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# AN IMPROVED SUPERSONIC COMBUSTION ANALYSIS PROCEDURE FOR SCRAMJETS

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### ABSTRACT

Dual-mode scramjets, which are the systems of primary interest in this study, have intricate dynamics, including complex and unsteady pseudo-shock phenomenon, thermal choking, and the potential performance issue of unstart, that need to be thoroughly understood in order to design realistic air-breathing hypersonic vehicles. Our interest focuses on the manner in which pressure is treated within the laminar flamelet framework to modeling turbulence-combustion interaction. The laminar flamelet method provides a highly efficient means of modeling combustion when the mass fractions of a large number of species are of interest. However, the original approach was developed for combustion in low-speed flows. Extension to high-speed flows has been done in several ways in our work, including the addition of pressure as an independent variable of the flamelet library and using several formulations for this. To further improve model fidelity, several progress variable interpolations from the S-curves of opposed-jet flames have also been investigated in our work. The observations from our studies emphasize the need to be critical about the precise sub-models when judging the accuracy of the flamelet method for supersonic combustion simulation.

**KEYWORDS:** Supersonic combustion, Air-breathing propulsion, Laminar flamelet method, Large-eddy simulation, Pressure scaling, Pressure modeling, Progress variable interpolation

### **1. INTRODUCTION**

Supersonic combustion [1,2] has many peculiarities when compared to its low-speed counterpart. For internal supersonic combustion systems such as those found in dual-mode scramjets, intricate dynamics, including complex and unsteady pseudo-shock phenomenon [3], thermal choking [4] and the potential performance issue of unstart, have to be thoroughly understood in order to design realistic air-breathing hypersonic vehicles. Of particular interest in the present work is the role of pressure fluctuations as they affect combustion dynamics under supersonic conditions. With this interest in mind, we focus on the manner in which pressure is treated in the laminar flamelet approach to modelling turbulence-combustion interaction in turbulent supersonic combustion. The laminar flamelet approach [5] was originally developed for combustion in low-speed flows. Thus, the need arises to extend the procedure to supersonic combustion. This has been done in several ways in our work [6], including the addition of pressure as an independent variable of the flamelet library and using several formulations for this. To further improve model fidelity, several progress variable interpolations from the S-curves of opposed-jet flames have also been investigated in our work. Some details are provided in this paper.

# 2. MODELING APPROACH

#### **2.1 The LES Equations**

The fully compressible form of the large-eddy simulation (LES) equations for continuity, momentum, and energy are solved together with the filtered transport equations for the mixture fraction, Z, and progress

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variable, *C*. Appearing in the equations are independent variables (t, x, y, z) which are time and the three spatial coordinate directions, respectively. The equations are Favre-filtered, to give the dependent variables  $\overline{\rho}$  the density,  $\overline{p}$  the static pressure,  $\tilde{u}_i$  the velocity component in the *i*<sup>th</sup> physical-coordinate directions  $x_i$ , and  $\tilde{E}$  the total specific energy:

$$\widetilde{E} = \int_0^T c_p dT - \frac{\overline{p}}{\overline{\rho}} + \frac{\widetilde{u}_j \widetilde{u}_j}{2} + k^{SGS} , \qquad (1)$$

where T is temperature,  $c_p$  is specific heat at constant pressure and  $k^{SGS}$  is the sub-grid turbulent kinetic energy. Bilger's equation is used to define the mixture fraction. In the equations, overline on a variable implies Reynolds-averaging, tilde denotes Favre-averaging and the subscript "t" refers to turbulence quantities. The filtered viscous stress tensor,  $\tau_{ij}$ , and the heat flux vector,  $q_j$ , are based on the filtered flow variable. The sub-grid scale (SGS) terms are resolved using the Smagorinsky model and the parameters are determined empirically, or are dynamically computed using the formulation in, with the modifications proposed by Lilly:

$$\tau_{ij}^{SGS} = \overline{\rho u_i u_j} - \overline{\rho} \widetilde{u}_i \widetilde{u}_j, \qquad (2)$$

$$H_{j}^{SGS} = -\overline{\rho} \, \frac{\nu_{t}}{\Pr_{t}} \left( \frac{\partial \widetilde{h}}{\partial x_{j}} + \widetilde{u}_{i} \, \frac{\partial \widetilde{u}_{i}}{\partial x_{j}} + \frac{1}{2} \, \frac{\partial k^{SGS}}{\partial x_{j}} \right), \tag{3}$$

where *h* is the enthalpy, *v* is the kinematic viscosity and the unclosed viscous work,  $\sigma_j^{SGS}$ , is assumed to be zero. The heat release rate,  $\tilde{Q}$ , and reaction rate of progress variable,  $\tilde{\omega}_c$ , are obtained from flamelet table. The CFD code used for solving the compressible flow equations is called AEROFLO [7], which is a significantly enhanced version of the high-order FDL3DI code developed at the Computational Sciences Branch of Excellence at the Wright-Patterson Air Force Base [8]. AEROFLO is based on high-order curvilinear, finite difference schemes, with advanced overset capabilities. The large-eddy simulation (LES) procedures in AEROFLO include the standard and dynamic Smagorinsky models, Vreman's version of the Smagorinsky model, and the approach by Menon which involves the solution of an evolution equation for the sub-grid scale turbulence kinetic energy. AEROFLO supports the sixth-order compact schemes and several versions of the fifth-order weighted essentially-non-oscillatory (WENO) schemes. Second- and third-order spatial discretization with the MUSCL schemes is also supported in the tool. The time integration methods in the code include backward Euler, the trapezoid rule, fourth-order Runge-Kutta, third-order total-variation-diminishing (TVD) Runge-Kutta, and Beam-Warming-type approximate factorization. For the present study, MUSCL and the Beam-warming schemes are used for spatial and temporal integrations, respectively.

## 2.2 Generation of the Flamelet Library

The flamelet libraries are generated by solving the governing equations for opposed-jet flames (OJF) [9]:

$$-G + \frac{dU}{dx} = 0, \tag{4}$$

$$\frac{dH}{dx} = 0, (5)$$

$$\frac{3}{\rho}G^2 - 2\frac{d}{dx}\left(\frac{UG}{\rho}\right) + \frac{d}{dx}\left(\mu\frac{d}{dx}\left(\frac{G}{\rho}\right)\right) + H = 0 , \qquad (6)$$

$$2U\frac{dT}{dx} - \frac{1}{c_p}\frac{d}{dx}\left(\kappa\frac{dT}{dx}\right) + \frac{\rho}{c_p}\sum_{i}^{N}Y_iV_ic_{p,i}\frac{dT}{dx} + \frac{1}{c_p}\sum_{i=1}^{N}\dot{\omega}_ih_iW_i = 0,$$
(7)

$$2U\frac{dY_i}{dx} + \frac{d}{dx}(\rho Y_i V_i) - \dot{\omega}_i W_i = 0; i = 1, 2, \dots N , \qquad (8)$$

where  $G = -\frac{\rho v_r}{r}$ ,  $U = \frac{\rho v_x}{2}$  and  $H = \frac{1}{r} \frac{\partial p}{\partial r}$ ,  $v_r$  and  $v_x$  are radial velocity and axial velocity, respectively,  $\kappa$  is

the thermal conductivity,  $W_i$  is the molecular weight of species *i*, and  $\mu$  is the dynamic viscosity.

To solve OJF equations above, we use the arc-length continuation method. Thus the equations are written as [10]:

$$F_i(\widetilde{\phi};\lambda) = 0, \qquad (9)$$

where  $\tilde{\phi}$  is the solution vector:

$$\widetilde{\phi}_{j} = (Y_{i}, T, G, U, H)_{j}, j = 1, \dots, N_{p} \cdot (N_{Y} + 4),$$
(10)

where  $N_p$  is the number of grid points,  $N_Y$  is the number of species in the mechanisms and  $\lambda$  is a suitably selected physical parameter. To improve the conditioning of the equations, a new variable, pseudo-arc-length, s, is introduced to re-parameterize the solutions in the form  $(\tilde{\phi}(s), \lambda(s))$ , where  $\lambda$  then becomes an eigenvalue. An extra scalar equation is adopted such that the dependence of s on the augmented solution vector is written as

$$N = \dot{T}_{\max,0} \left( T_{\max} - T_{\max,0} \right) + \dot{\lambda}_0 \left( \lambda - \lambda_0 \right) - \Delta s = 0,$$
(11)

where the phase space ( $T_{\max}(s), \lambda(s)$ ) has been used instead of the standard ( $\tilde{\phi}, \lambda$ ) that is commonly used in the literature. A predictor-corrector method is used to obtain the solution vector. Details are available in [10].

#### 2.3 Pressure Treatment in the Flamelet Library

Pressure has been added as an independent variable in the flamelet library, for the purpose of accounting for the effects compressibility-induced pressure fluctuations on supersonic combustion. Three seven-pressure-level (SLP) flamelet libraries are generated for the simulation of hydrogen-air flame (10-species, 19-reactions [11]) to represent the three branches of the S-Curve, with the pressures being: 0.2, 0.4, 0.6, 0.8, 1.0, 1.5, and 2.5 atm. In addition to SLP, separate background pressure values of 0.2, 1.0, and 2.5 atm. are also included in the flamelet library.

#### 2.4 Progress Variable Interpolation from the S-Curve

One flamelet library is generated for each of the three branches of the S-curve. The subscripts "0", "1/2", and "1" are used to represent the stable burn library, unstable burn library, and pure mixing library, respectively. The stoichiometric progress variable value,  $C_{st}$ , is used to measure the local reaction progress. Since hydrogen-air flame is of interest in this work, the mass fraction of water is chosen to define the progress variable:  $C = Y_{H_2O}$ . Several progress-variable-based interpolation methods have been investigated, as follows. In Linear Progress Variable Interpolation (LPVI), the variables  $\phi \equiv \left(Y_i, Q, \dot{\omega}_c\right)$  are linearly interpolated depending on the values of the progress variable

(PV) obtained from the solution of its filtered transport equation, vis-à-vis the values obtained from the flamelet library. For the Stable Branches PV model, only the stable (upper and lower) branch libraries are used, whereas in the Upper Branch Only model, only the stable burn library is used. In the Middle Branch Only model, only the unstable burn library is used.

#### **3. VALIDATION AND RESULTS**

Two problems have been used to validate the models proposed in this work. The first is the supersonic hydrogen-air jet flame in [12]. The non-dimensional heat release distribution versus the non-dimensional flame length was compared between our simulations and the experimental results in [57]. It was found that SLP pressure model combined with LPVI gives the correct distribution of the heat release rate, which has a log-normal profile. The goodness-of-fit,  $R^2$ , is 91%, meaning that the log-normal model explains 91% of the variability of the numerical data around its mean. An alternative numerical simulation using a more typical flamelet condition – that is, the single pressure (1.0 atm.) library and Upper-Only PV interpolation, gives a Gaussian profile, which is the distribution associated with low-speed combustion using the standard library generation procedure. Details of the validation exercise are contained in [6].

A supersonic combustor [13], with a height of 20 cm and a length of 131 cm, has also been investigated. The geometry (Fig. 1) has a close resemblance to the HyShot test model. A transverse fuel injector is placed 14 cm from the inlet. The schematic of the combustor can be found in Fig. 1. Only half of the domain is simulated on the assumption of symmetry and, as in the source of the test case [13], two-dimensional grids are used. Hydrogen fuel is injected sonically into the combustor through a vertical choked port of 0.1 cm in diameter. The minimum grid spacing adjacent to the wall is chosen to be 20  $\mu$ m, which gives a wall  $y^+$  value of unity. Grid convergence using three grids was established for the calculations. Additional validation of the flamelet procedures has been obtained in this study by calculating the same problem using the transported species approach and laminar chemistry. Details of similar procedures can be found in [14]. Qualitatively, the results agree quite well [6].



Fig. 1 Schematic of the supersonic combustor.

Sample results are shown in Figs. 2 and 3 below, respectively for the pressure and progress variable models. Significant effects of pressure and progress variable modeling are evident in these results.

#### REFERENCES

- [1] Ferri, A., "Mixing-controlled Supersonic Combustion," Annual Review of Fluid Mechanics, Vol. 5, pp. 301-338 (1972).
- [2] Ladeinde, F. "A Critical Review of Scramjet Combustion," AIAA Paper 2009-0036. (2009).
- [3] Matsuo, K., Miyazato, Y. and Kim, H.-D., "Shock Train and Pseudo-Shock Phenomena in Internal Flows, *Progress in Aerospace Sciences*, Vol. 35, pp. 93-100 (1999).
- [4] Fotia, M. L. and Driscoll, J. F. "Isolator-combustor Interactions in a Direct-Connect Ramjet-Scramjet Experiment, J. Prop. Power, Vol. 28, No. 1, pp. 83-95 (2012).
- [5] Peters, N., "Laminar Flamelet Concept in Turbulent Combustion," 21st Symposium on Combustion, The Combustion Institute, pp. 1231-1250, (1986).
- [6] Ladeinde, F., Lou, Z. and Li, W., "New Results from Improved Pressure and Progress Variable Modeling of Turbulent Supersonic Combustion," AIAA 2017 Joint Propulsion Conference, Atlanta, GA, (2017).
- [7] Ladeinde, F., Cai, X.C., Alabi, K., and Safta, C. "The First High-Order CFD Simulation of Aircraft: Challenges and Opportunities," AIAA Paper 2006-1526 (2006).

[8] Gaitonde, D. and Visbal, M.R., "High-Order Schemes for Navier–Stokes Equations: Algorithm and Implementation into FDL3DI," Technical Report# AFRL-VA-WP-TR-1998-3060, (1998).

- [9] Kee, R. J., Rupley, F. M., and Miller, J. A., "Chemkin-II: A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics," Report No. SAND-89-8009). Sandia National Labs., Livermore, CA (USA), (1989).
- [10] Lou, Z. and Ladeinde, F. "On the Unstable Branch in Non-Premixed Opposed-Jet Laminar Flames," Submitted to Journal of Combustion (2017).
- [11] Conaire, Ó, Curran, M., , Simmie, H. J., Pitz, J. M., and Westbrook, C. K. "A Comprehensive Modeling Study of Hydrogen Oxidation," International Journal of Chemical Kinetics, Vol. 36, No. 11, pp. 603-622 (2004).
- [12] Yoon, Y., Donbar, J. M., Huh, H., and Driscoll, J. F., "Measured Supersonic Flame Properties-Heat-Release Patterns, Pressure Losses, Thermal Choking Limits," Journal of Propulsion and Power, Vol. 12 No. 4, pp. 718-723 (1996).

- [13] Choi, J. Y., Ma, F., and Yang, V. "Combustion Oscillations in a Scramjet Engine Combustor with Transverse Fuel
- [15] Choi, S. F., Ma, F., and Fang, V. Combustion Oscillations in a behangle Engline Combustor with Transverse Face Face Figure 11, 1997 [11] Fureby, C., "Comparison of Flamelet and Finite rate Chemistry LES for Premixed Turbulent Combustion," AIAA Paper 2007-1413, January 2007.



Fig. 2 Effects of pressure model on reaction progress variable in supersonic combustion.



Fig. 3 Effects of progress variable model on the temperature field in supersonic combustion.