Large eddy simulations of the HIFiRE scramjet using a compressible flamelet/progress variable approach

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Abstract

In this study, large eddy simulations (LES) of supersonic combustion using a compressible flamelet/progress variable (CFPV) approach are performed for the HIFiRE scramjet at Mach 8 flight conditions. The LES results show good agreement with the ground test experimental measurements. The combustion model is based on an efficient flamelet approach, where compressibility corrections are devised based on assumed functional forms of important thermo-chemical quantities. Specifically, the source term of the progress variable is rescaled with the local density and temperature in the LES, leading to improved predictions relative to existing flamelet models. A modified equilibrium wall-model, capable of predicting the viscous heating, is used in the viscous near-wall region. Temperature near the wall increases significantly due to viscous heating, enhancing the reaction rate and heat-release. This is shown to be a crucial step for accurately predicting the pressure rise in the combustor.

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1. Introduction

Scramjet engines have the potential to provide economical air-breathing propulsion at high Mach numbers for applications such as transportation, reusable launch vehicles, and hypersonic cruise missiles. Designing stable high-speed combustion systems remains a major challenge for scramjet propulsion, where fuel must be mixed, ignited, and burned to completion all within a few milliseconds. The large scale and extreme thermodynamic conditions in hypersonic flight vehicles make experiments costly and challenging [1]. Data are often limited to relatively sparse measurements of pressure, temperature, thrust, or combustion efficiency using conventional instrumentation. Validated numerical models are the most promising option to bridge the gap between sub-scale ground testing and full-scale flight-testing.

The vast majority of computational work in supersonic turbulent combustion has relied on simplified/reduced chemistry mechanisms and the explicit transport of the involved species [2].
Such approaches require the closure of the chemical source term in the species transport equations due to nonlinear interactions with the turbulent flow field. Although many types of closure models have been investigated [3–10], research is ongoing to construct models that describe fundamental physics, reduce computational expense, and increase accuracy and robustness of simulation tools.

Flamelet models present an alternative to traditional finite rate chemistry approaches for CFD. The approach is based on the flamelet concept [11,12], which assumes that the chemical time scales are shorter than the turbulent time scales, such that the flame can be approximated as an ensemble of laminar flamelets. The flamelet approach allows the chemistry to be computed independently of the flow simulation and stored in tabulated form as a function of a small number of scalars. During the CFD simulation, thermochemical quantities are interpolated from the chemistry table, thus, dramatically decreasing the overall computational cost and allowing the use of complex chemical mechanisms.

In this study, a computationally efficient flamelet combustion model is developed for high-speed flows. Flamelet-based models that are currently used in low-Mach applications are extended and validated for hypersonic conditions. The target configuration is the HIFiRE Direct-Connect Rig experiments from the NASA Langley Arc-Heated Scramjet Test Facility [13].

2. Mathematical model

In this section, the filtered transport equations for LES of compressible reacting flows are presented, the combustion model based on the flamelet/progress variable approach is described, and the wall modeling approach is summarized.

2.1. Governing equations

The Favre averaged or filtered variables (indicated by · and ·, respectively), \( \bar{\rho} \), \( \bar{\rho} \bar{u} \), \( \bar{\rho} \bar{E} \), \( \bar{\rho} \bar{Z} \), \( \bar{\rho} \bar{Z}^2 \), and \( \bar{\rho} \bar{C} \) are solved in the conservative form, where \( \bar{\rho} \) is the density, \( \bar{u} \), the components of the velocity vector, \( \bar{E} \) the total energy (including the chemical energy), \( \bar{Z} \) the mixture fraction, \( \bar{Z}^2 \) the variance of the mixture fraction, and \( \bar{C} \) a reaction progress variable [14].

The mixture composition depends directly on \( \bar{Z} \), \( \bar{Z}^2 \), and \( \bar{C} \). In order to close this system, the pressure and the temperature need to be determined. This is achieved by using an equation of state and the energy of the mixture as explained in the following section. For the current study, the progress variable is defined as

\[
\bar{C} = Y_{H_2O} + Y_{H_2} + Y_{CO_2} + Y_{CO}.
\]

2.2. Combustion model

The combustion model used in this study is based on the compressible flamelet/progress variable approach (CFPV) [15,14]. In the CFPV approach, flamelet equations are solved in a preprocessing step using detailed kinetic mechanisms (GRI 3.0 mechanism [16] in this study) and stored in a chemistry table. Appropriate compressibility corrections are introduced [14] to decrease the size of the chemistry table. The CFPV model has been extensively validated in a priori and a posteriori studies using direct numerical simulation data [14]. In this section, the CFPV approach is briefly explained, and the compressibility corrections are summarized.

The CFPV approach is designed to account for variations due to compressibility, while maintaining roughly the same computational efficiency as its low-Mach-number counterpart. In this approach, the thermochemical state of the compressible flow is approximated as a perturbation about nominal low-Mach-number flamelet solutions. Appropriate expressions are derived from the physical behavior of each variable, and are used to correct the value from the low-Mach-number flamelet library.

Quantities of interest that are necessary to close the transport equations include the gas constant, specific heat ratio, temperature, pressure, molecular viscosity and thermal diffusivity. Corrections that account for the effects of compressibility on these quantities are described in detail in Refs. [14,17].

The source term of the progress variable is very sensitive to perturbations in temperature and concentration. A rescaling of this term is applied as

\[
\frac{\bar{\omega}_C}{\bar{\omega}_{C_0}} = \left( \frac{\bar{\rho}}{\rho_0} \right)^{a_\rho} \exp \left[ -T_a \left( \frac{1}{T} - \frac{1}{T_0} \right) \right],
\]

where \( \bar{\omega}_{C_0} \) is the tabulated source term computed at a background pressure \( \rho_0 \). This equation is the dimensionless ratio of the progress variable source term from the LES to its value from the chemistry table. It is used to adjust the tabulated production rate for consistency with the local temperature and density in the LES. The values of the baseline density \( \rho_0 \), the density exponent \( a_\rho \), and the activation temperature \( T_a \) are computed in a preprocessing step to describe the dependency of the source term on the mixture temperature and pressure, and are then tabulated as a function of \( \bar{Z} \), \( \bar{Z}^2 \), and \( \bar{C} \). The form of this equation is motivated by the Arrhenius behavior of elementary reactions, where density (to some order) appears in the species concentration terms. For hydrocar-
bon fuels, the value of $a_p$ is close to two, because the majority of reactions are bimolecular. The value of $T_a$, in general, depends on the chemical mechanism. For the conditions studied in this work, $T_a$ at stoichiometric conditions is approximately 15,000 K.

It should be noted that all of the variables with the “0” subscript are obtained directly from the base-state flamelet data, while the other parameters, $a_p$ and $T_a$, are determined by local data fitting using flamelet solutions at perturbed conditions. All of the parameters are tabulated as functions of $Z$, $Z^{02}$, and $C$ in the chemistry table. The functional form of the compressibility corrections are general and can be used for different conditions and fuels (e.g., see [14] for hydrogen fuel). However, most of the compressibility coefficients are not universal (e.g., $T_a$), and are precomputed as functions of $Z$, $Z^{02}$, and $C$ for the chemistry and conditions of interest. For more details on the CFPV model along with validations of the above expressions refer to Refs. [15,14].

2.3. Wall modeling

Wall-resolved LES of scramjets is not practical with the current computational resources [18], therefore, a wall model for the wall shear stress and heat flux is applied. The unstructured LES grid extends all the way to the wall and is designed to resolve outer-layer scale motions of the boundary layer [19]. The wall model then solves the compressible equilibrium boundary layer equations for momentum and energy as described in Refs. [20,21]. In the current work, the manner of exchanging data between the LES and wall model has been modified from Bodart and Larsson [20] to use an integral constraint based on the wall-adjacent LES cell. The following equations,

$$
\frac{1}{\delta} \int_0^{\delta} u_d d\eta = \bar{u}, \quad \frac{1}{\delta} \int_0^{\delta} T d\eta = \bar{T},
$$

(2)

are solved iteratively at each wall-adjacent LES cell, ensuring that the average streamwise velocity and temperature from the wall model match the filtered values from the LES. The wall-shear stress computed by the wall-model is applied as a flux in the LES momentum equation. This integral approach allows for the wall-modeled viscous heating to be passed as a source term to the LES energy equation. In prior wall-modeling implementations, thermal feedback to the LES solution was limited to the wall heat flux and was simply zero in the adiabatic case.

3. HIFiRE simulations

Figure 1 shows the HIFiRE Flight 2 (HF2) scramjet [22] with relevant dimensions shown. At each streamwise fuel injection station shown in Fig. 1, there are four injectors (spaced equally in the spanwise direction) on the body side (upper surface) and four injectors on the cowl side (lower surface). The primary injectors have a diameter of 3.175 mm, and are canted at 15° relative to the combustor wall. The secondary injectors are normal to the combustor wall with a diameter of 2.388 mm. For more details on the HF2 geometry refer to Ref. [23].

The fuel is a JP-7 surrogate with molar composition of 64% ethylene and 36% methane. The total equivalence ratio is 1.0, where 40% of the fuel by mass is injected from the primary injectors and the balance from the secondary injectors [23].

The experimental measurements [13] of the full-scale HIFiRE scramjet are conducted at NASA’s Arc-Heated Scramjet Test Facility [24]. In this study, the experimental results corresponding to the highest Mach number are considered, where the Mach number at the isolator inlet is 3.46 (equivalent to the Mach 8 HF2 flight test).

3.1. Boundary conditions

The LES is performed on one-quarter of the HF2 domain (including the cowl-side surface and one side wall), with symmetry boundary conditions applied at the mid-plane in both the spanwise and lateral directions. The use of symmetry boundary conditions reflects a compromise between computational costs and the need to provide adequate resolution in boundary layers, shear layers, and reaction zones. Unfortunately, the resolution requirements of the HF2 configuration made it infeasible to simulate the entire domain with the computational resources that were available. The symmetry boundary condition is obviously an approximation to the physical combustor and carries implications for the overall fidelity that can be achieved. Despite this, it is a reasonable concession given the cost constraints and has been used in other investigations [25,26]. Simulations of the full HF2 domain (i.e., no
symmetry boundary condition) are planned as future work; however, results are not available for the current paper.

Specific inflow boundary conditions of the isolator, primary injectors, and secondary injectors are shown in Table 1. At the isolator inlet, synthetic turbulence is generated using a digital filtering approach [27,28]. Profiles of the Reynolds stress tensor from the boundary layer DNS data of Wu and Moin [29] are rescaled and used as inputs. As the turbulent conditions inside the HIFiRE isolator are not well characterized [23,22], the objective of this approach is simply to develop a fully turbulent boundary layer prior to the primary fuel injectors. This is similar to the approach taken in Brès et al. [30], where for practical design studies the synthetic turbulence inside a jet nozzle is prescribed in a manner to ensure realistic turbulence levels at the nozzle exit. Simulation of the full isolator provides a sufficiently long development length for the boundary layer to equilibrate before reaching dynamically important regions of the flow. All of the walls are assumed to be adiabatic due to the long duration of the experiment [13], and wall modeling is applied to all surfaces. Characteristic boundary conditions are applied at the outflow boundary.

### Table 1: Inflow boundary condition parameters.

<table>
<thead>
<tr>
<th>Boundary Condition</th>
<th>Pressure [kPa]</th>
<th>Temperature [K]</th>
<th>Mach number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isolator</td>
<td>40.3</td>
<td>736.2</td>
<td>3.46</td>
</tr>
<tr>
<td>Primary injector</td>
<td>105.7</td>
<td>293.3</td>
<td>1.0</td>
</tr>
<tr>
<td>Secondary injector</td>
<td>290.7</td>
<td>301.1</td>
<td>1.0</td>
</tr>
</tbody>
</table>

3.2. Numerical implementation

The unstructured finite volume LES solver “Chris” developed at Cascade Technologies, Inc. [31] is employed in this study. Numerical stencils based on higher-order polynomial expansions are used to minimize numerical dissipation. The spatial discretization relies on a second-order hybrid central/ENO method, in which a shock sensor is used to identify the cells where the ENO scheme should be applied. An explicit third-order Runge–Kutta scheme is used for temporal integration. All sub-grid turbulent quantities are modeled using the dynamic procedure [32,14].

A body-fitted, block-refined, unstructured mesh [31] is used for all of the simulations in this study. Several embedded zones of refinement are defined to provide sufficient resolution in regions where gradients are large, e.g., in boundary layers, fuel/air mixing layers, and the cavity. The simulations are performed using a coarse mesh with 21 M cells, and a fine mesh with 96 M cells to evaluate the grid independence of the solution. For the fine case, grid spacing in the wall normal direction near the primary injectors is approximately 100 wall units and is around 3% of the diameter of the primary injectors in the mixing layer of fuel and air. Grid spacing is approximately 35% larger in the coarse mesh. Although the coarse mesh includes the full length of the HF2 geometry, the fine mesh utilizes a shortened isolator in order to reduce the cost of the simulations. The impact of these decisions on the results are discussed below.

3.3. Results

Figure 2 shows the LES wall pressure distribution in the symmetry plane normal to the spanwise direction (centerline between the injectors). Experimental measurements on the body and cowl sides are also plotted for comparison. Statistics from the LES are obtained by time-averaging instantaneous flow-fields after 10 flow-through times (when the LES results are statistically steady). A schematic of the HF2 domain is shown on the plot for reference.

Comparisons with the experimental measurements show relatively good agreement. Combustion heat-release causes a sharp pressure rise beginning just upstream of the primary injectors. The pressure reaches a plateau in the cavity, and rises again due to compression on the ramp wall of the cavity. Strong turbulent mixing produces a relatively homogeneous flow in the cavity, and
nearly constant pressure in this region. The coarse LES under-predicts the pressure in the cavity by about 4.5%, while the fine LES attains the correct pressure levels. The pressure drops suddenly as the supersonic flow expands at the end of the ramp wall. The pressure is under-predicted in the expansion region downstream of the secondary injectors on both the fine and coarse mesh; however, experimental uncertainty is uncharacteristically high in this region for reasons that are not explained in Ref. [13]. For example, note the large variations in the experimental measurements on the body and cowl sides around the secondary injectors. For this reason, the LES results are believed to be in the range of experimental uncertainties.

There are notable differences between the fine and coarse LES results in Fig. 2. The fine mesh outperforms the coarse grid in predicting trends and peak pressures in the cavity, ramp, and secondary injection regions. The coarse mesh, however, seems to better predict the initial pressure rise around the primary injectors. This discrepancy is most likely the result of the truncated isolator that was used in the fine grid simulations. The shorter development length resulted in jet/boundary-layer interactions that were sufficiently different from the coarse mesh to suppress mixing and combustion until the cavity. These differences will be clarified in future simulations.

It should be noted that the current combustion model uses a single mixture fraction that cannot fully represents the interactions between the primary and secondary fuel jets. Properly modeling this interaction could enhance the combustion around the secondary injectors, and increase the pressure in this region. The addition of a second mixture fraction and modeling of cross-dissipation effects in the flamelet equations are the subjects of ongoing research. Using a multi-stream model could potentially improve the results in the regions after the secondary injectors.

Figure 3 shows the mixture fraction contours and the pressure rise on the combustor walls (the isolator wall is excluded for clarity). The primary jets are confined near the wall by the relatively strong cross-flow. The secondary jets, which are injected normal to the cross-flow and have a higher momentum flux ratio, penetrate more deeply into the combustor interior. Figure 4 shows the iso-surface of the stoichiometric mixture fraction colored by the progress variable. Upstream of the cavity, the primary jets burn mostly in the low speed boundary layer, and the mixing region between the injectors. In fact, Figs. 3 and 4 indicate that the fuel streams merge before entering the cavity. Mixing is enhanced in this region as the boundary layer separates just prior to the cavity due to the strong adverse pressure gradient (see Fig. 2). This can be clearly seen in Fig. 5a, where a small recirculation zone is visible between the primary injectors and the cavity step.

Contours of the progress variable near the primary injectors are plotted in Fig. 6a. The oxidizer stream in the mixing layer has low velocity and high temperature due to conversion of the kinetic energy to thermal energy. This provides favorable conditions for the mixture to ignite [14]. Auxiliary simulations were also performed to independently evaluate the effect of the source term correction outlined in Eq. (1), and the effects of the wall model. Figure 2 compares the pressure distribution from the full CFPV model with a second LES where the source term correction was not applied. It is clear from the delayed pressure

Fig. 3. Contours of the mixture fraction on six slices normal to the streamwise direction at $x_1 = 0.25, 0.3, 0.35, 0.4, 0.45,$ and $0.5 \text{ m}$. Combustor wall is colored by pressure.
response in the case with no correction term that Eq. (1) is an indispensable step in the CFPV approach. Contours of the progress variable from these two cases are plotted in Fig. 6b and c, which shows that combustion cannot be sustained at the primary injectors without correcting the progress variable source term for compressibility. A third LES simulation was performed that included the source term correction but did not apply the wall model. Comparing Fig. 6a and c shows that the viscous heating provided by the wall model is equally important in stabilizing the flame at the primary injectors. The viscous heating in the isolator boundary layer transfers the kinetic energy of the flow into sensible energy. The corresponding increase in the fluid temperature enhances the reactions and stabilizes the flame near the primary injectors. Equation (1) provides a mechanism to couple these two phenomena in the CFPV model.

4. Analysis and discussion

Flamelet models assume that a turbulent reacting flow can be approximated by asymptotically-thin laminar flame structures embedded in a turbulent flow field [11]. Implicit in this model is the assumption that the chemical length and time scales of the flamelet are much smaller than the representative turbulent scales. Also, because flamelet manifolds are derived from collections of canonical flame structures, the target system must persist more or less within the prescribed mixing and turbulence regimes for the approach to be valid. In this section, the results from the HF2 simulations are evaluated in terms of assumptions common to the flamelet paradigm.

The CFPV model presented in Section 2.2 is based on non-premixed diffusion flamelets. It is instructive to compare characteristic flame structures from the compressible LES to the original incompressible flamelet solutions. Figure 7 shows a scatter plot of instantaneous temperature versus mixture fraction from the HF2 simulation. Data from two separate $z$-planes are shown — the dark symbols represent data from a slice along the centerline of the fuel injectors, and the lighter symbols show data from midway between the two jets. Laminar flamelet solutions depicting isenthalpic mixing ($\nu_{st} = 500 \text{s}^{-1}$) and near equilibrium chemistry ($\nu_{st} = 1 \times 10^{-4} \text{s}^{-1}$) are also presented for reference.

Deviations from the incompressible flamelet manifold due to compressibility are immediately apparent in Fig. 7. Differences of over 1000 K relative to the baseline flamelets are observed in and around the reaction zone, with even larger temperature excursions near the lean boundary. These high temperatures arise from the shocked air flows in the isolator upstream of the primary mixers. Data sampled from the fuel jets (dark symbols) show temperature fluctuations around the baseline fuel inlet condition and a variety of reacting and intermediate states in the interior of the flamelet. Data sampled from between the fuel injectors (lighter symbols) suggest a more consistent transition to burning, as hot air is entrained with burning gases in this highly unsteady region. Profiles with similar flame structure and temperature range have been reported in previous RANS [33] and LES [25] studies of this configuration.

Although the global flame structure in Fig. 7 appears to have significant non-premixed character, more careful analyses are required to evaluate the suitability of the diffusion flamelet approach for the HF2 combustor. The Takeno Flame Index [34] is a useful indicator for identifying mixing regimes in reacting flows. It assumes that
gradients in the fuel and oxidizer fields are aligned in premixed flames and anti-aligned in non-premixed flames

\[ G_{FO} = \frac{\nabla \bar{Y}_F \cdot \nabla \bar{Y}_O}{|\nabla \bar{Y}_F||\nabla \bar{Y}_O|}, \]  

so that non-premixed regimes are characterized by negative values of \( G_{FO} \) and premixed regimes are identified by positive values of \( G_{FO} \). Contours of \( G_{FO} \) are shown in Fig. 5d. Non-premixed combustion modes are widespread in shear layers and the cavity; however, pockets of premixed combustion are peppered throughout the flow.

(a) Streamwise velocity (white line indicates the \( u_1 = 0 \) boundary)

(b) Pressure

(c) Scalar dissipation rate, \( \chi \) (logarithmic scale)

(d) Takeno Flame Index, \( G_{FO} \)

(e) Damköhler number (logarithmic scale)

Fig. 5. Flow variables from LES of the HIFiRE scramjet.
With the diverse range of flame states shown in Fig. 5d, it is interesting to consider which structures are contributing most strongly to the combustion. Figure 8 shows an iso-surface of progress variable reaction rate, a quantity that is closely correlated with heat release. The surfaces are colored according to the local value of the Flame Index. Non-premixed combustion is observed in the shear layer rollup at the windward base of the injectors, but there appears to be significant premixed zones in entrainment regions of the jet-in-crossflow vortex systems.

A time-scale analysis is used to examine these reactive zones in more detail. The analysis is based on estimates of the local Damköhler number,
Da = \tau_{flow}/\tau_{chem}. For non-premixed combustion, the scalar dissipation rate provides an inverse time scale for mixing. We use the equilibrium model for scalar dissipation rate proposed by De Bruyn Kops et al. [35]

\[ \frac{1}{\tau_{flow}} = \bar{Z} = \left( \frac{\bar{v}}{Pe} + \frac{v_i}{Sc_t} \right) |\nabla \bar{Z}|^2, \tag{4} \]

with the primary jet diameter as a representative length scale in the Peclet number. The computed dissipation rates are shown in Fig. 5c and are largely insensitive to the choice of length scale due to large contributions from the SGS term \( v_i/Sc_t \). The characteristic chemical time scale for the CFPV model is

\[ \tau_{chem} = \frac{\bar{\rho} \bar{C}}{\partial \bar{C}/\partial t}. \tag{5} \]

Contours of Damköhler number based on Eqs. (4) and (5) are shown in Fig. 5e.

The flamelet assumptions are valid for \( Da \gg 1 \), a criteria that can be loosely interpreted as \( Da > 10 \). The regions shown in Fig. 8 are evaluated using this criteria in conjunction with the Flame Index to determine the suitability of the CFPV model for the HF2 case. Figure 9 shows the volume-weighted joint PDF of Damköhler number and Flame Index for the heat release regions shown in Fig. 8. The \( Da = 10 \) line is represented by the horizontal dashed line and the non-premixed (\( G_{OF} < 0 \)) and premixed (\( G_{OF} > 0 \)) regions are divided by the vertical dashed line. A substantial fraction of the heat release region (67%) lies in the upper left quadrant, where the flamelet assumptions are valid and diffusion flamelets properly characterize the combustion regime. A non-negligible fraction (26%) of the heat release region falls in the upper right quadrant, indicating that time scale ratios are amenable to flamelet modeling but that the combustion model should consider premixed flame structures as a basis. The remaining 7% of the heat release region lies below the \( Da = 10 \) line, suggesting that flamelet methods are unlikely to properly describe all of the important reaction phenomena under these conditions.

5. Conclusions

Large eddy simulations using the CFPV combustion model are reported for the HIFiRE scramjet at Mach 8 flight conditions. Results are compared with experimental measurements from the HIFiRE Direct-Connect Rig at NASA Langley. The CFPV model utilizes functional corrections to a nominal flamelet solution to account for compressibility, thus providing an efficient description of high-speed combustion with a low memory footprint. Turbulent wall modeling of the viscous near-wall region is used to accurately predict the wall shear stress and heat flux in the LES. The numerical results show good agreement with the experiment when both compressibility and wall effects are modeled. Neglecting either of these factors, however, leads to reduced combustion and poor prediction of the pressure trends observed in the experiment. Corrections to the progress variable source term are particularly important, as they provide strong coupling between the combustion chemistry and compressible phenomena such as shocks, expansions, and viscous heating. The present results also suggest that jet/boundary-layer interactions are important in sustaining proper mixing and combustion in the near field of the primary injectors. All of these effects must be considered to stabilize combustion in the proper location. A time-scale analysis showed that assumptions about flamelet time scales are valid throughout a large fraction of important heat release regions of the HIFiRE combustor. However, analysis of the mixing regime suggested that premixed combustion plays a non-negligible role in this flow and should be considered in future simulations.

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