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A Critical Review of Scramjet Combustion Simulation (Invited)

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A review of scramjet combustion simulation is provided in this paper. The topics covered include the fundamental problem of supersonic mixing layers, high-speed combustion modeling efforts, and actual calculations of realistic scramjet combustors. The review shows that the RANS approach dominates the turbulence modeling of the system, with only a handful of LES work. Also, virtually all the numerical works are based on low-order schemes, and the combustion models that have been used for realistic simulations solve the species evolution equations with assumed PDF closures, although there seems to be a growing use of the flamelet methods. Spray modeling for scramjet combustion has not received enough attention.

Nomenclature

2D = two-dimensional
3D = three-dimensional
C_p = specific heat at constant pressure
CFL = Courant-Friedrichs-Lewy
D = diffusion coefficient
DES = detached eddy simulation
k = kinetic energy of turbulence
P = probability density function (PDF)
P_{rt} = turbulence Prandtl number
p = pressure
S = stoichiometric coefficient
S_{ct} = turbulence Schmidt number
T = temperature
t = time
TVD = total-variation diminishing
u = velocity
Y = mass fraction
Z = mixture fraction
δ = Kronica delta
ε = kinetic energy dissipation rate
ζ = variance of fluctuating vorticity
κ = parameter in the MUSCL scheme
μ = absolute or dynamic viscosity
ρ = density
σ = shear stress tensor
φ = function of species and/or temperature, equivalence ratio
χ = mixture fraction dissipation rate
$\dot{\omega}$ = reaction rate

Subscripts
airc = inlet to combustor
airct = total (stagnation) at inlet to combustor
f = fuel
i = coordinate direction; 1, 2, 3
j = coordinate direction; 1, 2, 3
k = index for species
o = oxidizer
p = products
∞ = free stream

I. Introduction

EXPERIMENTAL facilities for scramjet combustion measurements are extremely complicated, such that only a few run-time facilities are available worldwide. The computational fluid dynamics (CFD) approach, which can be developed to a high-fidelity level, offers the modeling and simulation alternative, and has been investigated extensively. A critical review of this simulation approach, covering the aerothermodynamics and combustion aspects in supersonic combustion and scramjets is presented in this paper. It is the objective of this review to provide fairly detailed and current information on the subject, to complement other relevant reviews. One of such reviews is that of Baurle,[1] who provides an overview of the modeled equations typically employed by commercial-quality CFD codes

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for high-speed combustion applications, emphasizing on the salient features and shortcomings of the averaged equation set. Some of the models in Ref [1] have been implemented in VULCAN, a widely-used, multi-grid, flux-difference-split, finite-volume code, developed by the Air Force and NASA for high-speed (ramjet, scramjet) reacting flow simulation. The precise models and solution procedure in this code are documented in White and Morrison.[2] Tishkoff et al.[3] presents the state of supersonic combustion research, including modeling and simulation, as an outcome of a joint AFRL/NASA meeting in May of 1996, in which the state-of-the-art in hydrocarbon and/or hydrogen-fueled scramjet research was examined, with suggestions for the future direction and needs of basic research in support of scramjet technology.

Other relevant reviews, albeit applicable mostly to low-speed combustion, include Givi,[4] who provides a review of the state-of-the-art in subgrid scale modeling as required for large-eddy simulation (LES) of turbulent combustion. Closure complexities caused by chemical reactions are the focus, while Givi[5] presents a review devoted primarily to subgrid scale (SGS) closure based on the filtered density function (FDF), which is a method that is analogous to the probability density function (PDF) modeling. A more recent review of the FDF method is provided in Ref [6]. Heinz[7] highlights the fundamental differences between the Reynolds-averaged Navier-Stokes (RANS) and LES combustion models for premixed and non-premixed turbulent combustion.

Finally, Grinstein[8] addresses modeling issues relevant to CFD of turbulent non-premixed jet flames, including subgrid and supergrid modeling. Transitional jet diffusion flames of the hydrogen/air and propane/air types are reviewed, while the jets studied involve laminar initial conditions, preferential diffusion effects, weak axial forcing, negligible streamwise vorticity, and negligible azimuthal non-uniformities, as well as the impact of aspect ratio-dependent vortex topological and dynamical features on the development of the jet diffusion flame. Models for turbulence, chemical reactions, volume expansion, and heat release are discussed, as are models for the dominant features of the couplings between the various phenomena.

Unlike the foregoing reviews, which either did not dwell much on the complexities of scramjet engines or omitted scramjets entirely, it is the intricate aerothermodynamic, combustion, and mixing aspects of the scramjet system that are of interest in this review, since they pose challenges to accurate and computationally-efficient modeling of the engine.

It is well-known that air-breathing propulsion at high supersonic speeds encounters some novel and troublesome constraints on the combustion problem.[9,10,11] In a scramjet, the inlet compresses the free-stream air from a hypersonic Mach number to roughly one-third of the inlet value by the time it reaches the combustor. However, the decelerated flow at the combustor in a scramjet is supersonic, so that the fuel residence time in the combustor is of the order of 1 ms, during which time the fuel and oxidant must be mixed on a molecular scale and reactions must be completed before leaving the engine. Thus, supersonic combustion is very difficult to maintain. The ignition delay time of a fuel-air mixture continues to be a limiting factor for all scramjet engine designs; a decrease in this quantity allows the use of a shorter combustor and/or higher flight velocities. The effects of fuel and/or air stream temperature, pressure, and equivalence ratio on ignition delay ratio have been investigated. However, mixing remains a serious problem for scramjet combustion because of the high speed and the fact that reaction will not occur without it, independent of the temperature, pressure, or equivalence ratio. It is therefore understandable that the fuel injection pattern could be critical for a successful scramjet engine operation, explaining the numerous investigations on injector systems.[12-15] Another technological challenge associated with the scramjet engine arises from the fact that reactants may start to dissociate prior to combustion due to their high temperatures. This leads to significantly lower heat release and the attendant reduction in combustion efficiency or fuel-specific impulse. In addition, ignition at the high velocities encountered in scramjets poses problems.

II. Theoretical Foundation

The theoretical foundation for the flow and/or combustion in scramjet combustors have been based on the canonical model of supersonic mixing layers. Insights on the problem have been obtained from linear stability analysis of both the temporal and spatial waves (Michalke[16-18]), while the characteristics of large coherent structures have been investigated experimentally by Brown and Roshko.[19] They discuss the central instability mode for two-dimensional incompressible, non-reacting flows, while Lesson, Fox, and Zien[20] analyze the inviscid temporal stability of compressible mixing layers that were subjected to two-dimensional and three-dimensional disturbances. The spatial case was investigated by Goldstein and Leib,[21] Grosch and Jackson,[22] and Jackson and Grosch.[23] In addition to the central mode, they also report on two outer modes, which were further investigated by Day, Reynolds, and Mansour[24] in studies that were extended to the reacting, supersonic case. The combined effects of compressibility, heat release, density ratio, equivalence ratio, and velocity ratio on the instability characteristics of each mode were also investigated. Planché and Reynolds[25] observe that heating favor the outer instability modes in

linear, small-amplitude disturbance theory. The linear stability studies in Ref [24] were extended to the nonlinear case by Ladeinde and Wu,[26] whereby second-order nonlinear spatial stability to the three-dimensional perturbation waves is analyzed by expanding the perturbations into amplitude-dependent harmonic waves and truncating the Landau equation to the second term. Ragab and Wu[27] examine the viscous and inviscid stability, from which they conclude that the disturbance could be calculated accurately from the inviscid theory if the Reynolds number was greater than 1000. (The inviscid results yield the upper bound for the growth rate since viscosity damps out the perturbations.) The studies by Schade[28] also show that viscosity does not have a destabilizing effect in an unbounded flow. The effects of compressibility studied[24,29,31] subsequent to the work of Papamoschou and Roshko,[30] which suggests the use of "convective Mach number" to study compressibility effects of mixing layers. The general results are that compressibility enhances stability at low to moderate Mach numbers, while three-dimensional characteristics evolve at higher Mach numbers.

Numerical studies on high-speed, non-premixed combustion in supersonic, spatially-developing mixing layers include Drummond,[32] who report the dominance of vertical structures in supersonic mixing layers, in the same manner that they are present in subsonic flows. Marked effects of the structures on chemical reaction are reported, such as the significant burning that takes place in the eddies on the edges of the mixing layer, broadening the reaction zone relative to the layer thickness defined by the velocity gradient. Figure 1 is a schematic of vortex system in mixing layers. The vertical structures are also found to result in the roll-up of unburned reactants inside a layer of partially- or fully-burned products. This phenomenon, which is often called "unmixedness" in subsonic flows, prohibits the reaction of captured reactants and reduces the overall efficiency of the combustion process. However, insertion of a splitter plate between the fuel and air streams provides the disturbance that triggered transition and turbulence in the latter fourth of the domain being studied, leading to significant improvement in the mixing of the fuel and air in that region. No reactions are observed in the early part of the mixing layer, and the reaction is mainly endothermic further downstream. However, well downstream in the transition-like region, the reaction is highly exothermic. Givi et al.[33] use direct numerical simulation (DNS) to investigate low Reynolds number compressibility and combustion heat release effects in a high-speed mixing layer, but they consider only a single step reaction.

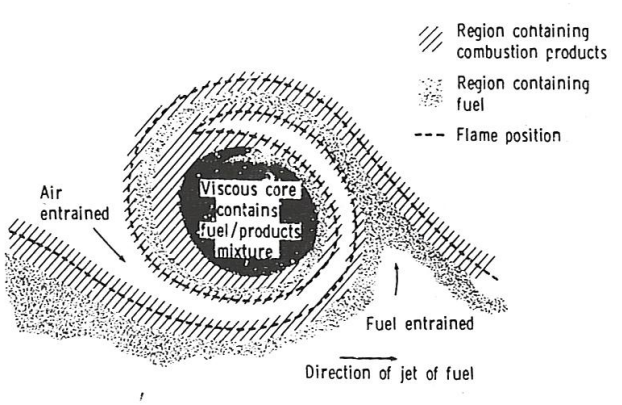

Figure 1. Cross section of transitional "vortex" eddy in gas diffusion flame (Ref [32]).

Other studies of reacting mixing layers show that the heat release may delay the turbulence development.[32,34-37] Vuillermoz et al.,[38] who had earlier studied the effects of viscosity and molecular diffusion on the mixing of hydrogen and oxygen streams for a nonreactive, temporally-evolving mixing layer, parametrically variy the chemical reaction rate in a time-dependent study of supersonic reacting mixing layers to examine the way in which the time of energy release affects the evolution of the flow. Such calculations provide a way to investigate the effects of changes in the Damköhler number. Two distinct mixing regimes are identified: a convective mixing regime and a diffusive mixing regime. Large-scale structures dominate the former regime, while in the latter regime, the structures have decayed and fine structures developed. The computations showed that the timing of the chemical energy release had a marked effect on the development of the supersonic mixing layer. For the fast chemistry, energy release and product formation occur almost instantaneously, leading to a highly-stretched flame, and the chemical reactions are completed by the end of the convective-mixing period. For the slow chemistry, the initial chemical reactions are almost extinguished by turbulent convection before the system re-ignites. The flame regions are much more compact and burning occurs well into the diffusive-mixing regime. Dimotakis[39] reviews some experimental data on turbulent mixing layer growth, mixing, and chemical reactions. The dependence of these phenomena on such fluid and flow parameters as Reynolds number, Schmidt number, and Mach number are discussed.

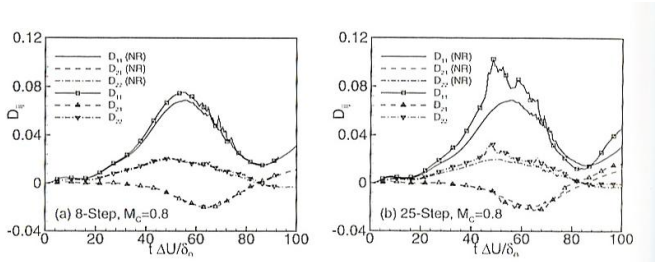

Figure 2. Evaluations of the evolution with the eddy turnover time of turbulence of $D_{ij} = \bar{\rho}\varepsilon_{ij}$, where $\bar{\rho}\varepsilon_{ij} = \overline{\sigma'_{ik}u'_{j,k}} + \overline{\sigma'_{jk}u'_{i,k}}$ and $\sigma_{ij} = \mu\left(u_{i,j} + u_{j,i} - \frac{2}{3}u_{k,k}\delta_{ij}\right)$, for the 8-step and 25-step kinetic models at a convective Mach number $M_c = 0.8$. (Ref [43]). The various kinetic mechanisms are given in the appendix.

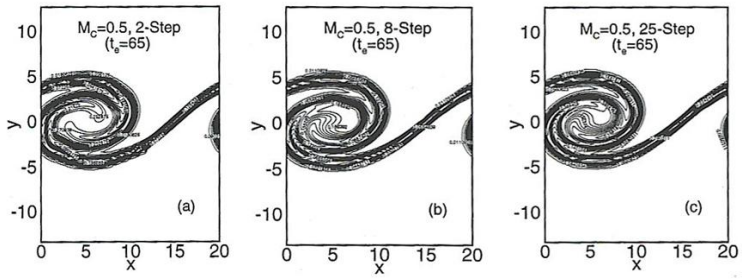

Figure 3. Contour maps of water mass fraction for supersonic combustion in mixing layers as a function of the kinetic model. Results were obtained from a transported joint PDF for supersonic combustion (Ref [45]). The various kinetic mechanisms are given in the appendix.

Chakraborty et al.[40] calculate reacting mixing layers with multi-step chemistry models consisting of a 7-step, 8-species model, while Evans and Schexnayder[41] study the influence of using a 25-step, 12-species kinetics and unmixedness on burning supersonic hydrogen flame. However, the RANS approach is used, so that the studies are more applied. Ladeinde et al.[42] used DNS to carry out fundamental studies that compare the performance of an 8-step, 7-species model consisting of twenty-five steps and twelve species for a convective Mach number of M_c=0.8. Various definitions of the layer growth rate are used in an attempt to differentiate compressibility effects of high speeds from those of chemical reactions. Three of the definitions show considerably different temporal evolution for the two chemistry models. In general, the twenty-five step model shows more rigorous reaction, as they account for more radicals. With this kinetics model, more energy is extracted from the system because of the endothermic nature of some of the reaction steps. The effects of combustion on the second moments of turbulence, $\rho\widetilde{u_i u_j}$, are investigated in Ladeinde et al.[43] and Liu.[44] See Fig. 2 for sample results.

The differential temperature distribution due to the foregoing kinetic models and mass fraction PDF have also been studied by the present author[45,46] using the transported PDF approach (see Fig. 3). Eifler and Kollman[47,48] also derive and model the transport equation for the joint PDF of velocity, density, internal energy, mixture fraction, and dilation.

III. Combustion Modeling Efforts

Raman measurements of mixing and finite-rate chemistry in supersonic hydrogen/air non-premixed flame[49] show that this type of combustion is significantly different from combustion in low-speed flows. Cheng et al.[49] suggest that finite-rate effects become particularly important in supersonic flows and that higher fluctuations of temperature and species concentrations are observed in supersonic flames compared to subsonic flames. The latter effect is attributable to the interaction of velocity and temperature in supersonic compressible flow. Studies by Balakrishan and Williams[50,51] of supersonic combustion on hypersonic aircraft, such as the National Aerospace Plane (NASP) over the range of flight Mach numbers up to 25 and altitudes from 30 to 75 km, indicate that laminar flamelets are likely to exist in supersonic combustion under the conditions of their studies.

Although the transported joint PDF approach used in Refs [47, 48] is the most comprehensive treatment of supersonic combustion, there are issues related to computational efficiency, chemical non-equilibrium, and the modeling of compressible turbulence. Thus, simplified, albeit finite-rate, models, such as the flamelet[52-58] and the linear eddy models,[59-66] are of interest.

The use of the laminar flamelet model for scramjet combustion simulation in engineering is not as common as its application to low-speed combustion. Baurle et al.[67] use assumed and evolution PDFs to compare their relative performance in the modeling of turbulent reacting flow. The evolution PDF formulation is found to give improvements over assumed PDF although, as alluded to earlier in this paper, the former is significantly less computationally efficient (in terms of computer storage and solution turnaround). Eklund, Baurle, and Gruber[68]

employed the assumed PDF approach in the VULCAN code to investigate ethylene-fueled scramjet combustor. An assumed PDF model that has been widely used for scramjet simulation, for example, by Baurle and his co-workers, and in the VULCAN code, is Girimaji's approach, in which a multivariate β PDF is used for species mass fraction fluctuations and a Maxwellian distribution for temperature fluctuations.

Unfortunately, assumed PDFs were found to be unable to accurately predict high-order correlations, such as terms involving chemical production source. Similar results have been reported by Keistler et al.,[69] who report that the PDF approach in Girimaji[70] has a highly dissipative effect on the concentration variance, resulting in poor agreements with the measurements. To avoid the high computational cost of the PDF approach, Xiao et al.[71] model the high-order terms using evolution equations for the variance of mass fraction and enthalpy and by applying the procedure to two hydrogen/air chemical kinetic mechanisms for a scramjet combustor.

The resulting algorithm is found to be computationally efficient, in comparison to assumed or transported PDF methods, especially for three-dimensional models characteristic of scramjet geometries. Xiao et al. point out that their formulation is dimensionally and tensorially consistent, Galilean invariant, coordinate-system independent, and free of damping and wall functions.

The flamelet approach is reviewed in this paper, and this is limited to the non-premixed case. Zheng and Bray[72-74] and Zheng[75] extend this model to supersonic combustion of non-premixed gases. However, in their treatment, the pressure term is $\frac{\partial p}{\partial t}$ in the stagnation enthalpy equation which Sabel'nikov[76] suggests is a serious assumption for supersonic flamelet modeling because of the role played by dynamic compressibility.

Even for the flamelet method reviewed in this paper, only aspects appropriate for high Mach number combustion are included, as the low-speed combustion treatments have already received a significant amount of attention.[7,77-79] The appearance of flow kinetic energy in the enthalpy equation for high-speed flows implies that the functional dependence of temperature and composition on the mixture fraction, Z, and scalar dissipation rate, $\chi = D(\nabla Z)^2$, now includes a third parameter (velocity, u):

$$T = T(Z, \chi, u), \tag{1}$$

$$Y_k = Y_k(Z, \chi, u), \tag{2}$$

where T is temperature, Z is mixture fraction, and χ is mixture fraction dissipation rate. The functional dependence on u in Eq. (2) is implicit through the dependence of the reaction rate, $\dot{\omega}_k$, on temperature: $\dot{\omega}_k = \dot{\omega}_k(Y_k, Z, u)$. Thus, an appropriate flamelet model that includes the effect of the kinetic energy requires the knowledge of the joint PDF of Z, χ, and u, or $P(Z, \chi, u)$, in order to correctly calculate the mean flow properties. The classical Kolmogorov's hypothesis of statistical independence[80] can be applied if we recognize that χ has the characteristics of small scales, while Z and u are dependent on the large turbulence scales:

$$P(Z, \chi, u) = P(Z, u)\, P(\chi). \tag{3}$$

Furthermore, the Bayes theorem can be used to express $P(Z, u)$ as

$$P(Z, u) = P(Z)\, P(u \mid Z), \tag{4}$$

where $P(u \mid Z)$ is the conditional PDF of velocity at a given value of Z.

Zheng[75] and Zheng and Bray[72-75] suggests a simple, empirical model to account for the conversion of kinetic energy to thermal energy. Basically, a correction $\Delta T(Z, \chi, u)$ is introduced:

$$T_n(Z, \chi, <u>) = T(Z, \chi) + \Delta T(Z, \chi, <u>), \tag{5}$$

whereby

$$\Delta T(Z, \chi, <u>) = \frac{1}{2C_p}\left\{\left[Y_f(Z,\chi) + \frac{1}{1+s}Y_p(Z,\chi)\right]u_f^2 + \left[Y_o(Z,\chi) + \frac{s}{1+s}Y_p(Z,\chi)\right]u_o^2 - <u>^2\right\}, \tag{6}$$

where Y denotes mass fraction, and subscripts f, o, and p correspond to fuel, oxidizer, and products, respectively, and s is the stoichiometric coefficient of chemical reaction. Thus, the expectation $\langle\varphi\rangle$ of an arbitrary function of temperature and species mass fraction, $\varphi(T, Y_k)$, can be written as

$$\langle\varphi\rangle = \int\int\int \varphi\big(T(Z,\chi,u), Y_k(Z,\chi,u)\big)P(Z)P(\chi)\,P(u|Z)\,dZd\chi du. \tag{7}$$

The conditional moment closure technique[81] can be used. If we assume that the fluctuations around conditionally-averaged velocity $\langle u \mid Z\rangle$ are negligible, or $\mathrm{P}(u|Z) = \delta(u - \langle u|Z\rangle)$, then

$$\langle\varphi\rangle = \int\int \varphi\big(T(Z,\chi,\langle u|Z\rangle), Y_k(Z,\chi,\langle u|Z\rangle)\big)P(Z)P(\chi)\,dZd\chi. \tag{8}$$

Note that

$$\dot{\omega}_k = \dot{\omega}_k(Z,\chi,\langle u|Z\rangle), \tag{9}$$

and in the Peter's approach to the flamelet equations, the conditionally-averaged values of mass fraction, $\tilde{Y}_k = Y_k(Z,\chi,\langle u|Z\rangle)$, and temperature, $\tilde{T} = T(Z,\chi,\langle u|Z\rangle)$, can be solved as a function of Z. A linear relationship between $\langle u|Z\rangle$ and Z can be assumed as a simple closure:

$$\langle u|Z\rangle = a_1 + b_1 Z. \tag{10}$$

More details are contained in Sabel'nikov.[76] It is important to note that the foregoing description pertains to the simple approach of the flamelet method, in which the species mass fractions and temperature are directly written in differential equations with Z and time t as the independent variables. The more complicated flamelet approach[82-85] involves the solution of the spatially-dependent continuity, momentum, energy, and the species transport equations for freely-propagating and opposed jet problems.

IV. Sample Scramjet Combustion Calculations

In this section, we review a few calculations of scramjet combustion, with respect to the governing equations solved, the numerical procedures (in terms of the schemes for spatial and temporal integration of the equations, limiters, CFL limit, the use of sub-iterations, etc. We also discuss the model in terms of the dimensionality (2D or 3D), grid resolution in terms of the number of cells, and y^+, the type of combustion configuration, inflow conditions and the conditions at the combustor inlet. The kinetics mechanisms are presented, as are the turbulence models and the procedure for turbulence-chemistry interactions. Table 1 gives the summary of the sample calculations. It is evident from the table that the majority of the schemes used in the analysis of realistic scramjet combustor are based on the finite volume method and the turbulence models are of the RANS type; as opposed to LES or DNS. The exception in the table is Berglund and Fureby,[92] who used the LES approach. It is also evident that the combustion models are fairly standard – evolution equations for the species mass fractions with assumed PDF closure. Figure 4 shows a sample species concentration from the scramjet simulation of Xiao et al.,[71] while Figs. 5 and 6 represent the computational domain and results from the simulation of Berglund et al.[92]

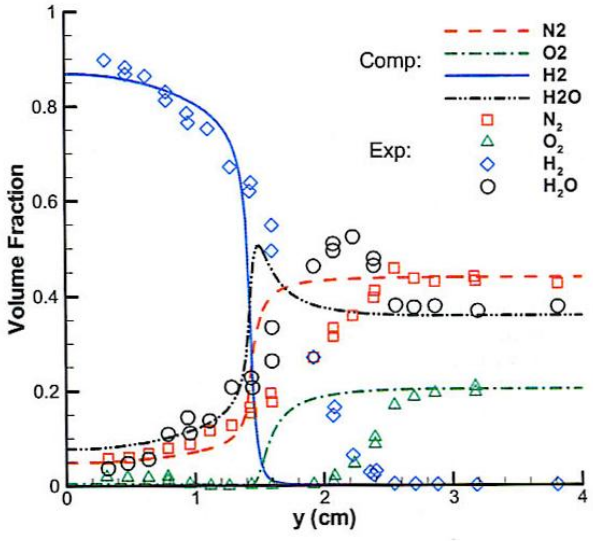

Figure 4. Composition profiles, reacting case, variable Sc_t, $(\mathrm{Pr}_t = 0.5)$, $k-\zeta$ model, with turbulence/chemistry interaction (Ref [71]).

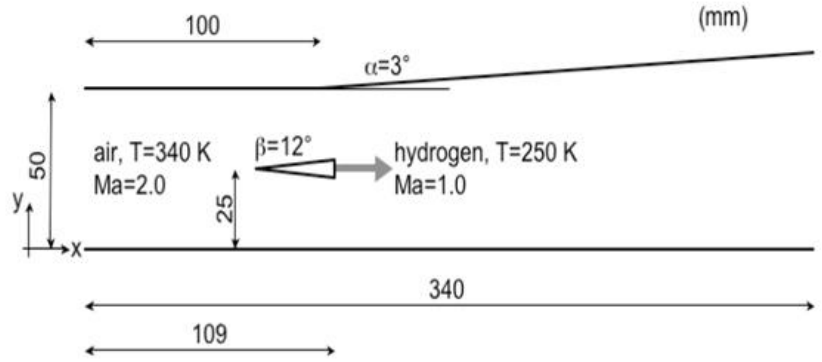

Figure 5. Schematic of the computational domain of the DLR scramjet model in Berglund and Fureby.[92]

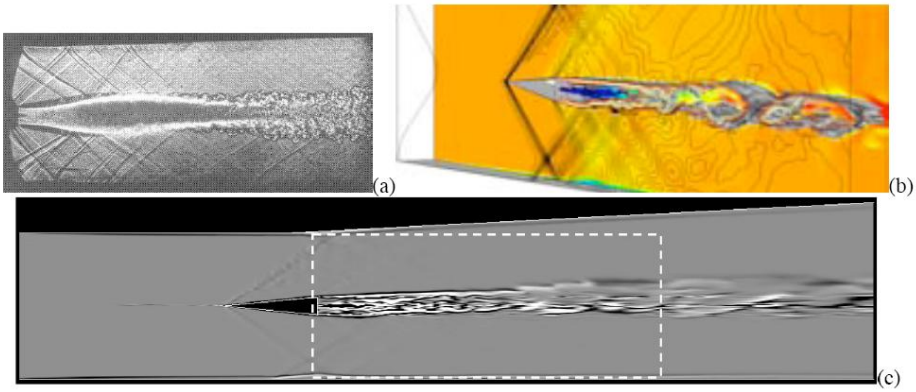

Figure 6. Results from Berglund et al.[92] for supersonic flow in the scramjet combustor with hydrogen injection and combustion. a) Shadowgraph photographs from the experiments, b) a perspective view from the rear of the simulated flow and c) a numerical shadowgraph image from the reacting LES calculations. The size and location of the experimental image a) is superimposed on c).

Author(s)	Jeung et al.[87]	Xiao et al.[71]	Baurle and Eklund[91]	Berglund and Fureby[92]
Equations Solved	Compressible Navier-Stokes, energy equations; species transport equations	Compressible Navier-Stokes, energy equations; species transport equations	As in VULCAN: compressible RANS equations for calorically or thermally perfect gas, species transport equations	Filtered LES equations for flow, energy, passive scalar, reactive scalar.
Numerical Methods	Finite volume, Roe's flux-difference splitting, differentiable limiter function, MUSCL, spatial TVD, second-order implicit time integration with 4 Newton sub-iterations per time step, CFL=2.	North Carolina State University REACTMB code: multi-component, multiphase, spatial TVD upwind with flux splitting method of Edwards[89]; second-order ENO, central difference for viscous and diffusion terms, planar relaxation.	Structured grid topology, cell-centered finite volume, low-diffusion flux-split model of Edwards[89], MUSCL, with $\kappa = 1/3$, van Leer flux limiter, steady state, diagonalized approximate factorization scheme, $1.5 \leq CFL \leq 2.0$. (No steady state solutions were found for some problems.)	Unstructured finite volume, reconstructions of the convective terms, second-order flux limiter-based spatial TVD scheme, central difference for viscous terms , explicit TVD Runge-Kutta temporal scheme.

Model/Maximum number of cells for combustor, etc	2D, 936×160 cells, $y^+ \leq 5$	2D, 104,428 cells	3D, 2×10^6 cells for combined isolator and combustor, $y^+ \leq 50$ (wall functions used).	3D, 3.2×10^6 cells, $y^+ \leq 50$ (wall functions used)
Combustor configuration and inflow conditions	The HyShot geometry, $5 \leq M_\infty \leq 6$ (altitude of 20 km), M_{airc}=3, P_{airc}=1.0 MPa, T_{airc}=600K, M_f = 1, T_{fuel}=151K, $.167 \leq \varphi \leq 0.5$, vertical injection of fuel	Supersonic combustor setup in Ref [90], with injection parallel to vitiated main flow; M_{airc}=2.44, P_{airc}=1.0 atm, 1250K$\leq T_{airc} \leq$1270K, M_f = 1.	AFRL/PRA-designed combustor, $4 \leq M_\infty \leq 6.5$ (Dual Mode), $1.8 \leq M_{airc} \leq 3$, 574.5kPa$\leq P_{airct} \leq$2634kPa, 902K$\leq T_{airct} \leq$ 1187K, M_f = 1.	DLR scramjet experimental rig.[93-96] Expanded pre-heated air enters combustor at Mach 2, wedge-shaped strut in combustor acts as flame holder. H_2 injected at base of strut. M_{airc}=2, $P_{airc}=10^5$ Pa, T_{airct}=340K, M_f = 1, $P_f=10^5$Pa , T_f=250K.
Kinetic Mechanisms	H_2/Air, GRI-Mech 3.0[87], 8-step/25-species	H_2/Air, 2 mechanisms: 7-step/7-species, 9-step/19-species	Ethylene (C2H4), 3-step/6-species (Mawid's), reaction rate adjusted for OH in vitiated freestream. Arrhenius activation temperature of each step reduced by a factor of 2 to force ignition. Values reset after ignition.	H_2/Air, 2-step/5-species
Turbulence Models	Menter's SST (k-ω), DES is used their Ref [88] paper	k-ζ, ζ is variance of fluctuating vorticity, variable P_{rt}	Menter's Baseline model, Menter's SST (k-ω), wall functions, constant P_{rt}.	Subgrid scale models with logarithmic velocity distribution, mixed models[97] for subgrid turbulent viscosity, species diffusion, scalar dissipation rate, mixture fraction variance.
Turbulence-Chemistry Interaction	None, turbulence does not affect chemical reactions!	Variable S_{ct} , evolution equations for variance of mass fraction and enthalpy	Assumed PDF in conjunction with the solution of the species evolution equations; constant S_{ct}.	Two flamelet models : a) transport equation for passive scalar and algebraic equation for its variance, b) transport equations for a passive scalar and a reactive scalar. No Arrhenius rate expression needed. Laminar flame speed provides finite rate chemistry effects.

Table 1. Sample Scramjet Combustion Calculations.

V. Conclusion

A review of scramjet combustion simulation is provided in this paper, covering the fundamental problem of supersonic mixing layers, the high-speed combustion modeling efforts, and actual calculations of realistic scramjet combustors. The review shows that the RANS approach dominates the turbulence modeling of the system, with only a handful of LES work. Also, virtually all the numerical procedures used are based on low-order schemes, and the combustion models that have been used for realistic simulations solve the species evolution equations with assumed PDF closures, although there seems to be a growing use of the flamelet methods. Areas of future research in this

field includes the investigation of high-order methods for scramjet combustor calculations, more advanced turbulence-chemistry interaction models, including the conditional PDF procedure discussed in Section III, and the application of such flamelet-based methods to realistic scramjet systems. Even for LES, more advanced subgrid-scale models are needed for the high enthalpy flows in scramjets. Finally, spray modeling for scramjet combustion is an area that has not received enough attention.

Appendix

The 1-step, 3-species reaction is given by

$$2H_2 + O_2 \underset{k_b}{\overset{k_f}{\rightleftharpoons}} 2H_2O + \text{Heat}.$$

The 2-step, 4-species kinetics model is

$$H_2 + O_2 \underset{k_b}{\overset{k_f}{\rightleftharpoons}} OH$$

$$H_2 + 2OH \underset{k_b}{\overset{k_f}{\rightleftharpoons}} 2H_2O.$$

The 8-step, 7-species kinetics model and its constants are

No.	Reaction	A_f	B_f	C_f	A_b	B_b	C_b
1	$H_2 + M \rightleftharpoons H + H + M$	5.5×10^{18}	-1.0	51987	1.8×10^{18}	-1.0	0
2	$O_2 + M \rightleftharpoons O + O + M$	7.2×10^{18}	-1.0	59340	4.0×10^{17}	-1.0	0
3	$H_2O + M \rightleftharpoons OH + H + M$	5.2×10^{21}	-1.5	59386	4.4×10^{20}	-1.5	0
4	$OH + M \rightleftharpoons O + H + M$	8.5×10^{18}	-1.0	50830	7.1×10^{18}	-1.0	0
5	$H_2O + O \rightleftharpoons OH + OH$	5.8×10^{13}	0	9059	5.3×10^{12}	0	503
6	$H_2O + H \rightleftharpoons OH + H_2$	8.4×10^{13}	0	10116	2.0×10^{13}	0	2600
7	$O_2 + H \rightleftharpoons OH + O$	2.2×10^{14}	0	8455	1.5×10^{13}	0	0
8	$H_2 + O \rightleftharpoons OH + H$	7.5×10^{13}	0	5586	3.0×10^{13}	0	4429

The 25-step, 12-species kinetics model and its constants are

No.	Reaction	A_f	B_f	C_f	A_b	B_b	C_b
1	$HNO_2 + M \rightleftharpoons NO + OH + M$	5.0×10^{17}	-1.0	25000	8.0×10^{15}	0	-1000
2	$NO_2 + M \rightleftharpoons NO + O + M$	1.1×10^{16}	0	32712	1.1×10^{15}	0	-941
3	$H_2 + M \rightleftharpoons H + H + M$	5.5×10^{18}	-1.0	51987	1.8×10^{18}	-1.0	0
4	$O_2 + M \rightleftharpoons O + O + M$	7.2×10^{18}	-1.0	59340	4.0×10^{17}	-1.0	0
5	$H_2O + M \rightleftharpoons OH + H + M$	5.2×10^{21}	-1.5	59386	4.4×10^{20}	-1.5	0
6	$OH + M \rightleftharpoons O + H + M$	8.5×10^{18}	-1.0	50830	7.1×10^{18}	-1.0	0
7	$HO_2 + M \rightleftharpoons H + O_2 + M$	1.7×10^{16}	0	23100	1.1×10^{16}	0	-440
8	$H_2O + O \rightleftharpoons OH + OH$	5.8×10^{13}	0	9059	5.3×10^{12}	0	503
9	$H_2O + H \rightleftharpoons OH + H_2$	8.4×10^{13}	0	10116	2.0×10^{13}	0	2600
10	$O_2 + H \rightleftharpoons OH + O$	2.2×10^{14}	0	8455	1.5×10^{13}	0	0
11	$H_2 + O \rightleftharpoons OH + H$	7.5×10^{13}	0	5586	3.0×10^{13}	0	4429
12	$H_2 + O_2 \rightleftharpoons OH + OH$	1.7×10^{13}	0	24232	5.7×10^{11}	0	14922
13	$H_2 + O_2 \rightleftharpoons H + HO_2$	1.9×10^{13}	0	24100	1.3×10^{13}	0	0
14	$OH + OH \rightleftharpoons H + HO_2$	1.7×10^{11}	0.5	21137	6.0×10^{13}	0	0
15	$H_2O + O \rightleftharpoons H + HO_2$	5.8×10^{11}	0.5	28686	3.0×10^{13}	0	0
16	$OH + O_2 \rightleftharpoons O + HO_2$	3.7×10^{11}	0.64	27840	1.0×10^{13}	0	0
17	$H_2O + O_2 \rightleftharpoons OH + HO_2$	2.0×10^{11}	0.5	36296	1.2×10^{13}	0	0
18	$H_2O + OH \rightleftharpoons H_2 + HO_2$	1.2×10^{12}	0.21	39815	1.7×10^{13}	0	12582
19	$O + N_2 \rightleftharpoons N + NO$	5.0×10^{13}	0	37940	1.1×10^{13}	0	0

20	$H + NO \rightleftharpoons N + OH$	1.7×10^{14}	0	24500	4.5×10^{13}	0	0
21	$O + NO \rightleftharpoons N + O_2$	2.4×10^{11}	0.5	19200	1.0×10^{12}	0.5	3120
22	$NO + OH \rightleftharpoons H + NO_2$	2.0×10^{11}	0.5	15500	3.5×10^{14}	0	740
23	$NO + O_2 \rightleftharpoons O + NO_2$	1.0×10^{12}	0	22800	1.0×10^{13}	0	302
24	$NO_2 + H_2 \rightleftharpoons H + HNO_2$	2.4×10^{13}	0	14500	5.0×10^{11}	0.5	1500
25	$NO_2 + OH \rightleftharpoons NO + HO_2$	1.0×10^{11}	0.5	6000	3.0×10^{12}	0.5	1200

The twelve species in the most complex model are: H, O, H_2O, OH, O_2, H_2, N_2, N, NO, NO_2, HO_2, and HNO_2. The Arrhenius approach is used to model the reaction rates for the steps; the constants in the various models can be found in Evans and Schexnayder[41], except for the 2-step reaction whose constants are available in Vuillermoz et al.[38]

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