Turbulence / Chemistry Interactions in a Ramp-Stabilized Supersonic Hydrogen-Air Diffusion Flame

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Abstract

Hybrid large-eddy / Reynolds-averaged Navier-Stokes simulations of turbulence / chemistry interactions occurring within a ramp-injected, hydrogen-fueled scramjet combustor are presented in this work. The experimental geometry is one of several studied at the University of Virginia as part of the National Center for Hypersonic Combined Cycle Propulsion and consists of an isolator, a combustor, and an extender section. Data collected includes coherent anti-Stokes Raman spectroscopy (CARS) measurements of major species composition and temperature at several streamwise planes, stereoscopic particle image velocimetry (PIV) measurements, hydroxyl planar-induced fluorescence (OH-PLIF) imagery, wall pressure distributions, and line-of-sight profiles of temperature and water concentration obtained using tunable diode laser spectroscopy (TDLAS). This paper focuses on an equivalence ratio of 0.17, which does not produce enough heat release to force a shock train into the isolator. The computational methods utilize a hybrid fourth-order central-difference / upwind strategy to enable accurate resolution of turbulent structures and employ a nine-species hydrogen oxidation mechanism. Generally accurate predictions of temperature, velocity, and nitrogen mole fraction are achieved through a ‘laminar chemistry’ assumption for the filtered species production rates, though results do improve slightly with the use of a simple turbulence / chemistry subgrid closure model. The predictions are most sensitive to the choice of isolator inflow boundary condition, with the use of a recycling / rescaling technique to sustain turbulent fluctuations resulting in an ‘over-mixing’ effect immediately downstream of the fuel injector. Turbulence-chemistry interactions in the flameholding region are examined from the standpoint of laminar flamelet theory. A region of high scalar dissipation rate, coincident with the breakdown of the fuel plume and the interaction of a reflected shock wave with the plume, inhibits flame propagation, forming a ‘hole’ in the flame. Advection of cooler fluid downstream into regions of moderate scalar dissipation enlarges the ‘hole’, but eventually the flame reconnects. These results point to one potential disadvantage of fuel-air mixing technologies that enhance axial vorticity – even if conditions for combustion are favorable, high strain rates generated by the interaction and breakdown of vortex pairs can lead to flame suppression.

1 Introduction

The path to extend airbreathing flight to hypersonic speeds has been accompanied by many technical challenges. As combustor flow speeds become supersonic, the flow residence time in the combustor decreases; as a consequence, there is now the problem of maintaining mixing and reaction rates high enough to permit complete combustion before the flow exits the combustor. The Reynolds number of the engine fluid flow also increases with Mach number, leading to thick turbulent boundary layers which may interact with shock waves and may respond to heat release generated through combustion. In order for airbreathing hypersonic propulsion systems to be successfully designed and operated, a thorough understanding of the complex reacting flow in ramjet and scramjet combustors is necessary. Achieving this knowledge through experimentation alone is accompanied by many difficulties, such as test-time limitations, optical access limitations, and the inability of ground-based experiments to properly match flight conditions.

These issues in hypersonic research have been alleviated to some extent with the ongoing maturation of numerical simulation technology. However, there are still aspects of a high-speed propulsion system's operation which lack much understanding. Of these, one which requires perhaps the most attention is the interaction between turbulence, mixing, and reactive kinetics within a scramjet combustor. Large-eddy simulation (LES) and hybrid LES/RANS simulation methods offer several advantages over state-of-the-practice Reynolds-Averaged Navier-Stokes (RANS) methods in capturing this interaction, as they are able to directly capture large-scale turbulent structures and their corresponding effects. However, since molecular mixing and combustion take place at the unresolved subgrid scales, there is still a need to model the effects of reactivity as observed at the resolved scales.

Several recent studies have utilized LES or LES/RANS techniques for modeling scramjet combustion. A combustor mapped at DLR [1] has been studied by Berglund and Fureby [2], Potturi and Edwards [3], and Genin and Menon [4]. The results showed variations in the prediction of shear layer spreading rate and peak temperatures depending on the mesh resolution, the assumed degree of three-dimensionality, and the subgrid and combustion models employed. A combustor tested at Japan's National Aerospace Laboratory has been the subject of recent studies using LES methods by Berglund, et al. [5], Fedina et al. [6], and Sabelnikov, et al. [7] These simulations studied two strut injector orientations. The results provided insights into the combustion behavior and produced combustor wall-pressure data which agreed well with experimental measurements.[8]

More recent efforts using partially-stirred reactor (PaSR) [9] and flamelet-type [10] combustion models have focused on the hydrogen-fueled HyShot combustor, ground-tested at DLR. Good agreement with available wall-heating and wall-pressure data has been generally observed, irrespective of the combustion model employed. Large-eddy simulations have also been performed by Koo et al. [11] and Fureby et al.[12] for a hydrogen-fueled combustor tested at the University of Michigan [13]. These studies utilized very different turbulence-chemistry interaction models but were able to predict the observed transition between cavity-stabilized and jet-wake stabilized modes of operation.

Some LES and hybrid LES/RANS studies of hydrocarbon-fueled scramjet combustion have also been performed, with simulations of the HiFire combustor using a flamelet / progress-variable method [14] and simulations of cavity-stabilized ethylene combustion experiments performed at the University of Virginia (UVA) [15] being two recent examples. Comparisons with observed wall pressures and (in the case of the University of Virginia

experiments) tunable diode laser spectroscopy (TDLAS) measurements have revealed adequate agreement with experimental observations.

A common thread, however, among all of the studies previously mentioned, is the relative paucity of experimental data upon which to base a substantive assessment of the interplay among the various factors that might affect the outcome of a large-eddy simulation. In addition to the subgrid-closure issues previously mentioned, these factors may include facility-dependent effects, such as variable wall heating loads and inflow non-uniformities, as well as numerical effects, such as the choice of spatial discretization and the mesh resolution. A clearer evaluation of the potential of large-eddy simulations for high-speed combustion requires more detailed experimental data.

The National Center for Hypersonic Combined-Cycle Propulsion (NCHCCP) was a program developed to provide a mechanism for intense collaboration between numerical and experimental groups in order to gain a deeper understanding of hypersonic propulsion. One of the primary goals in this center was to provide benchmark-quality datasets for scram- and dual-mode hydrogen combustion using the Supersonic Combustion Facility (SCF) located at the University of Virginia. Previous studies focusing on the ‘Configuration A’ combustor geometry without an isolator have been described in [16-19] while companion numerical predictions using a hybrid LES/RANS method have been reported in [20, 21]. The general outcome of these studies was that even simple closures, such as the ‘laminar chemistry’ assumption often invoked for high-speed combustion, were able to provide adequate agreement with mean-flow experimental data (determined from Coherent Anti-Stokes Raman Spectroscopy (CARS), Stereoscopic Particle Image Velocimetry (SPIV), Wave Modulation Spectroscopy (WMS), and OH-Planar Induced Fluorescence (OH-PLIF) measurements, among other diagnostics). The influence of the choice of reaction mechanisms on the obtained predictions was stronger than any tested variation in subgrid combustion model (though only relatively simple closures were assessed). [21]. A disadvantage of the Configuration A studies is that the spatial resolution of the CARS measurements was not as desired due to problems in the stepper motor used to position the lasers. A further disadvantage is the absence of an isolator, which restricted the equivalence ratio to low values (< 0.3). These issues were addressed through the construction of a new rig, termed ‘Configuration C’, and the development of detailed maps of the flow field using the diagnostics mentioned above at conditions that yield ‘scram mode’ operation ($\Phi = 0.17$; no shock train in the isolator) and ‘dual-mode’ operation ($\Phi = 0.49$; shock train in the isolator).

This paper describes some of the computational studies performed for the Configuration C experiments at ‘scram-mode’ conditions, with one objective being to evaluate aspects of the computational model through quantitative comparisons with some of the available experimental data. Another objective is to utilize the computational results, processed according to concepts from flamelet theory, to examine aspects of flame stabilization in the near field of the fuel injector.

2 Facility

The University of Virginia’s Supersonic Combustion Facility (SCF) is a small-scale direct-connect dual-mode experimental scramjet combustor apparatus whose operation is designed to simulate flight conditions at Mach 5 flight enthalpy – see Figures 1 and 2. It is vertically mounted and consists of an inlet nozzle, constant-area isolator, combustor, and extender, from which the exhaust gases are vented to the atmosphere. Figure 1 shows an older flowpath configuration; Figure 2 gives detailed dimensions of Configuration C, which was the actual configuration used in this study.

Figure 1: SCF configuration C, 'side' view (top) and 'top' view (bottom). Dimensions given are nondimensionalized by ramp height (0.25" or 6.35 mm)

The Mach 2 inlet nozzle, located upstream of the isolator and combustor apparatus, is responsible for bringing the incoming airflow up to the speeds at the isolator entrance that would normally be seen during low hypersonic flight, after the freestream air was slowed and compressed in the inlet section of a hypersonic aircraft. In addition, the incoming air is compressed to a stagnation pressure of roughly 300 kPa using an oil-free compressor, and a 300 kW, 14-stage electrical resistance heater raises the stagnation temperature to 1200 K without introducing flow vitiates – a significant advantage of this facility. The facility is capable of operating continuously for long durations, limited only by the available fuel supply during combustor experiments.

For the work presented here, hydrogen is used as the fuel for the SCF. The fuel is introduced into the airflow via a single, wall-mounted, unswept, 10-degree raised compression ramp injector. The height of the injector at its end plane is 0.635 cm and its width is 1.27 cm. The fuel-injection nozzle is a converging-diverging conical design that accelerates the fuel to approximately Mach 1.7 at its exit. At lower equivalence ratios, the facility operates in scramjet mode; as the equivalence ratio is increased, it transitions to dual-mode operation.

Operational data for the SCF, as well as some other parameters, are summarized in Table 1.

Table 1: SCF run conditions.

Inflow pressure, kPa	38.4 (static), 300 (stag.)
Inflow temperature, K	667 (static), 1200 (stag.)
Inflow Mach number	2.0
Outflow Backpressure, kPa	99.0
Fuel Stag. Pressure, kPa	458 ($\phi = 0.17$)
Fuel temperature, K	298
Fuel Nozzle Mach number	1.7

Experimental data was gathered from the SCF experiments using various non-intrusive measurement techniques, such as coherent anti-Stokes Raman spectroscopy (CARS) (George Washington University), OH planar laser induced fluorescence (OH-PLIF) (NASA Langley, University of Calgary, and George Washington University), stereoscopic particle image velocimetry (SPIV) (University of Virginia), focusing Schlieren (University of Virginia and Tohoku University) and tunable diode laser spectroscopy (Stanford University, University of Virginia). The present study focuses on OH-PLIF [22], wall pressure [23], SPIV [23] and CARS [24] data taken from Configuration C at an equivalence ratio of 0.17; comparisons with other diagnostic data for this configuration can be found in [25-27].

3 Numerical Methods

This work employs North Carolina State University's REACTMB flow solver. REACTMB solves the compressible Navier-Stokes equations, expanded to include separate species continuity equations, on multi-block, structured meshes using finite volume techniques. The code is parallelized using MPI. The inviscid flux terms are evaluated using Edwards' low-diffusion flux-splitting scheme [28] and viscous flux terms are calculated using central differencing. REACTMB blends a TVD reconstruction scheme with a fourth-order central scheme using the well-known vorticity / divergence switch of Ducros, et al. [29] Time integration of the

equation system is accomplished using an implicit Crank-Nicholson discretization. In this, a block incomplete lower-upper scheme is used for approximate factorization of the equation-system Jacobian matrix. A dual time-stepping approach is employed to reduce temporal discretization errors – the factorization of the system Jacobian is held constant over the duration of the sub-iterations employed.

LES can be very expensive for high-speed internal flows. REACTMB reduces this cost by using RANS techniques near viscous walls and LES everywhere else, resulting in a hybrid LES/RANS simulation. A flow-dependent blending function (called Γ) is used to switch between RANS and LES formulations approximately where an turbulent attached boundary layer shifts from its logarithmic to wake-like structure. This function is defined as follows [30]:

$$\begin{aligned}\Gamma &= \frac{1}{2} \left[1 - \tanh \left(C_s \left(\frac{1}{\lambda_N^2} - 1 \right) \right) \right] \\ \lambda_N &= C_N \sqrt{10 + \frac{\langle k \rangle + \langle k_R \rangle}{\nu \langle \omega \rangle}} \frac{\sqrt{\nu}}{C_\mu^{(1/4)} \kappa d \sqrt{\omega}} \\ C_s &= 15, \quad C_\mu = 0.09, \quad C_N = 1.5\end{aligned}\tag{1}$$

In the above, κ is the Von Kármán constant (0.41), and d is the wall distance. The turbulent kinetic energy k and specific dissipation rate ω are obtained from Menter's baseline model [31], integrated in a time-accurate manner fully coupled with the main flow equations. The brackets indicate that these quantities are ensemble-averaged to reduce fluctuations in the argument of the blending function. The ensemble-averaged, resolved turbulent kinetic energy $\bar{k}_R$ is calculated as follows:

$$\langle \bar{\rho} \rangle \langle k_R \rangle = \frac{1}{2} \left(\langle \bar{\rho} \tilde{u}_k \tilde{u}_k \rangle - \frac{\langle \bar{\rho} \tilde{u}_k \rangle \langle \bar{\rho} \tilde{u}_k \rangle}{\langle \bar{\rho} \rangle} \right)\tag{2}$$

The eddy viscosity is then defined as

$$\mu_t = \bar{\rho} \left[\Gamma \frac{k}{\omega} + (1 - \Gamma) \nu_{t,LES} \right]\tag{3}$$

The subgrid eddy viscosity $\nu_{t,LES}$ is obtained from the mixed-scale model of Lenormand, et al. [32].

The mesh developed for Configuration C simulations contains a total of about 66 million cells and covers the isolator, the combustor, and a 'dump region' outside the combustor. The latter is used to allow unsteady flow structures to propagate through the combustor outlet boundary without disruption. The average mesh spacing away from the boundary layer is 0.25 mm; the minimum spacing at solid walls is 0.005 mm. The average mesh spacing is chosen to be approximately 1/2 of a characteristic laminar flame thickness for the fuel-air mixture (~0.5 mm for stoichiometric hydrogen / air combustion). To reduce total simulation time, the facility nozzle as well as the internal fuel injector channel are not included in the computational domain. Inflow conditions for these boundaries were taken from separate simulations of the nozzle and injector. A no-slip, isothermal wall condition was enforced on all solid surfaces. The wall temperature was chosen as 600 K except for the backplane of the fuel injector and a region on the injector wall just downstream of the fuel injector, where a zirconia coating was applied to improve flameholding. The surface temperature in this region was set to 1000 K in accord with available

thermo-couple measurements.[16]

It was reported from CARS measurements [33] that the high-enthalpy air supplied to the UVa combustor was in a state of thermal nonequilibrium after passing through the Mach 2.0 inlet nozzle and was not spatially symmetric. Procedures described in [20] were used to calculate an equivalent equilibrium temperature distribution at the isolator inflow that maintained the degree of asymmetry noted in the CARS measurements. The boundary layer at the isolator inflow plane is 1.75 mm thick and is resolved using about 12 cells; the boundary layer upstream of the ramp injector is 5.54 mm thick and is resolved using about 25 cells. Resolution within the entrance viscous layers is clearly marginal, but the primary focus is on the dynamics of the much larger reactive plume.

Two approaches were used to model turbulence at the inflow of the isolator section. Initially, a continuous re-cycling / rescaling procedure was used to introduce resolved turbulent fluctuations at the isolator inflow, following Boles and Edwards [34]. As discussed later in this paper (see also [23]), this approach led to over-mixing of reactants downstream of the fuel injector, an effect likely due to marginal mesh resolution within the thin isolator boundary layers. This approach was then replaced in favor of an *ad hoc* procedure which forced the isolator region of Configuration C to operate in RANS mode before switching to hybrid LES/RANS further downstream (see Figure 3). This was done by modifying the LES/RANS blending function in Eq. (1) as follows:

$$\Gamma = \frac{1}{2} \left[1 - \tanh \left(C_s \left(\frac{1}{\lambda_N^2} - \frac{1}{b} \right) \right) \right]$$
$$b = (0.05)(1 - c) + (1.0)(c) \quad (4)$$

The value of C in Eq. (4) linearly varies from zero to one over a region coincident with half of the axial extent of the fuel injector.

4 Combustion Chemistry and Turbulence / Chemistry Closure

The nine-species, twenty-four reaction hydrogen-air oxidation model of Burke, et al. [35] was employed for all calculations presented. Two approaches for modeling subgrid-scale turbulence / chemistry interactions are considered in this study. The laminar chemistry assumption evaluates the filtered chemical production terms using filtered mean values of the species densities and temperature:

$$\overline{\dot{\omega}_s(\rho_s, T)} = \dot{\omega}_s(\overline{\rho_s}, \tilde{T}) \equiv \overline{\dot{\omega}_{s, lam}} \quad (5)$$

The laminar chemistry assumption thus implicitly neglects the effects of subgrid-scale fluctuations in composition and temperature. Its use does not necessarily lead to unacceptable results, especially if the mesh is fine enough to resolve part of the flame thickness. The simplicity of this method makes it attractive for use in initial combustion studies, and it may be used as a point of comparison for more sophisticated closures.

The second model is based on a partially-stirred reactor framework, which holds that a spatial inhomogeneity in reactive scalars will exist within a mesh cell. This inhomogeneity generally serves to reduce chemical production rates to a certain degree due to the additional time it takes for full molecular mixing to occur within the cell. The model (termed PaSR-SS) was developed and tested in [21] and utilizes scale-similarity concepts to estimate the degree of un-mixedness present in a particular mesh cell:

$$\overline{\dot{\omega}_s(\rho_s, T)} = \min(C_3, C_1 \frac{\|\overline{\dot{\omega}_s(\rho_s, \tilde{T})}\| + C_2 \mu / \Delta^2}{\|\overline{\dot{\omega}_s(\rho_s, \tilde{T})}\| + C_2 \mu / \Delta^2}) \dot{\omega}_s(\overline{\rho_s}, \tilde{T}) \quad (6)$$

An index-based test-filtering operation of the form

$$\bar{q}_{i,j,k} = \frac{1}{2} q_{i,j,k} + \frac{1}{12} (q_{i+1,j,k} + q_{i-1,j,k} + q_{i,j+1,k} + q_{i,j-1,k} + q_{i,j,k+1} + q_{i,j,k-1}) \quad (7)$$

is used to evaluate terms on the right-hand side of Eq. (6). The constants C_1, C_2 , and C_3 are assigned values of 1.0, 0.1, and 2.0, respectively. This model allows for enhancement as well as attenuation of the species production rates as calculated using laminar chemistry. *A priori* analyses described in [21] indicate that attenuation is more probable but enhancement may occur in fuel-lean and fuel-rich regions.

5 Comparisons With Experimental Data and Model Assessment

The Configuration C simulations which follow were performed at an equivalence ratio of $\Phi=0.17$, at which the facility was experimentally observed to be operating in ‘scram mode’, characterized by the absence of a shock train in the isolator. Each calculation was evolved for approximately seven combustor transit times, two of which were used to expel solution transients and five used for gathering statistics. A combustor transit time is defined as that required for a fluid element moving at the combustor inflow velocity to travel from the leading edge of the fuel injector to the exit of the combustor. Three cases are presented in this article. Case A-1 uses laminar chemistry and employs recycling / rescaling for inflow turbulence generation. Cases B-1 and B-2 use laminar chemistry and PaSR-SS, respectively, and use a RANS isolator inflow. Results from other cases may be found in [23]. Time averages shown were obtained from 350 discrete snapshots extracted over the averaging period. This number of frames approximates that used in the CARS measurements.

The general structure of the reacting plume is illustrated in Figure 4, which displays instantaneous and averaged temperature contours at the x - y centerplane for Case A-1, and in Figure 5, which compares OH mole fraction predictions with OH-PLIF intensity measurements. In Figure 4 and elsewhere, the axial location in the combustor is given as x/H , where H is the height of the ramp injector (0.635 cm) – $x/H = 0$ corresponds to the injector outlet location. The compression ramp creates a three-dimensional shock wave that wraps around it. Because the shock is generated by the angled upper ramp surface and not the sides of the ramp which are parallel to the airflow, a very strong transverse pressure gradient is created downstream of the shock which tends to force streamlines away from the ramp centerline and toward its sides. As flow spills over the sides of the ramp, it creates a pair of vortices whose axes are aligned parallel to the airflow and rotate in opposite directions.

Temperature contours in Figure 4 show that the flame is stabilized in the low-momentum region just behind the ramped injector. The action of the counter-rotating vortex pairs generated by the injector allows the flame sheet to propagate away from the upper wall, though as discussed later, flame propagation across the outer edges of the plume is inhibited due to locally high strain rates. A shear layer exists between the fuel jet and the airflow leaving the top face of the compression ramp. The shock wave created by the compression ramp is reflected a number of times between this shear layer and the combustor wall opposite the ramp. The shear layer is bent by the shock waves until it is parallel with the combustor walls and propagates down its length. This separates the downstream portions of the combustor into two general zones: a ‘core’ region

(located further away from the injector wall) and a ‘flame’ region. The core region is characterized by high speeds (supersonic during scram operation), low temperatures, and low to no reactivity. In contrast, the flame region is characterized by low speeds (usually subsonic) and very high temperatures and reactivity.

Flame temperatures peak upstream of $x/H=30$, and the majority of reactant consumption is completed by this point. Further downstream, the flame temperature reduces due to entrainment of cooler air. Comparisons of OH mole fraction with OH-PLIF signal intensity in Figure 5, while not quantitative, illustrate that the LES/RANS approach captures the effect of the vortex pairs on flame propagation. OH intensities near the injector are lower and regions of peak OH are more fragmented compared to regions further downstream, indicating the effects of incomplete fuel-air mixing and high local strain rates in this region.

Figure 6 compares wall pressure and wall-pressure standard-deviation distributions for Case A-1 with experimental data. The effect of the expanding reacting plume in initiating the compression process is evident, as is the start of a thermal choke at the end of the straight section. This effect is more clearly noted in the experimental data. Overall, agreement with experiment is very good. Wall pressure standard deviations peak near the edge of the ramp, indicating that unsteadiness is present in the shock structures emanating from the ramp injector.

The remaining examples highlight the effect of the RANS inflow and the PaSR-SS subgrid model on the obtained predictions. Figure 7 compares axial velocity predictions obtained by stereoscopic (S)PIV with those extracted from Cases A-1, B-1, and B-2. The PIV data field is limited as only the fuel jet was seeded; the computational data field is restricted to the same area as the PIV measurements. The general trend is that all LES/RANS models underpredict the degree of volumetric expansion of the plume in the vertical (y) direction. The results obtained using the RANS inflow are nearly identical, while the use of the unsteady inflow leads to slightly better predictions of the vertical displacement of the low-momentum region at $x/H=12$.

Figure 8 presents *rms* velocity (defined as $[(u')^2 + (v')^2 + (w')^2]^{1/2}$) for Cases A-1 and B-1 at $x/H = 6$ and $x/H = 12$. Case B-2 is similar to B-1 and is thus not shown. Only resolved data is processed, so the boundary-layer effects noted near the walls for Case A-1 are not present for Case B-1, which uses the RANS inflow. Neither approach captures the very low levels of turbulence intensity measured at $x/H = 6$. The case with the RANS inflow yields higher levels of turbulence intensity in the fuel-jet region at this location but produces slightly lower levels in the fuel-air mixing region and over much of interrogation region at $x/H = 12$. Broadly speaking though, the predicted turbulence intensity distributions between the cases are comparable. As shown later, the reactive-scalar trends are quite different in the near field of the injector, meaning that relatively small changes in turbulence intensity in the fuel-air mixing regions can result in larger observed changes in the reactive scalars.

Figures 9-12 compare predictions from Cases A-1, B-1, and B-2 with CARS measurements at four axial stations within the combustor ($x/H = 6$, $x/H = 18$, $x/H = 38$, and $x/H = 56$). In each figure, crosshairs indicate the axially-projected location of the fuel injection point and may be interpreted as the flame centerline. Figure 9 reveals that both runs with the RANS isolator inflow (B-1 and B-2) result in reduced temperatures at $x/H = 6$ and 18, relative to Case A-1. At $x/H = 6$ the temperature differences are slight and might be interpreted as simply a flame profile that is ‘thinner’ but just as intense as in Case A-1. At $x/H=18$, however, there is a marked drop in overall flame temperatures which brings the predictions much closer to experimental values. Case B-2, which uses the PaSR-SS model, predicts temperatures that are slightly lower than that of B-1, as expected. In addition, the temperature standard deviations, shown in Figure 10, are generally lower

for Cases B-1 and B-2, relative to A-1, and are in closer agreement with CARS measurements. Since the only difference between Cases B-1 and A-1 is the presence of resolved turbulence in the isolator region in the latter, it may be concluded that the use of the inflow turbulence-generation procedure increases the near-field mixing rates to levels higher than apparent in the experimental data. It can also be seen in Figure 10 that the degree of volumetric plume expansion in the vertical direction is lower for Case B-1, relative to Case A-1, and more in agreement with CARS data.

Further evidence of a decrease in initial mixing rates afforded by the use of the RANS inflow may be found in Figure 11, which plots nitrogen mole fraction contours at the different axial stations. This effect is also seen in Figure 9 in the form of a cooler region at $x/H = 6$, corresponding to the location of the hydrogen jet. Reduced mixing rates allow this jet to maintain its structure further downstream; in this case, however, the predictions of Cases B-1 and B-2 are in poorer agreement with CARS data, as the consumption of hydrogen is inhibited.

Figure 12 shows that the use of the RANS inflow in Cases B-1 and B-2 results in an overall increase in nitrogen concentration fluctuation intensity, relative to Case A-1 and the CARS data. The reason for this response is not completely clear. The CARS measurements indicate an asymmetric plume response in the far field that is not captured by any of the models – this could also affect the comparisons.

While the use of the PaSR-SS model does appear to improve predictive capability by reducing flame temperatures and variances in the near field, it appears that the dominant effect is the reduction of initial turbulence levels in the fuel-air mixing region afforded by use of the RANS inflow. With the RANS inflow, the transition to turbulence is afforded solely by the breakdown of the vortices generated by the ramp injector, and the initial intensity of this turbulence seems more in accord with experimental observations.

6 Analysis of the Flame Stabilization Region

As discussed earlier, comparisons with CARS, SPIV, and other diagnostic data reveal inaccuracies in temperature, species concentration, and velocity predictions that are most pronounced in the flameholding region ($x/H < \sim 18$). Furthermore, the effectiveness of attempts to model subgrid turbulence-chemistry interactions was found to be limited in this region, which is dominated by the action of counter-rotating vortices generated by the ramp injector. These types of injectors are designed to mix fuel and air as rapidly as possible to maximize combustion efficiency. At the speeds and Reynolds numbers that exist in a scramjet, it is possible that these vortices, along with the high-intensity turbulence induced by their breakdown, could lead to locally high strain rates impacting the flame. The result would be areas of diminished reactivity, which, if large enough, could lead to flame blowout. The objective of this part of the paper is to analyze the structure of the flameholding region from the standpoint of laminar flamelet theory, with a view toward identifying regions in which flame inhibition might occur.

The premise of flamelet theory is that a turbulent flame is a collection of laminar flames which have been deformed or strained by the influence of turbulent eddies.[36] A laminar flame's structure is often expressed as the well-known Burke-Schumann solution, shown as a solid red line in Figure 13. This is a plot of temperature versus mixture fraction, the latter being a measure of local equivalence ratio. Many differing definitions of mixture fraction exist; in this work, it is defined as [36]

$$Z = \frac{E_H - E_{H,ox}}{E_{H,fuel} - E_{H,ox}}$$

$$E_H = \sum_{s=1}^{NS} \frac{a_s W_H}{W_s} Y_s \quad (8)$$

where a_s is the number of atoms of hydrogen in species s . The subscripts ‘ox’ and ‘fuel’ refer to the fuel and oxidizer streams, respectively. On the oxidizer side of a non-premixed flame, Z is zero; on the fuel side, Z is unity. Between these two extremes exists the mixing-reactive zone of the flame. Within this zone is a point where the mixture fraction corresponds to stoichiometric conditions (Z_{st}). The effective flame surface is usually considered to be the locus of points near the stoichiometric mixture fraction value.

In Figure 13, it is shown that the temperature profile tends to reduce in intensity as the local strain rate increases. In flamelet theory, this strain rate is quantified by the scalar dissipation rate χ . The scalar dissipation rate is the rate at which the spatial variance of any scalar variable (such as temperature or species mass fraction) is dissipated at the smallest scales of turbulence due to molecular viscosity. The scalar dissipation rate is mathematically defined as

$$\chi = 2 \frac{\mu}{\rho S c} \frac{\partial Z}{\partial x_j} \frac{\partial Z}{\partial x_j} \quad (9)$$

It has been shown that χ is log-normally distributed throughout a flame.[37]

If the scalar dissipation rate reaches high enough levels, the flamelet will extinguish, resulting in the non-burning solution shown in blue in Figure 13. The relationship between flamelet temperature at Z_{st} and scalar dissipation rate is shown in Figure 14. At low scalar dissipation rates, there is no possibility of flamelet extinction. Between $\chi_{st,ign}$ and $\chi_{st,ext}$, the flamelet enters a region in which flame extinction *might* occur. Above $\chi_{st,ext}$, the scalar dissipation rate is so high that a reactive flamelet is not possible. An alternate way to describe flame extinction is an equivalence of turbulent and chemical reactive timescales. Under these conditions, a turbulent eddy is capable of penetrating into a flame surface and convecting heat and reactants out of it, resulting in a localized cessation of chemical reaction, or an extinction event.

To date, the phenomenon of strain-induced flame inhibition has not received much attention in the design and development of high-speed combustors for hypersonic propulsion systems. For example, it was not known if the turbulence levels in the SCF (as modeled in the LES/RANS simulations) were high enough to cause strain-induced flame inhibition. As a starting point toward answering this question, a combustion regime diagram [38] that incorporates length and velocity scales representative of LES is used to characterize the combustor flow. This diagram separates combustion into regimes based on the ratio of filter width to laminar flame thickness, Δ/l_F , and the square of the ratio of laminar flame thickness to the Kolmogorov scale, which is also

called the Karlovitz number, $Ka = \left(l_F / \eta \right)^2$. According to [35], the Karlovitz number may also

be expressed as $Ka = \sqrt{\left(\frac{u'_\Delta}{s_F} \right) \frac{l_F}{\Delta}}$ where u'_Δ is the *rms* SGS velocity fluctuation and s_F is the laminar burning velocity. The resulting regime diagram, along with sample data from a Configuration A simulation, is plotted in Figure 15.

For this diagram s_F and l_F are estimated to be 2.0 m/s and 0.5 mm, respectively, and the SGS *rms* velocity is calculated as $u'_\Delta = \sqrt{2/3} k$, where k is the subgrid turbulent kinetic energy

(estimated by test-filtering the resolved-scale velocity data [29]). The data shown was taken by sampling the flowfield for one transit time at twenty-five locations within the reaction zone while Configuration A operated at $\Phi=0.17$. As the filter size is fairly constant and the flame thickness is assumed constant, most of the data spread is in the horizontal direction and is related to the variation in the *rms* SGS velocity relative to the laminar burning velocity. The diagram reveals that the LES/RANS simulation results lie mostly within the ‘thin reaction zones’ regime, with some locations lying within the ‘resolved turbulence’ regime and others within the ‘broken reaction zones’ regime. It is in the latter that flame inhibition events are most probable. Additional analyses are necessary to determine if such events occur and if so, where they do occur within the combustor simulation. It should be noted that similar flame-regime diagrams were obtained for cavity-stabilized, hydrocarbon-fueled combustion in [15] and [39].

In a hybrid LES/RANS simulation, a direct calculation of χ is not possible. Instead, a filtered value $\tilde{\chi}$ must be calculated which contains both resolved and SGS-modeled parts:

$$\begin{aligned}\tilde{\chi} &= \chi^R + \chi^S \\ \chi^R &= 2 \frac{\nu}{Sc} \frac{\partial \tilde{Z}}{\partial x_j} \frac{\partial \tilde{Z}}{\partial x_j}\end{aligned}\quad (10)$$

The resolved part, χ^R , may be easily evaluated from filtered data. The subgrid contribution to filtered scalar dissipation rate, χ^S , is not as straightforward. Historically, this value has been estimated by direct analogy to the resolved portion:

$$\chi^S = 2 \frac{\nu_t}{Sc_t} \frac{\partial \tilde{Z}}{\partial x_j} \frac{\partial \tilde{Z}}{\partial x_j}\quad (11)$$

However, this is a rough estimate at best, and several models have been proposed to improve upon Eq. 11. Of these, a model for SGS dissipation rate was selected from [40]:

$$\begin{aligned}\chi^S &= \frac{C_{\chi}}{\Delta^2} \frac{\nu_t}{Sc_t^2} \frac{C_\epsilon}{C_\mu} \overline{Z''^2} \\ C_{\chi} &= 2.0 \quad \frac{C_\epsilon}{C_\mu} = 0.5\end{aligned}\quad (12)$$

Here Δ is the filter size, and the quantity $\overline{Z''^2}$ is the subgrid mixture-fraction variance. In this study, the subgrid mixture-fraction variance was estimated using a scale-similarity method similar to that employed in the PaSR-SS subgrid closure model.

Figure 16 plots instantaneous centerplane contours of pressure and filtered scalar dissipation rate, expressed using a base-10 logarithmic scale. Also shown in each plot is an isoline which represents the locus of instantaneous stoichiometric mixture fraction, $Z_{st} = 0.0284$. This generally represents the effective flame surface in the combustor. High scalar dissipation levels initially coincide with the fuel-air interface, and the termination of the hydrogen jet leads to a local region of elevated scalar dissipation. This region also coincides with the impingement of the reflected shock on the plume, implying that amplification of plume turbulence levels through baroclinic torque mechanisms may also contribute to the observed increase in scalar dissipation.

To analyze the role of compressibility on the observed increase in scalar dissipation, we first consider the transport equations for $\omega^2 \equiv \omega_k \omega_k$, where ω_k is the vorticity vector, and the scalar dissipation λ : As noted by others [42,43], the production terms within these equations are similar, with the first term on the right-hand side of each equation representing production via

strain rate and the second representing production via dilatation. The vorticity transport equation contains an additional production mechanism due to baroclinic torque.

$$\begin{aligned}\frac{D(\omega^2)}{Dt} &= 2\omega_i\omega_j \frac{\partial u_i}{\partial x_j} - 2\omega_i\omega_j \frac{\partial u_j}{\partial x_i} + 2\omega_i\epsilon_{ijk} \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \dots \\ \frac{D\chi}{Dt} &= -2 \left(2 \frac{\mu}{\rho Sc} \right) \frac{\partial Z}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial Z}{\partial x_j} + 2\chi \frac{\partial u_j}{\partial x_j} + \dots\end{aligned}\quad (13)$$

To determine the relative importance of these terms, an ensemble of pathlines emanating from the fuel jet and traversing the region of high scalar dissipation is extracted from a single snapshot of the 3D flowfield. The production terms, plotted in Figure 17, are calculated along the pathlines and are averaged over the ensemble members to reduce statistical scatter. The terms are evaluated using filtered mean data, as the intent is to determine only the general trends. Black bars indicate the $x/H = 3, 6, 12$, and 18 stations, respectively. These are used in analyses discussed subsequently. It is clear that strain-rate driven production is dominant over dilatation-driven production in both equations. Furthermore, vorticity production due to baroclinic torque is small where strain-rate production peaks. By this point, the small shocklets present in the fuel jet have dissipated, and the pressure is smoothly increasing. These results provide evidence that the observed increase in scalar dissipation is not significantly influenced by local compressibility effects but rather, by the interaction of the scalar field with resolved turbulence. The fact that the fuel jet plume breaks down at the location that it does, however, is a consequence of global compressibility and heat release - a tightly coupled response that forces the jet plume to negotiate an adverse pressure gradient as well as to turn toward the injector wall due to the shock / shear layer interaction.

Figure 18 shows contours of instantaneous and time-averaged $\tilde{\chi}$ at a number of crossplanes ($x/H = 3, 6, 12, 15, 18, 38$, and 56). Also shown are the instantaneous and time-averaged stoichiometric mixture-fraction contours. The region of high instantaneous scalar dissipation rate near the fuel jet appears as a red region within the stoichiometric contour; between $x/H=3$ and 6 , this region of high scalar dissipation seems to expand slightly, filling the area within the stoichiometric contour more completely. This causes the scalar dissipation rate seen at the stoichiometric contour to reach higher values, which would increase χ_{st} and therefore the possibility of flamelet extinction. The time-averaged contours must be examined with caution because these plots can only show *average* values of scalar dissipation rate with respect to the location of *average* mixture fraction, whereas flamelet theory requires that flamelets be examined in the instantaneous sense. However, the time-averaged plots may be used to estimate the ‘propensity’ of a flamelet to undergo strain-induced extinction in different regions of the combustor. In the time-averaged crossplanes of Figure 18, there is a region of the time-averaged stoichiometric contour which passes through a region of very high scalar dissipation rate at $x/H=3$ and 6 ; this region is located between the fuel jet and the core flow. Further downstream, the average scalar dissipation rate drops sharply. From this it is deduced that the possibility of instantaneous flamelet structures existing in regions of very high instantaneous scalar dissipation rate (and possibly leading to broken flame structures due to extinction) is highest for the two most upstream planes, where scalar dissipation values exceed 100 . However, this plot is not able to prove that broken flame behavior exists in this region. Further analysis is necessary to show this.

Figure 19 presents two-dimensional scatter plots of temperature versus mixture fraction in

comparison with CARS data at the $x/H=6, 18, 38$ and 56 data planes. On each data plane, CARS data for temperature (thermally-equilibrated) and mixture fraction are taken from four data points lying along a vertical line of crossplane symmetry. The computational data was also sampled at the same points on each plane to provide a direct comparison. Good agreement between computation and experiment is observed, with both showing a characteristic strained-flamelet structure at $x/H = 18, 38$, and 56 . It can be seen that fuel-air mixing and combustion lower the maximum mixture fraction as the flow proceeds downstream. These plots also show significant amounts of cooler fluid at $x/H=6$ throughout the range of mixture fraction values, but not nearly as many at the other locations. Whether or not these low-temperature points represent regions of possible flame extinction or simply the convection of cooler fluid into the flame zone cannot be determined from these maps – a third axis, representing scalar dissipation, is required at a minimum. Figure 20 plots temperature versus mixture fraction and scalar dissipation at the $x/H=3, 6$, and 12 stations. The data was extracted from three $y=\text{constant}$ lines bisecting the flame zone for each plane. The lower-temperature points seen at $x/H=3$ and 6 generally correspond to higher scalar dissipation rates, but at $x/H=12$, the low-temperature points correspond to values of the scalar dissipation that are significantly lower than at $x/H=3$ and 6 . This may imply that low temperatures in this region result from convection of cooler fluid rather than from local extinction.

The location of significant flame inhibition in the combustor may be determined by observing a consistent correlation between low instantaneous temperature and high instantaneous scalar dissipation rate at a particular location. Assuming that the reaction front is associated with the location of stoichiometric mixture fraction, this requires one to simultaneously observe four variables: temperature, scalar dissipation rate, and the y and z locations of the stoichiometric mixture fraction contour for a given crossplane. Because an extinction event is a highly transient phenomenon and the shape of the stoichiometric flame isosurface is also constantly changing, these observations must be made using a large number of instantaneous ‘snapshots’ of the flame. In this work, these observations were made using data extracted from a number of combustor crossplanes. Figure 21 illustrates the orientation of one crossplane. Figure 22 illustrates the process of constructing the spatial map which relates 2D instantaneous flame position, temperature, and scalar dissipation rate. First, two-dimensional y - z coordinates of all data points (mesh cell centroids) falling within a small range about the stoichiometric mixture-fraction value are determined (Figure 22 a). Next, the temperature is associated with the third dimension (Figure 22 b). These points are then colored by scalar dissipation rate and the procedure repeated for a large number of time instances, resulting in a cloud of points that show the influence of resolved turbulence on the data. (Figure 22 c). Figures 23-25 present these results for crossplanes located at $x/H = 3, 6$, and 12 , respectively. In each plot, $(y,z)=(0,0)$ roughly corresponds to the centroid of the data extraction plane. In Figures 23 and 24, corresponding to $x/H = 3$ and $x/H = 6$, points with low temperatures and high scalar dissipation rates are concentrated in the region between the fuel jet and the core flow; local extinction events appear to occur here as a result of very high instantaneous scalar dissipation rates. In Figure 25, corresponding to $x/H = 12$, low-temperature stoichiometric points are no longer associated with very high scalar dissipation rates but rather those comparable to the remainder of the points on this plane (evidenced here as a general uniformity of color between higher- and lower-temperature points). However, the points which exhibit low-temperature excursions are located at nearly same y - z locations as those at $x/H = 3$ and $x/H = 6$, implying that the low flame temperatures seen on this plane are a result of cooler fluid being convected downstream, not localized extinction events. Strong flame-inhibition effects appear to be confined to only the very high shear regions between $x/H = 3$ and $x/H = 6$ and are

associated with a spike in scalar dissipation resulting from the shock-flame interaction illustrated in Figure 16 and the breakdown of the fuel plume. From this analysis, it is hypothesized that the flame structure near the injector should have a ‘hole’ in it where reactivity is significantly reduced.

This hole in the flame structure can be clearly seen in Figure 26, which plots isosurfaces of instantaneous (a) and time-averaged (b-c) isosurfaces of stoichiometric mixture fraction, colored by heat release per unit volume ($-\sum_s h_s \dot{\omega}_s$). Also shown is an instantaneous stoichiometric

mixture fraction iso-surface colored by the logarithm of scalar dissipation (Figure 26d). Figure 26a reveals a distinct dark stripe of low heat release which originates downstream of the compression ramp lip and propagates to about ten to twelve ramp-heights downstream. Because this region of low-reactivity stoichiometric mixture contains fuel which was not ignited since the point at which it was first injected, it may be more appropriate to describe the flame response in this region as one of suppressed flame propagation, rather than one of flame extinction: the reactants in this region, which were otherwise well-mixed and prepared to react, are prevented from doing so by high strain rates. The flame hole is visualized better in a time-averaged sense, as shown in Figure 26b-c. In Figure 26c, the region of low heat release is seen to coincide very closely with the location of initial shock impingement on the flame, as indicated by the superimposed centerplane Schlieren image. Local flame reactivity is reduced after this point. It can be clearly seen that there is a small region of very high scalar dissipation rate about four to six ramp heights downstream of the fuel injector which coincides with a region of cooler fluid and low reactivity that extends further downstream. Overall, these results indicate a potential disadvantage of injector designs that utilize axial vorticity generation as a means of mixing enhancement – the ‘collision’ of the counter-rotating vortices and their subsequent breakdown leads to high local strain rates that can inhibit flame propagation.

7 Conclusions

Large-eddy / Reynolds-averaged Navier-Stokes (LES/RANS) simulations of supersonic combustion in the University of Virginia’s ‘Configuration C’ isolator / combustor rig have been described in this paper. The equivalence ratio is 0.17, a value small enough to ensure near complete combustion but with heat release insufficient to force a shock train into the isolator. Predictions have been compared with CARS measurements (mean and *rms*) of temperature and nitrogen mole fraction as well as wall pressure measurements, stereoscopic PIV measurements, and OH PLIF imagery. The predictions deviate the most from experimental observations in the near-field of the injector, where the breakdown of counter-rotating vortex pairs emanating from the ramp injector, combined with shock / plume interactions, lead to significant turbulence / chemistry interactions. Initial simulations performed using a recycling / rescaling turbulence generation technique yielded a pronounced over-mixing effect in the near field that was circumvented in subsequent calculations by forcing a full RANS solution in the isolator mesh. The inclusion of subgrid turbulence-chemistry interactions, as modeled by a partially-stirred reactor – type model, provided better overall agreement with experimental data, relative to laminar chemistry, but the effect was found to be minor compared with that due to the presence or absence of resolved turbulence in the combustor inflow. An analysis of turbulence / chemistry interactions within the flame-stabilization region downstream of the fuel injector was conducted using concepts from laminar flamelet theory. The analysis revealed a region of high instantaneous scalar dissipation rate initially concentrated within the fuel jet and enlarged as the fuel jet breaks down. Significant flame inhibition is observed where this region coincides with

the stoichiometric value of the mixture fraction, leading to a ‘hole’ in the flame that extends downstream into regions less affected by high strain rates.

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References

- [1] W. Waidmann, U. Brummund, and J. Nuding., Experimental investigation of supersonic combustion ramjet (SCRAMJET), 8th Symposium on Transport Phenomena in Combustion (1995) 1473-1484
- [2] M. Berglund and C. Fureby, LES of supersonic combustion in a scramjet engine model, Proceedings of the Combustion Institute, 31 (2006) 2497-2504
- [3] A. Potturi and J. Edwards, Hybrid large-eddy / Reynolds-averaged Navier-Stokes simulation of flow through a model scramjet, AIAA Journal, 52 (2014) 1417-1429.
- [4] F. Genin and S. Menon, Simulation of turbulent mixing behind a strut injector in supersonic flow, AIAA Paper 2009–0132, (2009).
- [5] M. Berglund, E. Fedina, C. Fureby, V. Sabelnikov, and J. Tegnér, Finite rate chemistry large-eddy simulation of self-ignition in supersonic combustion ramjet, AIAA Journal, 48 (2010) 540-550.
- [6] E. Fedina, C. Fureby, V. Sabelnikov, and J. Tegnér, On the sensitivity of subgrid turbulence chemistry interaction models in large eddy simulation of self-ignition in vitiated hot confined supersonic air flow, Proceedings of the 6th Mediterranean Combustion Symposium (2009)
- [7] V. Sabelnikov, Combustion in supersonic flow: finite-chemistry effects – LES simulation, NORDITA Workshop on Turbulent Combustion, Stockholm, Sweden (2010).
- [8] C. Fureby, LES for supersonic combustion, AIAA Paper 2012–5979, (2012).
- [9] C. Fureby, M. Chapuis, E. Fedina, and S. Karl, CFD analysis of the HyShot II scramjet combustor, Proceedings of the Combustion Institute, 33 (2011) 2399-2405.
- [10] J. Larsson, Large eddy simulations of the HyShot II scramjet combustor using a supersonic flamelet model, AIAA Paper 2012-4261 (2012)
- [11] H. Koo, P. Donde, and V. Raman, A quadrature-based LES/transported probability density function approach for modeling supersonic combustion, Proceedings of the Combustion Institute, 33 (2011) 2203-2210.

- [12] C. Fureby, J. Tegnér, R. Farinaccio, R. Stowe, and D. Alexander, A computational study of a dual mode ramjet combustor with a cavity flameholder. *International Journal of Energetic Materials and Chemical Propulsion*, 11 (2012) 487-510.
- [13] D. Micka and J. Driscoll, Combustion characteristics of a dual-mode scramjet combustor with cavity flameholder, *Proceedings of the Combustion Institute*, 32 (2009) 2397–2404.
- [14] A. Saghafian, S. Lee, D. Philips, and F. Ham, Large eddy simulations of the HIFiRE scramjet using a compressible flamelet/progress variable approach, *Proceedings of the Combustion Institute*, 35 (2015) 2163-2172.
- [15] A. Potturi and J. Edwards, Large-eddy / Reynolds-averaged Navier-Stokes simulation of cavity-stabilized ethylene combustion, *Combustion and Flame*, 162 (2015) 1176-1192.
- [16] R. Rockwell, C. Goyne, B. Rice, T. Kouchi, J. McDaniel, and J. Edwards, Collaborative experimental and computational study of a dual mode scramjet combustor, *Journal of Propulsion and Power*, 30 (2014) 530-538.
- [17] A. Cutler, G. Magnotti, L. Cantu, E. Gallo, R. Rockwell, C. Goyne, Dual-pump coherent anti-Stokes Raman spectroscopy measurements in a dual-mode scramjet, *Journal of Propulsion and Power*, 30 (2014) 539-549.
- [18] C. McRae, C. Johansen, R. Rockwell, C. Goyne, L. Cantu, P. Danehy, E. Gallo, J. McDaniel, OH PLIF visualization of the UVa supersonic combustion experiment: Configuration A, *Journal of Visualization* 17 (2014) 131-141.
- [19] I. Schultz, C. Goldenstein, J. Jeffries, R. Hanson, R. Rockwell, and C. Goyne, Diode laser absorption sensor for combustion progress in a model scramjet, *Journal of Propulsion and Power*, 30 (2014) 550-555.
- [20] J. Fulton, J. Edwards, H. Hassan, J. McDaniel, C. Goyne, R. Rockwell, A. Cutler, C. Johansen, and P. Danehy, Large-eddy / Reynolds-averaged Navier-Stokes simulations of reactive flow in a dual-mode scramjet combustor, *Journal of Propulsion and Power* 30 (2014) 558-575.
- [21] A. Potturi and J. Edwards, Investigation of subgrid closure models for finite-rate scramjet combustion, *AIAA Paper* 2013-2461 (2013)
- [22] C. McRae, C. Johansen, P. Danehy, E. Gallo, L. Cantu, G. Magnotti, A. Cutler, R. Rockwell, C. Goyne, J. McDaniel, OH PLIF visualization of the UVa supersonic combustion experiment: Configuration C, *AIAA Paper* 2013-0034 (2013)
- [23] B. Rice, C. Goyne, J. McDaniel, R. Rockwell, Characterization of a Dual-Mode Scramjet via Stereoscopic Particle Image Velocimetry, *AIAA Paper* 2014-0986 (2014)

- [24] A. Cutler, G. Magnotti, L. Cantu, E. Gallo, P. Danehy, R. Rockwell, C. Goyne, J. McDaniel, Dual-pump CARS measurements in the University of Virginia's dual-mode scramjet: Configuration "C", AIAA Paper 2013-0335 (2013)
- [25] I. Schultz, C. Goldenstein, J. Jeffries, R. Hanson, R. Rockwell, and C. Goyne, Spatially-resolved water measurements in a scramjet combustor using diode laser absorption. *Journal of Propulsion and Power* 30 (2014) 1551-1558
- [26] J. Fulton, Numerical simulation of a dual-mode scramjet using a RANS and hybrid LES-RANS approach, Ph.D. Dissertation, North Carolina State University (2013).
- [27] K. Busa, B. Rice, J. McDaniel, C. Goyne, R. Rockwell, J. Fulton, and J. Edwards, Direct measurement of combustion efficiency of a dual-mode scramjet via TDLAT and SPIV, AIAA Paper 2015-0357 (2015)
- [28] J. Edwards, A low-diffusion flux-splitting scheme for Navier-Stokes calculations, *Computers and Fluids* 26 (1997) 635-659.
- [29] F. Ducros, V. Ferrand, F. Nicaud, C. Weber, D. Darracq, C. Gachareiu, and T. Poinso, Large-eddy simulation of the shock / turbulence interaction, *Journal of Computational Physics* 152 (1999) 517-549.
- [30] D. Gieseeking, J. Edwards, and H. Hassan, Compressible flow simulations using a new LES/RANS model, *AIAA Journal* 49 (2011) 2194-2209.
- [31] F. Menter, Two equation eddy viscosity turbulence models for engineering applications, *AIAA Journal* 32 (1994) 1598-1605.
- [32] E. Lenormand, P. Sagaut, L. Phouc, and P. Comte, Subgrid-scale models for large-eddy simulations of compressible, wall-bounded flows, *AIAA Journal* 49 (2000) 1340-1350.
- [33] A. Cutler, L. Cantu, E. Gallo, R. Baurle, P. Danehy, R. Rockwell, C. Goyne, and J. McDaniel, Nonequilibrium supersonic freestream studied using coherent anti-Stokes Raman spectroscopy, *AIAA Journal* 53 (2015) 2762-2770.
- [34] J. Boles, J. Edwards, and R. Baurle, Multi-wall recycling / rescaling method for inflow turbulence generation, AIAA Paper 2010-1099 (2010).
- [35] M. Burke, M. Chaos, Y. Ju, F. Dryer, and S. Klippenstein, Comprehensive kinetic model for high-pressure combustion, *Journal of Chemical Kinetics* 44 (2012) 444-474.
- [36] N. Peters, *Turbulent Combustion*, Cambridge, New York, 2000
- [37] H. Pitsch and H. Steiner, Scalar mixing and dissipation rate in large-eddy simulations of non-premixed turbulent combustion, *Proceedings of the Combustion Institute*, 28 (2000) 41-49.

[38] H. Pitsch, Large-eddy simulation of turbulent combustion, Annual Review of Fluid Mechanics, 38 (2006) 453-482.

[39] J. Quinlan, J. McDaniel, T. Drozda, G. Lacaze, J. Oefelein, *A priori* analysis of flamelet-based modeling for a dual-mode scramjet combustor, AIAA Paper 2014-3743 (2014).

[40] M. Ihme and Y. See, Large-eddy simulation of a turbulent lifted flame in a vitiated co-flow, AIAA Paper 2009-329 (2009).

[41] J. Martin and C. Dopazo, "Turbulent mixing in combustion modeling", in Engineering Turbulence Modeling and Experiments, W. Rodi and N. Fueyo, eds., Elsevier, 2002.

[42] N. Swaminathan and K. Bray, Effect of dilatation on scalar dissipation in turbulent premixed flames, Combustion and Flame, 143 (2005), 549-565.

Figure Captions

Figure 2. Layout of UVa Supersonic Combustion Facility (SCF)

Figure 3. SCF configuration C, ‘side’ view (top) and ‘top’ view (bottom). Dimensions given are non-dimensionalized by ramp height (0.25” or 6.35 mm)

Figure 4. *Ad hoc* method of forcing RANS in isolator of configuration C

Figure 5. Temperature contours at X-Y centerplane (top: averaged, bottom: instantaneous)

Figure 5. Predicted OH mole fraction (bottom) versus OH-PLIF signal intensity (top)

Figure 6. Wall pressure and wall pressure standard deviation distributions

Figure 7. Near-field axial velocity comparison with SPIV data

Figure 8. *RMS* velocity magnitude at $x/H = 6$ and $x/H = 12$

Figure 9. Mean temperature predictions vs. CARS data

Figure 10. Temperature standard deviation predictions vs. CARS data

Figure 11. Mean N_2 mole fraction predictions vs. CARS data

Figure 12. N_2 mole fraction standard deviation predictions vs. CARS data

Figure 13. Non-premixed flamelet structure

Figure 14. Qualitative plot of scalar (temperature) vs. scalar dissipation rate, also known as the ‘S-curve’

Figure 15. Combustion regime diagram, after [38], containing configuration A sample data

Figure 16. Centerplane contours of static pressure (top) and logarithm of χ (bottom)

Figure 17. Production mechanisms for squared-vorticity and scalar dissipation

Figure 18. Instantaneous and averaged crossplane contours of logarithm of χ

Figure 19. Scatterplots of temperature vs. mixture fraction (CARS vs. CFD)

Figure 20. Scatterplots of temperature vs. mixture fraction and scalar dissipation ($x/H = 3, 6,$ and 12)

Figure 21. Extraction of flame-surface points on 2D crossplane slice, showing relative position and orientation of combustor flowpath, slice plane, and injector location

Figure 22. Visual explanation of spatial flame map generation ($x/H = 6$). (a) Locations of stoichiometric mixture fraction on 2D slice plane. (b) Projection of temperature in third dimension. (c) Coloration by instantaneous scalar dissipation rate and collection of large number of time instances

Figure 23. Spatial map of instantaneous stoichiometric temperature and scalar dissipation rate at $x/H = 3$

Figure 24. Spatial map of instantaneous stoichiometric temperature and scalar dissipation rate at $x/H = 6$

Figure 25. Spatial map of instantaneous stoichiometric temperature and scalar dissipation rate at $x/H = 12$

Figure 26. Isosurfaces of stoichiometric mixture fraction. (a) Instantaneous, colored by heat release. (b) Time-averaged, colored by heat release. (c) Time-averaged with Schlieren image. (d) Instantaneous, colored by scalar dissipation rate

Figure1

Figure2

Figure3

Figure4

Figure5

OH-PLIF

LES/RANS

Figure6

Figure7

Figure8

Figure9

Figure10

Figure11

Figure12

Figure13

Figure14

Figure15

Figure16

Figure17

Figure18

Figure19

Figure20

Figure21

Figure22

Injector Wall

(a)

(b)

(c)

Figure23

Figure24

Figure25

Figure26