. For combustion in hydrogen-fueled liquid rocket engines, the first two terms on the right-hand side are much greater than unity [44], indicating that the species distribution of the flamelet is able to directly respond to temperature variations by heat-loss effects because the characteristic chemical time is short compared to the time scales associated with diffusion and convection. It is thus justified to solve Eqs. (2) and (3) under steady-state conditions.

Equation (2) and (3) are implemented into the FlameMaster solver [45]. Sample solutions at conditions similar to those specified in Sec. V are shown in Fig. 2, where fuel, oxidizer, and wall temperatures are all set to be 500 K. The results in Figs. 2b–2d are obtained at $\chi_{st} = 200 \text{ s}^{-1}$ with Z_{wall} approaching the flame from the fuel side. The monotonic decrease of temperature shows an increasing level of heat loss as Z_{wall} approaches Z_{st} . Despite the fact that the maximum flame temperature decreases by 2000 K, the mass fraction of the product species H_2O shows much less sensitivity and is almost unaffected by the heat loss beyond the reactive region. In contrast, the hydroxyl-radical mass fraction is significantly reduced. This observation suggests that the difference between the mass fraction of OH and H_2O may serve as a diagnostic for the presence of convective heat losses to the wall.

B. Tabulation Approach

The procedure for generating the chemistry table for the proposed model and its coupling with the flow solver are schematically illustrated in Fig. 3. For a user-specified wall temperature, the steady-state solutions to Eqs. (2) and (3) are obtained with respect to a variation in χ and Z_{wall} . For a given value of Z_{wall} , the flamelets are obtained along the corresponding S-curve including the unstable middle branch. The procedure is repeated for different values of Z_{wall} . In the present study, the turbulence–chemistry interaction is modeled using a presumed probability density function (PDF) closure; a beta PDF is used for mixture fraction, and the distribution for the progress variable is described by a Dirac delta function. With this, the filtered flamelets are then used to generate the four-dimensional chemistry table, parameterized by filtered mixture fraction, mixture fraction variance, filtered progress variable, and Z_{wall} : $\tilde{\psi}_{FPV}(\tilde{Z}, \tilde{Z}^{1/2}, \tilde{C}, Z_{wall})$, where ψ represents the vector of all thermo-physico-chemical quantities. The tabulation procedure is similar to the adiabatic flamelet/progress variable (FPV) approach, with the exception of an additional

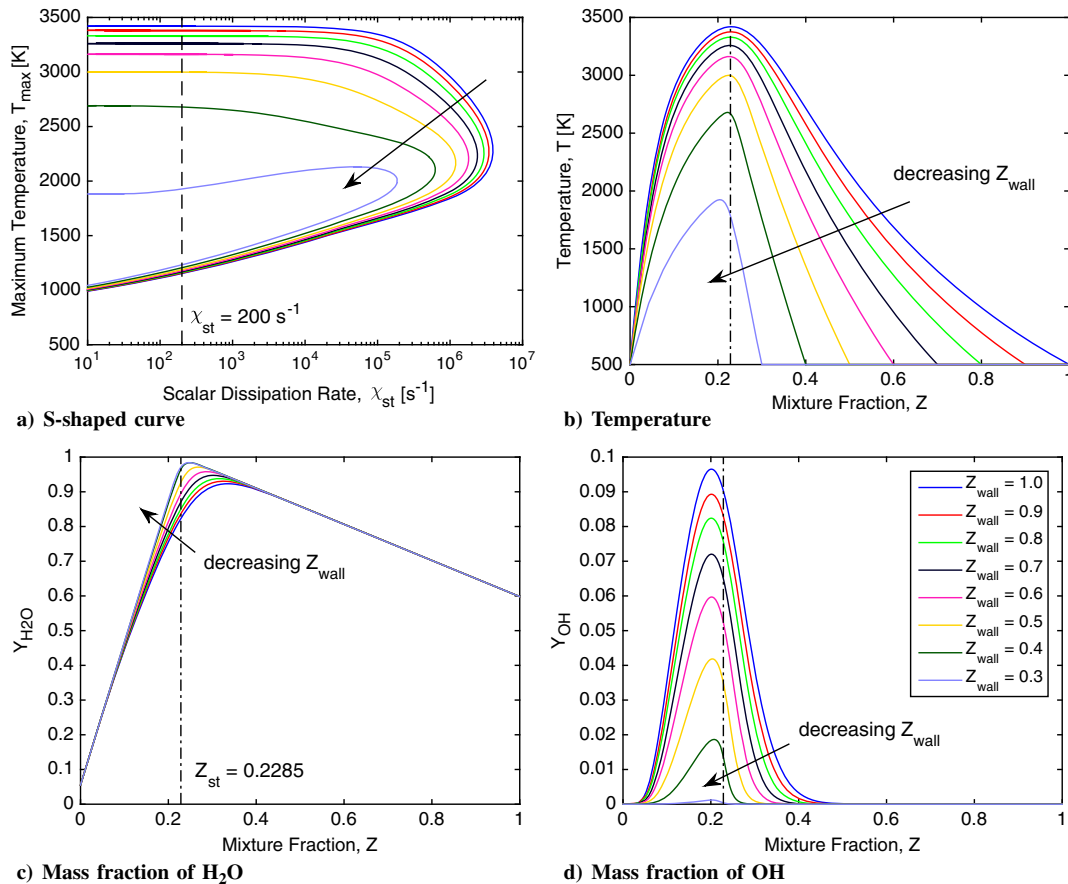


Fig. 2 Solutions of flamelet equations with heat-loss effects showing a) S-shaped curve, b) temperature, c) H_2O mass fraction, and d) OH mass fraction with respect to decreasing Z_{wall} from 1.0 to 0.3. Results in Figs. 2b–2d are calculated at $\chi_{st} = 200 \text{ s}^{-1}$.

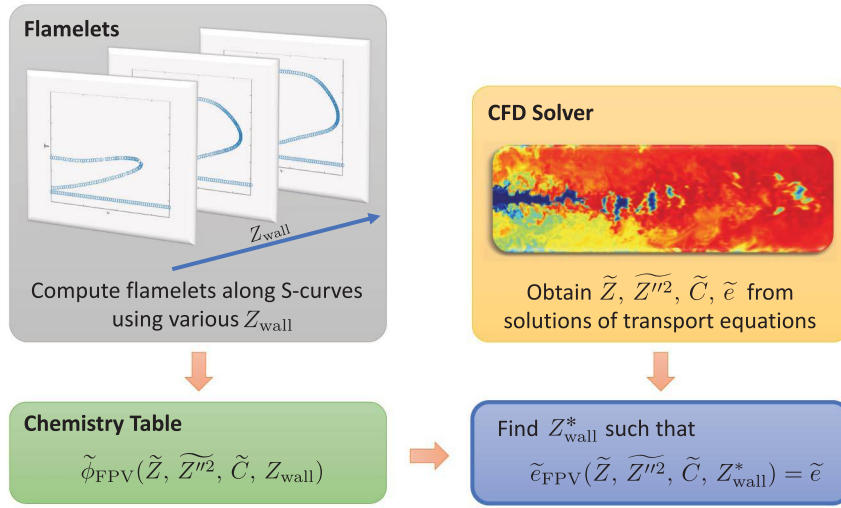


Fig. 3 FPV-WHT chemistry table generation and coupling with the computational fluid dynamics (CFD) solver.

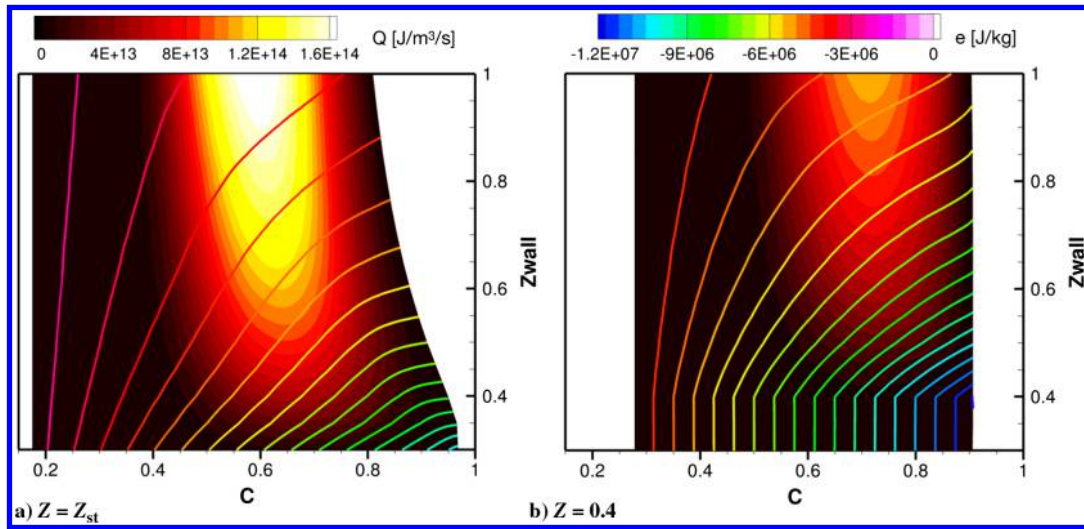


Fig. 4 Sample chemistry table generated using flamelet solutions shown in Fig. 2.

dimension to account for the variation of Z_{wall} . Slices of the table generated using sample flamelet solutions presented in Fig. 2 are shown in Fig. 4 along the $\tilde{C}$ - Z_{wall} plane for two different $\tilde{Z}$ values with zero $\tilde{Z}''^2$. The isolines of internal energy e are plotted on top of contours of the heat release rate Q . It is worth noting that the table look-up is not explicitly performed via Z_{wall} . Instead, for the compressible solver employed in this study, the internal energy from the flow solver is used, and the appropriate value of Z_{wall} is determined by matching it against the tabulated value.

In this context, it is noted that the total enthalpy is commonly used for the parameterization of nonadiabatic systems. However, for the case of flame quenching and variations in temperature-boundary conditions, the enthalpy is a nonmonotonic function [37]. In contrast, as shown in Fig. 2b, temperature provides a unique representation of the flame structure in the presence of wall heat losses. The aforementioned procedure is equivalent to the temperature-based parameterization, while being more efficient in memory for tabulations based on a Cartesian grid. In the following, this combustion model is referred to as flamelet/progress variable model with wall heat transfer (FPV-WHT). For comparison purposes, the flamelet/progress variable model developed by Saghafi et al. [46] for compressible flows will also be examined. In this model, the specific heat ratio is modeled as a linear function of temperature to evaluate primitive variables from conservative variables. This model is referred to as model FPV-LIN.

After presenting the numerical approaches employed, we will examine the performance of the FPV-WHT model by considering a DNS configuration to test the validity of essential modeling assumptions. This model is subsequently applied in an LES of a unielement rocket injector that was experimentally investigated by Pal et al. [47].

III. Governing Equations and Numerical Methods

The governing equations considered here are the conservation equations for mass, momentum, total energy, and transported scalars, written as follows:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (7a)$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) = \nabla \cdot \boldsymbol{\tau} \quad (7b)$$

$$\partial_t (\rho E) + \nabla \cdot [\mathbf{u} (\rho E + p)] = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q} \quad (7c)$$

$$\partial_t (\rho \phi) + \nabla \cdot (\rho \mathbf{u} \phi) = -\nabla \cdot \mathbf{j}_\phi + \dot{\omega}_\phi \quad (7d)$$

where ρ is the density; $\mathbf{u}$ is the velocity vector; p is the pressure; $E = e + \mathbf{u} \cdot \mathbf{u}/2$ is the specific total energy; $\boldsymbol{\tau}$ is the viscous tensor; $\mathbf{q}$ is the heat flux; ϕ represents transported scalars; $\mathbf{j}_\phi$ is the diffusion

flux; and $\dot{\omega}_\phi$ is the source term. The system is closed with the ideal-gas equation of state.

A control-volume-based finite volume approach is used for the discretization of the system of equations [48]. The convective flux is discretized using a sensor-based hybrid scheme in which a high-order, nondissipative scheme is combined with a low-order, dissipative scheme to minimize the numerical dissipation [48]. A central scheme that is fourth-order on uniform meshes is used along with a second-order essentially non-oscillatory scheme for the hybrid scheme and a density sensor [49,50] is adopted in this study. An entropy-stable flux-correction technique [50] is used to ensure the physical realizability of the numerical solutions including the positivity of scalars and to dampen the nonlinear instabilities in the numerical solutions. A strong stability-preserving third-order Runge–Kutta scheme [51] is used for time advancement.

IV. Direct Numerical Simulation Analysis

A. Configuration and Computational Setup

A DNS is performed to examine the effect of the convective wall heat flux on the flame structure and to evaluate the performance of the model. A schematic of the configuration is provided in Fig. 5. This setup follows the configuration studied by Wang and Trouvé [52] and considers the stabilization of a hydrogen/oxygen flame near a planar wall. The simulation is conducted in a three-dimensional, spanwise-periodic domain with an inflow boundary condition specified at $x/\delta = 0$, a wall boundary at $y/\delta = 0$, and convective outflow boundaries at $x/\delta = 15$ and $y/\delta = 6$. The temperature condition at the slip-free wall is either specified by a constant temperature of 300 K (nonadiabatic) or homogeneous Neumann condition (adiabatic). The velocity inflow profile is prescribed by a synthetic turbulent flow, of which the mean flow obeys the law of the wall [53] with boundary-layer thickness of $\delta = 1$ cm. The turbulent perturbations with turbulence intensity of 0.2 in the freestream are generated using the method of Klein et al. [54]. The mesh in wall-normal distance is discretized using 320 grid points following an exponential growth rate, and 10 grid points are used to resolve the viscous sublayer. The mesh in the streamwise and spanwise directions is uniform using 400 and 64 points, respectively.

The non-premixed combustion is overventilated with the fuel injected through a slit of height δ above the wall. Although the FPV-WHT model is equipped with the capability to account for detailed reaction chemistry, the present DNS study considers a single-step reaction to focus on convective heat-loss effects to the wall. The rate coefficients for this H_2/O_2 system are taken from Marinov et al. [55]. The consideration of detailed chemistry and complex transport properties is addressed in Sec. V. Relevant to preburner conditions, the fuel composition is $Y_{\text{H}_2} = 0.2$ and $Y_{\text{H}_2\text{O}} = 0.8$, and the composition in the oxidizer stream is $Y_{\text{O}_2} = 0.6$ and $Y_{\text{H}_2\text{O}} = 0.4$. The temperature in both streams is set to 300 K, and the pressure is 1 bar. Further model assumptions employed in this DNS include constant specific heat, temperature-dependent dynamic viscosity, a constant Prandtl number of $Pr = 0.7$, and unity Lewis numbers. The impact of these assumptions and choices are discussed by Wang and Trouvé [52].

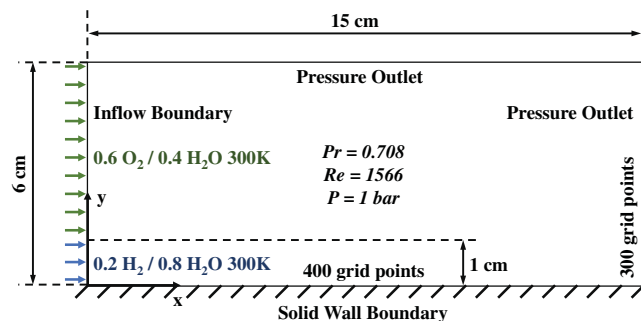


Fig. 5 Computational domain and boundary conditions for the DNS configuration.

In the following, we will evaluate the accuracy of the FPV-WHT model through direct comparisons against DNS data. The DNS solves transport equations for species mass fractions:

$$\partial_t(\rho Y_{\text{H}_2}) + \nabla \cdot (\rho \mathbf{u} Y_{\text{H}_2}) = \nabla \cdot (\rho D \nabla Y_{\text{H}_2}) + \dot{\omega}_{\text{H}_2} \quad (8a)$$

$$\partial_t(\rho Y_{\text{O}_2}) + \nabla \cdot (\rho \mathbf{u} Y_{\text{O}_2}) = \nabla \cdot (\rho D \nabla Y_{\text{O}_2}) + \dot{\omega}_{\text{O}_2} \quad (8b)$$

where Y represents the mass fraction, D is the diffusion coefficient, and $\dot{\omega}$ is the chemical source term, which is directly evaluated from the chemical mechanism. In contrast, the FPV-WHT model retrieves all thermochemical quantities from a flamelet table $\psi(Z, C, Z_{\text{wall}})$, which requires the solution of conservation equations for mixture fraction, and progress variable:

$$\partial_t(\rho Z) + \nabla \cdot (\rho \mathbf{u} Z) = \nabla \cdot (\rho D \nabla Z) \quad (9a)$$

$$\partial_t(\rho C) + \nabla \cdot (\rho \mathbf{u} C) = \nabla \cdot (\rho D \nabla C) + \dot{\omega}_C \quad (9b)$$

where $C = Y_{\text{H}_2\text{O}}$. The chemistry table is generated from the solution of flamelets [Eqs. (2) and (3)] by varying the wall-boundary location between $Z_{\text{st}} \leq Z_{\text{wall}} \leq 1$. All simulations are spatially resolved so that no turbulence closure is employed. To examine the importance of heat-loss effects on the flame, an additional FPV-WHT calculation is performed in which the wall is described by adiabatic boundary conditions. All simulations are performed on the same mesh and using the same boundary conditions.

B. Simulation Results

Comparison of the instantaneous temperature fields for these three simulations are presented in Fig. 6. To facilitate a direct comparison, results are shown at the same time instance. In this figure, the solid black line represents the location of the stoichiometric mixture, $Z_{\text{st}} = 0.273$. This direct comparison shows good agreement between DNS (Fig. 6a) and FPV-WHT (Fig. 6b) calculations. Clearly visible is the thermal boundary layer and the onset of thermal quenching at $x/\delta \approx 8.5$. The high turbulence level of the inlet stream leads to the formation of unburned fuel pockets that burn out as they are advected downstream. Results from the FPV-WHT calculation with adiabatic wall (Fig. 6c) provide a direct indication of the importance of convective heat-loss effects on the flame. Specifically, substantial flame–wall interaction is observed for $x/\delta \geq 5$. Associated with a lower temperature in the boundary layer due to the heat transfer is the reduction of dilation. This results in a thinner boundary layer, thereby pushing the flame closer to the wall.

Quantitative comparisons of simulation results are presented in Fig. 7, showing wall-normal profiles of mean temperature and mean water mass fraction at different streamwise locations. For both quantities, the FPV-WHT model provides an accurate prediction compared with the DNS results. Effects of heat losses are observed to be more significant for temperature than for species. The impact becomes stronger with increasing downstream position as the convective heat loss accumulates, which is indicated by the larger deviation between both FPV simulations. In this figure, the importance of thermal wall quenching is apparent at the location of $x/\delta = 13$, where the adiabatic FPV-WHT calculation shows the highest wall temperature of 1650 K, whereas the FPV-WHT calculation with isothermal walls predicts quenching.

Figure 8 presents conditioned statistics of temperature profiles in mixture fraction space for results from DNS and FPV-WHT simulations with both adiabatic and isothermal wall boundary conditions. It can be seen that a good agreement is obtained between DNS and the FPV-WHT model with isothermal wall conditions. Near the inlet, the flame is far from the isothermal wall so that the flame shape closely resembles the adiabatic flamelet solution in mixture fraction space. However, because of significant heat-loss effects, the temperature drops substantially on the fuel-rich side farther downstream. It is worth noting that the flame evolution in mixture fraction space as shown in Fig. 8 can adequately be represented by

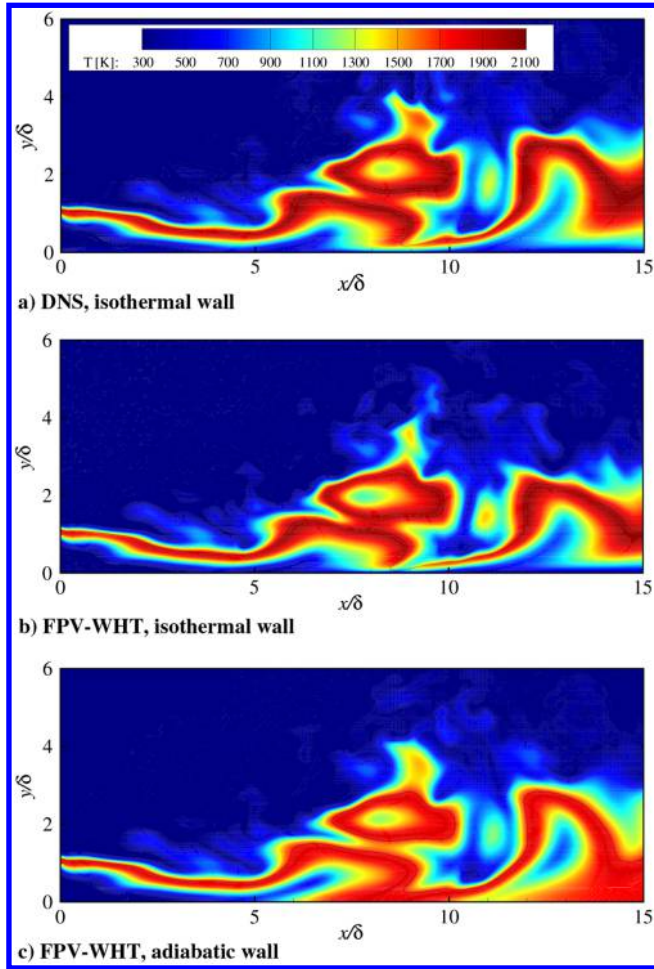


Fig. 6 Instantaneous temperature field obtained from a) DNS, b) FPV-WHT with isothermal wall, and c) FPV-WHT with adiabatic wall; solid black lines represent the stoichiometric mixture with $Z_{st} = 0.273$.

flamelet solutions with variations in parameter Z_{wall} as illustrated in Fig. 2.

The accurate prediction of the heat flux is essential for engineering applications. Here, we also compare the predictions for wall heat flux between DNS and the FPV-WHT model. As shown in Fig. 9, the maximum heat flux is approximately 110 kW/m^2 and appears at $x/\delta = 8$. It is seen that the herein proposed FPV-WHT formulation accurately predicts the heat flux profile along the wall, and deviation with the DNS results is less than 5%. Next, we will extend this model formulation to perform LES calculations of a uni-element rocket injector.

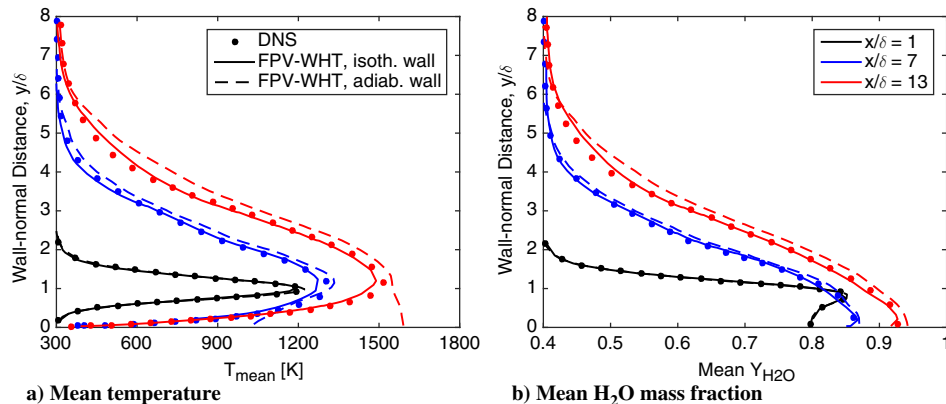


Fig. 7 Comparison of a) mean temperature and b) mean mass fraction of H_2O obtained at different streamwise locations between DNS, FPV-WHT with isothermal wall, and FPV-WHT with adiabatic wall.

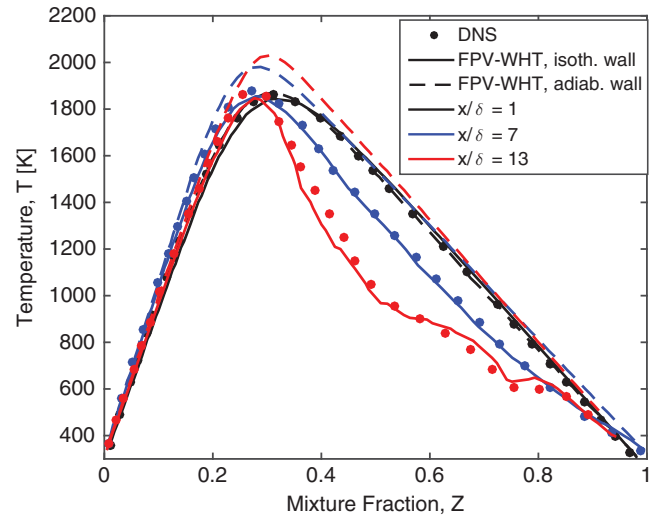


Fig. 8 Conditioned statistics of temperature profiles in mixture fraction space at different streamwise locations from DNS and FPV-WHT simulations with adiabatic and isothermal wall boundary conditions.

V. Application to Large-Eddy Simulation of Single-Injector Rocket Combustor

A. Configuration and Computational Setup

In this section, the FPV-WHT model is applied to LES of a uni-element rocket injector that was experimentally investigated by Pal et al. [47]. The experimental configuration is illustrated in Fig. 10a and consists of the main rocket chamber having a diameter of $D = 38.1 \text{ mm}$. Two propellant preburners supply gaseous hydrogen and oxygen to the coaxial injector. The central injector nozzle has a diameter of 5.26 mm and supplies the oxidizer, with a composition of $Y_{\text{O}_2} = 0.9458$ and $Y_{\text{H}_2\text{O}} = 0.0542$ at a temperature of $T = 700 \text{ K}$. The fuel is supplied by an annulus surrounding the inner oxidizer stream, with inner and outer diameters of 6.3 and 7.49 mm , respectively. The fuel composition is $Y_{\text{H}_2} = 0.4018$ and $Y_{\text{H}_2\text{O}} = 0.5982$, and the temperature is $T = 811 \text{ K}$. The post separating the fuel and oxidizer stream is recessed with respect to the injector end wall, and the recess height was estimated to be 0.43 mm at fired condition [47]. The pressure in the chamber during the steady-state operation was reported to be 54.2 bar [47]. The bulk exit velocities of the injector are 154 m/s for the oxidizer stream and 764 m/s for the fuel stream. The corresponding Reynolds numbers based on the hydraulic diameter are 6×10^5 and 1.7×10^5 , respectively.

To perform LES of this configuration, we solve Favre-filtered conservation equations for mass [Eq. (7a)], momentum [Eq. (7b)], and energy [Eq. (7c)], together with Favre-filtered conservation equations for mixture fraction, mixture fraction variance, and progress variable:

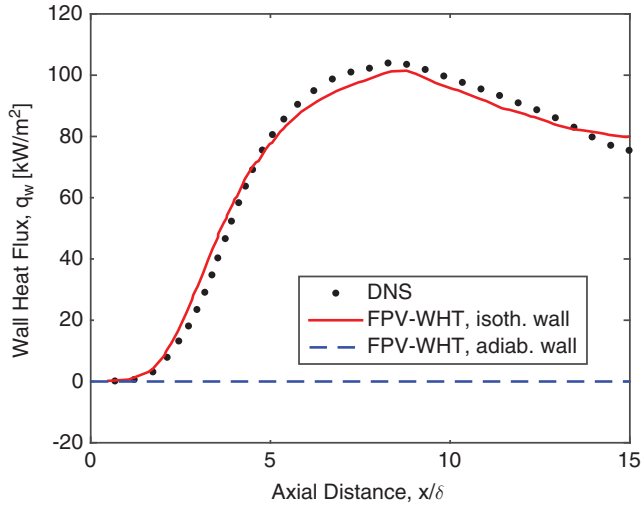


Fig. 9 Comparison of wall heat flux obtained from DNS and FPV-WHT models with adiabatic and isothermal wall boundary conditions.

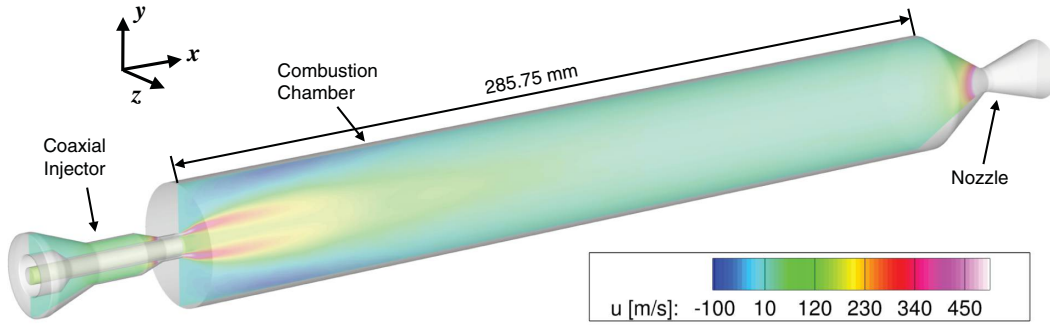
$$\partial_t(\bar{\rho} \tilde{Z}) + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{Z}) = \nabla \cdot \left[\left(\bar{\rho} \tilde{D} + \frac{\mu_t}{Sc_t} \right) \nabla \tilde{Z} \right] \quad (10a)$$

$$\begin{aligned} \partial_t(\bar{\rho} \tilde{Z}'^2) + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{Z}'^2) \\ = \nabla \cdot \left[\left(\bar{\rho} \tilde{D} + \frac{\mu_t}{Sc_t} \right) \nabla \tilde{Z}'^2 \right] + 2 \frac{\mu_t}{Sc_t} |\nabla \tilde{Z}|^2 - \bar{\rho} \tilde{\chi} \end{aligned} \quad (10b)$$

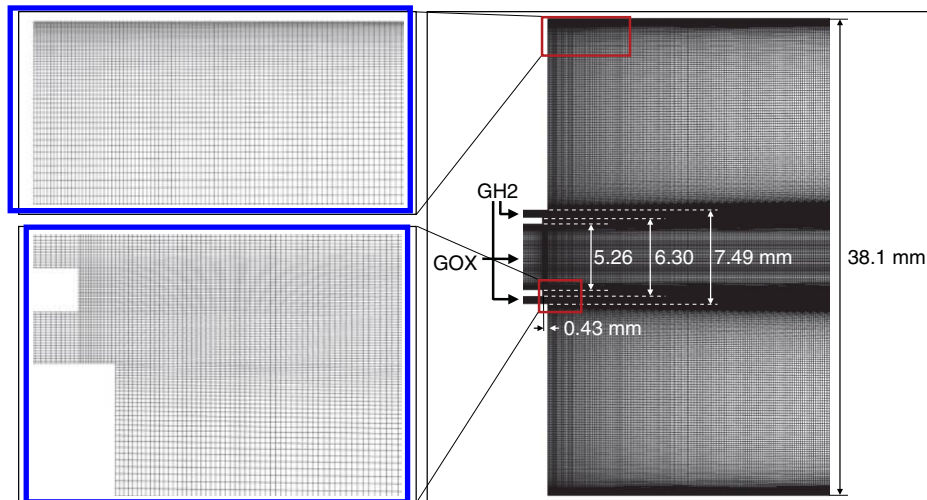
$$\partial_t(\bar{\rho} \tilde{C}) + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{C}) = \nabla \cdot \left[\left(\bar{\rho} \tilde{D} + \frac{\mu_t}{Sc_t} \right) \nabla \tilde{C} \right] + \tilde{\omega}_C \quad (10c)$$

where χ is the scalar dissipation rate, μ_t is the turbulent viscosity, and Sc_t is the turbulent Schmidt number. A Vreman subgrid-scale model [56] is applied for the closure of μ_t and a constant Sc_t of 0.9 is used. The pressure is evaluated from the ideal-gas equation of state, $\bar{p} = \bar{\rho} \tilde{R} \tilde{T}$. Further details regarding the LES equations can be found in Ma et al. [23]. The H_2/O_2 chemistry was described by the detailed mechanism due to Burke et al. [57].

A multiblock structured mesh is used for the discretization of the computational domain, which is shown in Fig. 10. The axial direction is discretized with 600 grid points for the combustion chamber following a linear growth rate, and 250 grid points are used in the radial direction. The circumferential direction is equally spaced and uses 120 points. To avoid additional uncertainties associated with the wall modeling, the thermoviscous boundary layer is fully resolved to capture the heat flux at the wall. The minimum wall spacing along the chamber wall is $10 \mu\text{m}$, which gives $y^+ < 2$ for most of the cells at the chamber wall. The grid is clustered in the near-injector region with minimum spacing of $20 \mu\text{m}$, as shown in Fig. 10b. Mass flow rate and temperature are specified at the inflow boundary conditions. Synthetic turbulence is generated for both inflow streams using the digital filter method [54]. Supersonic outflow boundary conditions are specified at the nozzle outlet. No-slip conditions are applied at all wall surfaces. Injector wall surfaces are assumed to be adiabatic. The face of the combustion chamber and oxidizer post tip have a temperature of 755 K. The temperature profile along the chamber wall is obtained from measurements as a one-dimensional axial profile [25], and a spline interpolation is used to evaluate intermediate temperatures between experimental data. The wall temperature in the nozzle is



a) Computational domain



b) Center-plane mesh near injector

Fig. 10 Computational domain and mesh. Mean axial velocity at the center plane is also shown in Fig. 10a.

assumed to be fixed at 510 K. The flowfield is initialized with hot products in the chamber and fuel and oxidizer at corresponding temperatures in the two injectors. The initial velocity field is set based on the overall mass flow rate and the density of the hot products. The flow inside the nozzle is initialized with a one-dimensional solution for converging-diverging nozzles. Simulations over two flow-through times are performed to flush out the initial transient and reach a statistically steady state. The simulations are conducted for another two flow-through times to obtain statistics, which are averaged in both time and azimuthal direction. Statistical convergence of LES results was confirmed by comparing with results averaged for the first flow-through time, which showed nearly identical results. The Courant-Friedrichs-Lewy (CFL) number is set to unity during the simulation, which gives a typical time step size of 5 ns during steady state.

Thermocouples were mounted to the chamber wall to measure wall temperature and heat flux in the experiment, and these heat flux measurements are used for comparison. To enable a direct comparison with experiment, the heat flux from LES is evaluated from the temperature gradient at the wall without considering subgrid-scale contributions.

B. Simulation Results

To assess effects of wall-heat transfer on the flowfield structure and the performance of the developed combustion model, LES calculations with both the FPV-WHT and FPV-LIN model are conducted. Three cases are considered: the FPV-LIN model with adiabatic wall, the FPV-LIN model with isothermal wall, and the FPV-WHT with isothermal wall. The simulation with adiabatic wall conditions is conducted to evaluate effects of wall heat transfer on the flowfield and flame structure. For this case, the FPV-LIN and FPV-WHT models are expected to yield similar results because no heat-loss effects are present. The FPV-LIN model, which uses an adiabatic flamelet table without taking into account heat-loss effects, is used as a baseline model for comparison with the FPV-WHT model.

Figure 11 shows instantaneous results of the temperature field at the center plane obtained from the three models. Black lines in the figures indicate the location of the stoichiometric mixture fraction. It can be seen from Fig. 11 that, near the injector, a diffusion flame separates the hydrogen and oxygen streams. The oxygen core extends downstream for about 50 mm (1.31D) until it breaks down. A recirculation zone is present at the corners of the combustor chamber, which is induced by the mixing of the hydrogen stream and the hot

combustion products. The flow accelerates after the breakdown of the oxygen core due to the recirculation zone and thermal expansion. The chemical equilibrium is almost reached farther downstream.

Comparing the three temperature fields in Fig. 11, the effects of the heat loss at the wall can clearly be seen. The instantaneous temperature fields obtained from both the FPV-LIN and FPV-WHT models with isothermal wall boundary conditions show lower temperatures both in the recirculation zone and the downstream equilibrium region. The equilibrium flame temperature of the hydrogen/oxygen flame is reached in the adiabatic case, which is about 3500 K, as can be seen from Fig. 4b. The reduction in temperature compared with the adiabatic case is about 300 and 200 K for the isothermal case with FPV-LIN and FPV-WHT models, respectively. The shape of the diffusion flame is not significantly affected by the presence of the wall heat loss, although relatively low temperature is convected toward the hydrogen stream from the recirculation region. The difference between FPV-LIN and FPV-WHT models explains the importance of including heat-loss effects on the flame structure. Specifically, slightly higher temperature in the combustor chamber can be observed with the FPV-WHT model.

Figure 12 shows the mean temperature profiles at the center plane for the three simulations performed in this study. Radial profiles of the mean temperature are plotted at several axial locations to better interpret the simulation results. As shown in Figs. 12 and 13, the case with adiabatic wall conditions shows significantly higher mean temperature near the injector, where the difference can exceed 500 K. With increasing downstream distance, the temperature inside the combustor core equilibrates, and heat-loss effects become increasingly confined to the combustor-wall region. Comparing the two cases with isothermal boundary conditions, the FPV-WHT shows consistently higher temperatures in comparison with the FPV-LIN model.

Figures 14 and 15 show the mean mass fraction fields of H_2 and H_2O at the center plane for the three cases considered. It can be seen from Fig. 14 that the difference in the H_2 mass fraction from the three models is not significant, with the two isothermal cases having slightly lower values of H_2 mass fraction downstream. The three simulations show comparable results for the mass fraction of O_2 , and the results are omitted here. For the mass fraction of H_2O shown in Fig. 15, noticeable differences can be observed downstream of the chamber, and the FPV-WHT model predicts higher levels of H_2O compared with the FPV-LIN model. This is consistent with the flamelet solution shown in Fig. 2c, where higher levels of H_2O are generated with increasing heat-loss effects.

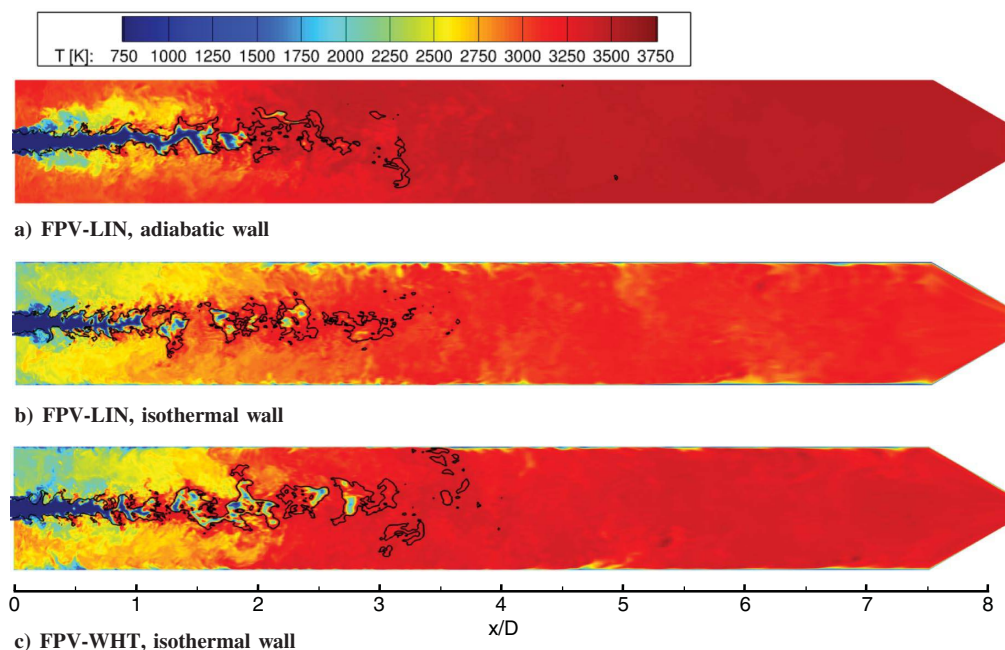


Fig. 11 Instantaneous temperature field at the center plane for a) FPV-LIN with adiabatic wall, b) FPV-LIN with isothermal wall, and c) FPV-WHT with isothermal wall. Black lines indicate the location of the stoichiometric mixture.

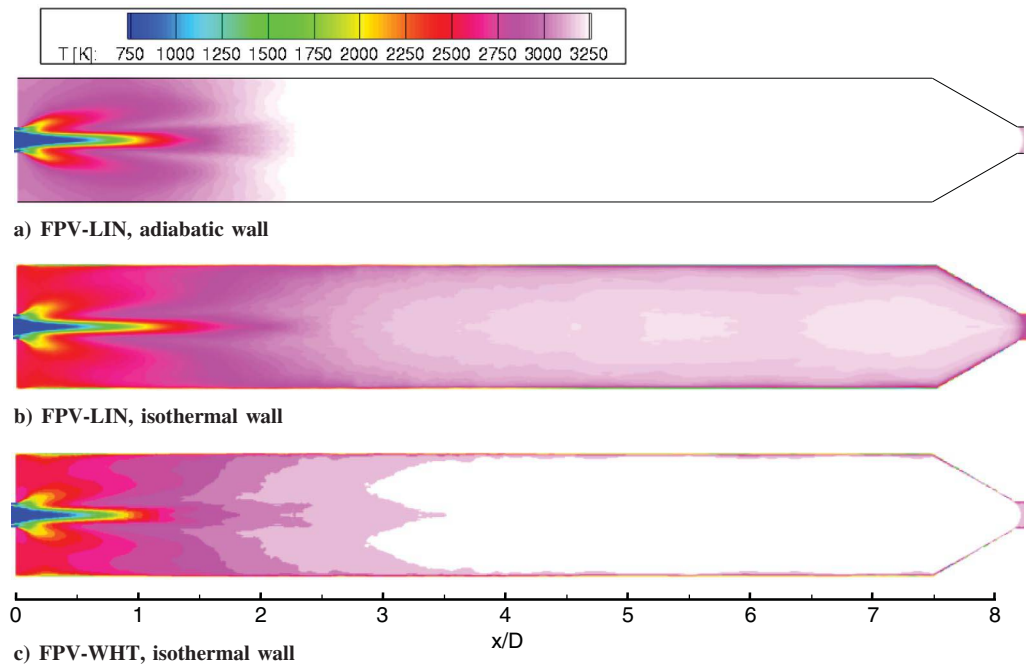


Fig. 12 Mean temperature field at the center plane for a) FPV-LIN with adiabatic wall, b) FPV-LIN with isothermal wall, and c) FPV-WHT with isothermal wall.

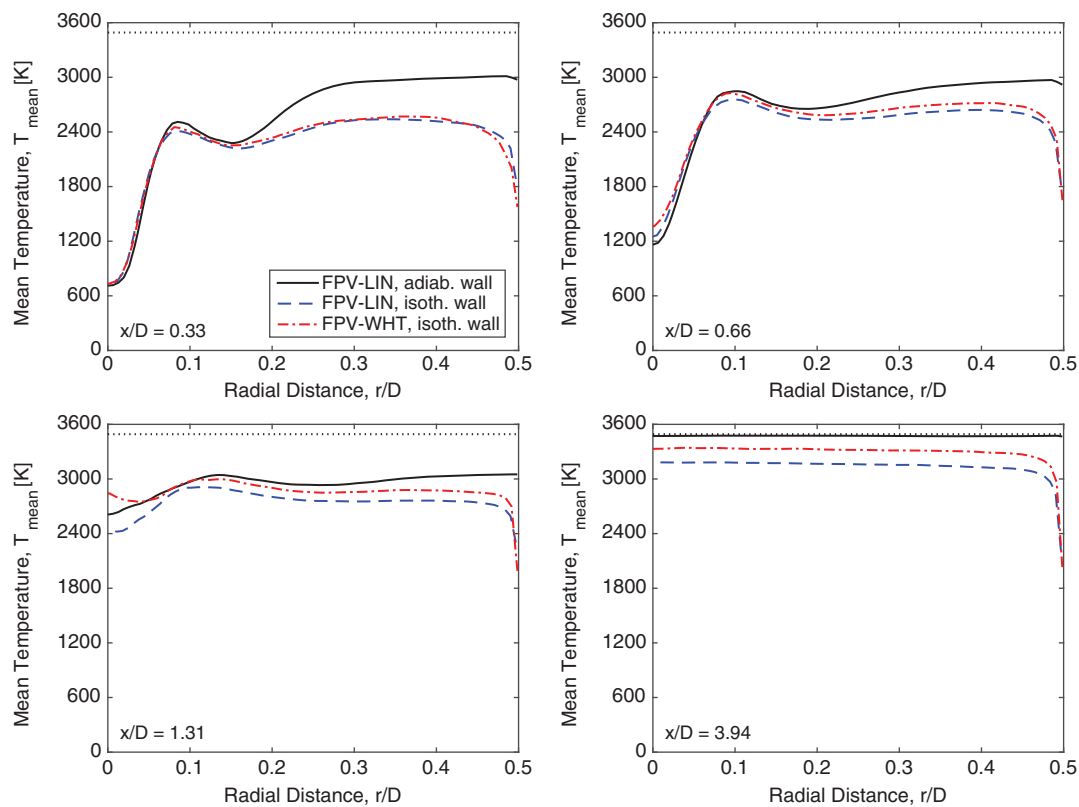


Fig. 13 Radial mean temperature profiles predicted for three different combustion models at axial locations of $x/D = 0.33, 0.66, 1.31$, and 3.94 . Dotted line indicates the value of equilibrium flame temperature, which is 3492.2 K.

Results for mean OH mass fraction profiles are presented in Figs. 16 and 17, in the form of isocontours at the center plane and radial profiles at several axial locations, respectively. Interestingly, even with a flamelet table generated under adiabatic conditions, the FPV-LIN model with isothermal wall predicts significantly lower OH mass fractions downstream of the combustor compared with the case with adiabatic wall boundary conditions. For the regions near the injector, the FPV-LIN model predicts similar levels of OH mass

fractions regardless of the wall boundary conditions applied, which can clearly be seen in Fig. 17. For comparison, between the two isothermal cases, simulation results obtained with the FPV-WHT model show significantly lower levels of OH mass fractions compared with the FPV-LIN model in the near-wall regions, emphasizing effects of the wall heat loss on the kinetics. These results are consistent with the flamelet solution, as shown in Fig. 2d, where the OH mass fraction is reduced in the presence of wall heat transfer.

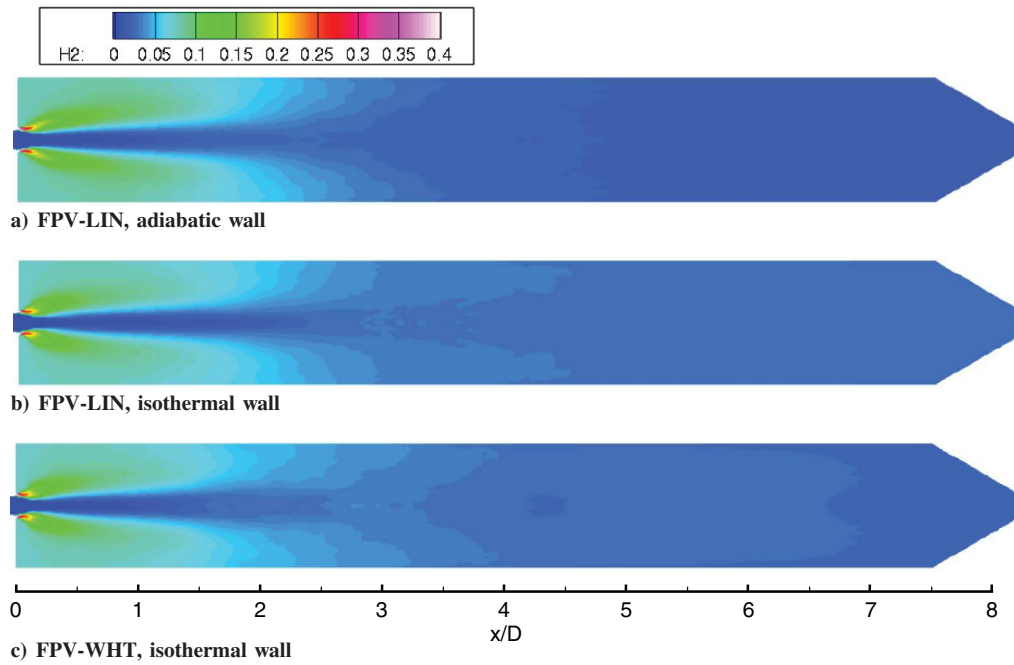


Fig. 14 Mean mass fraction field of H_2 at the center plane for a) FPV-LIN with adiabatic wall, b) FPV-LIN with isothermal wall, and c) FPV-WHT with isothermal wall.

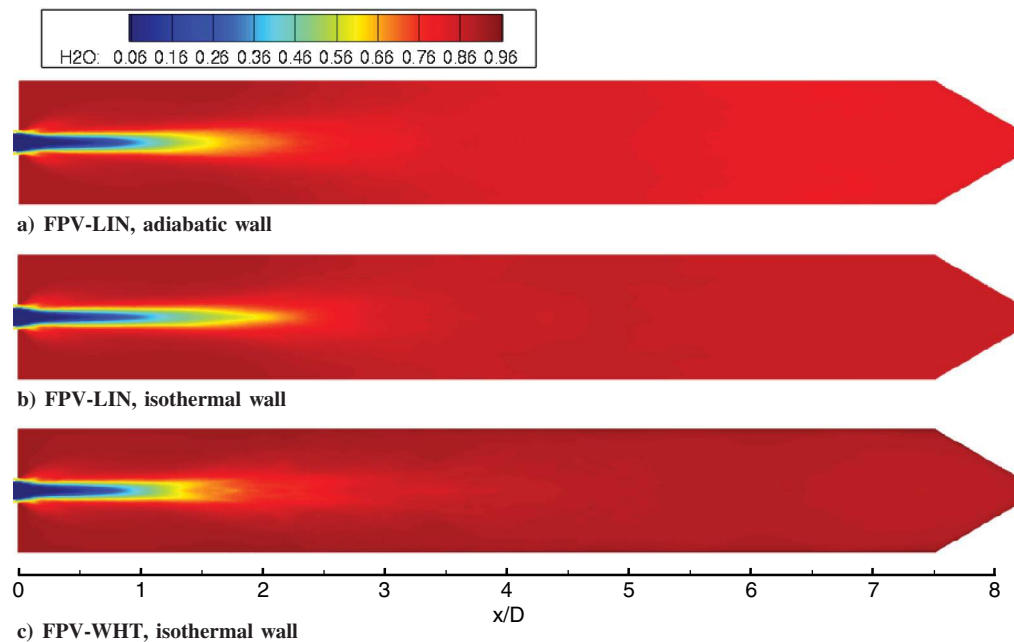


Fig. 15 Mean mass fraction field of H_2O at the center plane for a) FPV-LIN with adiabatic wall, b) FPV-LIN with isothermal wall, and c) FPV-WHT with isothermal wall.

Because no heat-loss effects are taken into account in the adiabatic table for the FPV-LIN model, the OH mass fraction profiles show almost zero gradient along the chamber wall. However, for the FPV-WHT model, with wall heat transfer effects considered, a boundary-layer-type profile can clearly be seen in Figs. 16 and 17 for the OH mass fraction profiles.

The effects of wall heat transfer and model performance can better be explained using Fig. 18 in which the mean profile of the variable Z_{wall} from the case with FPV-WHT model is shown at the center plane. Recall that this variable defines the location where the wall boundary condition in mixture fraction space is placed; see Sec. II. The value of Z_{wall} is also tabulated in the chemistry table for

visualization purposes. As can be seen from Fig. 18, the majority of the region inside the combustion chamber has a Z_{wall} value close to unity, meaning that the diffusion flame can be represented by an adiabatic flamelet solution. However, for regions near the wall, significant heat-loss effects are evident by deviation of Z_{wall} from nonunity. A large region at the corners of the recirculation zone near the injector shows Z_{wall} values significantly deviating from unity. The nonunity region of Z_{wall} near the wall downstream of the combustor increases with increasing axial location.

Finally, the predictions of the wall heat flux using both the FPV-LIN and FPV-WHT models are compared with experimental measurements along the chamber wall in Fig. 19. The wall

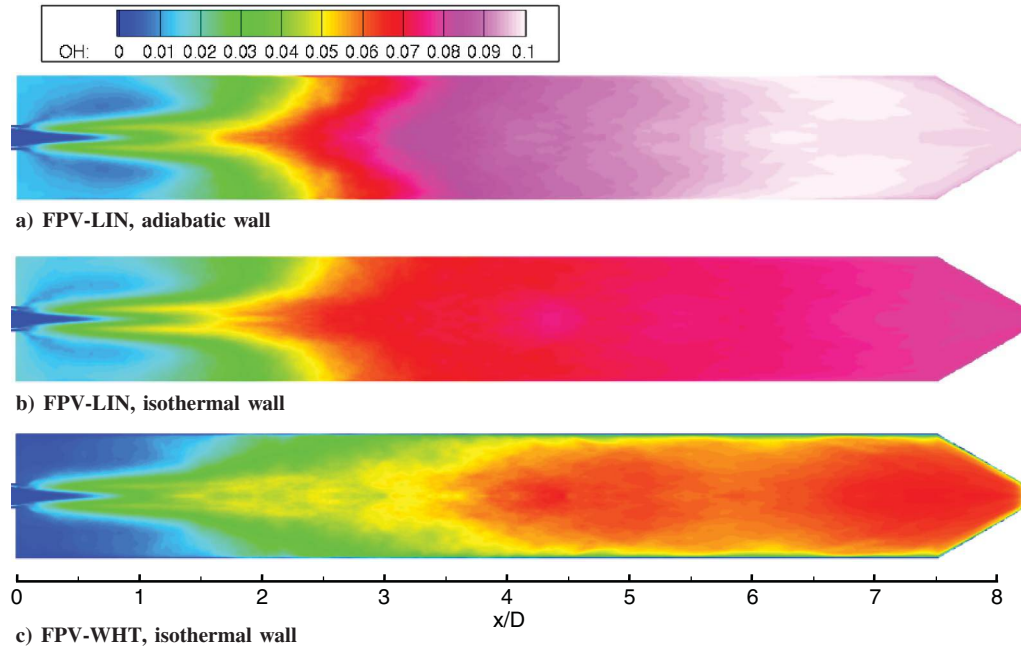


Fig. 16 Mean mass fraction field of OH at the center plane for a) FPV-LIN with adiabatic wall, b) FPV-LIN with isothermal wall, and c) FPV-WHT with isothermal wall.

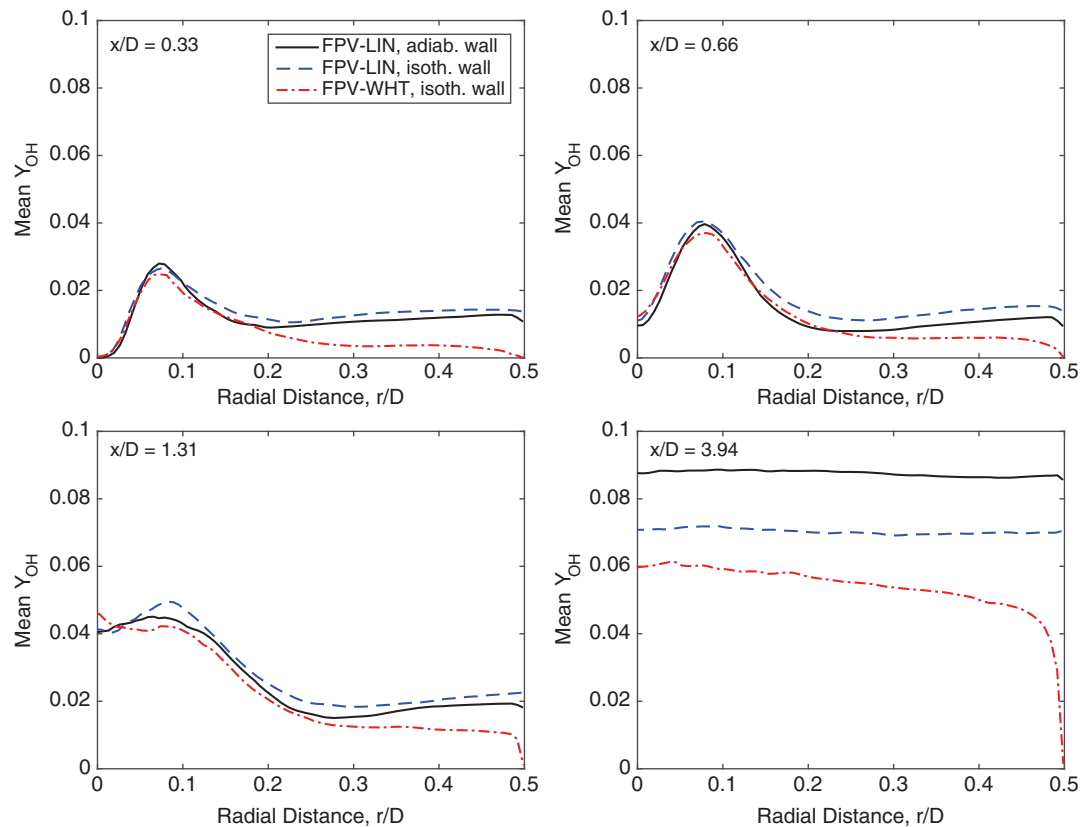


Fig. 17 Radial mean OH mass fraction profiles predicted from three different combustion models at axial locations of $x/D = 0.33, 0.66, 1.31$, and 3.94 .

temperature profile, which is applied as the isothermal wall boundary conditions, is also shown for reference. The wall heat flux and wall temperature were measured using coaxial thermocouples, with the uncertainty in wall heat flux measurements reported to be about 0.2 MW/m^2 [47,58]. It can be seen from Fig. 19 that the FPV-LIN model underpredicts the wall heat flux for all measurement locations. The results from the FPV-WHT model show improvement both in the

region of the peak heat flux at $1.31 < x/D < 2.62$ and downstream of the combustor chamber. However, overpredictions near the injector can be observed in comparison with the measurements at the first measurement station. The effect of heat losses on the reaction process can be further analyzed if joint statistics of the species mass fractions and temperature are considered. Such analysis as carried out in [59] is subject of future work.

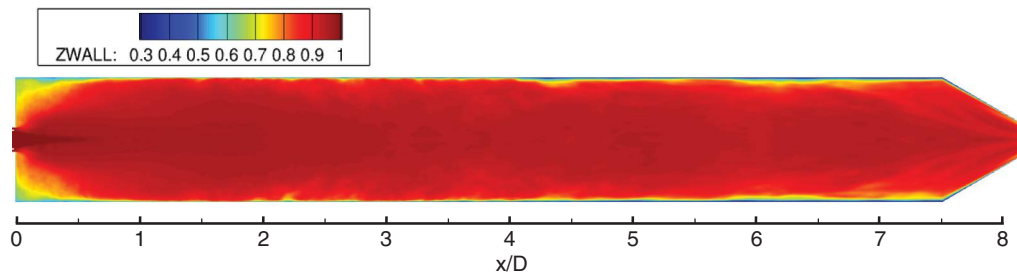


Fig. 18 Mean profile of variable Z_{wall} at the center plane for the case with isothermal wall using the FPV-WHT model.

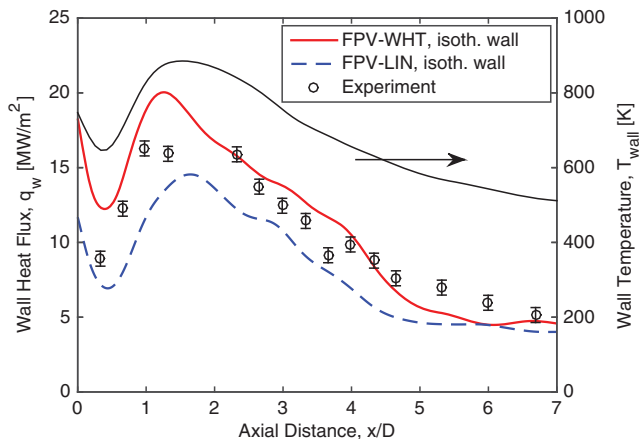


Fig. 19 Distribution of heat flux along the chamber wall predicted by different models in comparison with measurements. Temperature profile along the wall is also shown for reference.

VI. Conclusions

A turbulent combustion model for the prediction of wall heat transfer was developed. This model extends the adiabatic flamelet formulation by introducing a permeable thermal boundary condition into the flamelet equations, which allows for prescribing isothermal boundary conditions. This model is self-contained and does not introduce additional constraints on prescribed enthalpy profiles or other parameters. Flame quenching is also naturally incorporated in this formulation.

This flamelet formulation with wall heat transfer was incorporated into a flamelet/progress variable approach, and the performance of this model was examined in the context of direct simulations of a turbulent H_2/O_2 diffusion flame that is stabilized at an inert isothermal wall. Model predictions for mean-flow quantities and wall heat flux were compared with DNS-results, and it was shown that this formulation provides an adequate description of convective heat-loss effects.

The model was subsequently applied to a wall-resolved LES of a uni-element rocket injector. Model predictions obtained with a nonadiabatic combustion model show pronounced effects of wall heat losses on the temperature and minor species. These effects are not only confined to the near-wall region but are also evident in the combustor core region and the recirculation region, which is characterized by long residence times. The developed model shows significantly improved predictions of the wall heat flux compared with the model using an adiabatic chemistry table. Future work will address the development of wall models to enable wall-modeled LES [15,19].

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