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Advanced Computational-Fluid-Dynamics Techniques for Scramjet Combustion Simulation

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The simulation of supersonic mixing and combustion, with a focus on the supersonic combustion ramjet (scramjet), poses many challenges. Even for the nonreacting limit of the problem, the way to properly treat compressibility effects on turbulence when the Mach number is sufficiently high is far from being resolved, independent of previous studies that have advocated the decomposition of the turbulence dissipation of kinetic energy into dilatational and solenoidal components. Complex geometries posed additional difficulties. When combustion dynamics are added to the problem, uncertainty exists in the turbulence–chemistry interaction, shock-wave–chemistry interaction, and the general lack of adequate knowledge of the effects of supersonic conditions on turbulence, reaction rates, and flame regimes.

Of the three common approaches for modeling turbulence [direct numerical simulation (DNS), large-eddy simulation (LES), and Reynolds-averaged Navier–Stokes equations (RANS)], it is well known that the RANS approach is the most computationally efficient and has the chance of completely modeling realistic aerospace systems. This is followed by LES, whereas DNS is still too costly for realistic engineering problems. However, the success of the RANS approach is problem-dependent, and the procedure needs to be calibrated for every class of problem, making it nonuniversal. Moreover, the approach is inherently steady and cannot deal with unsteady large-scale structures that determine the dynamics of many important flow problems. The main issue with LES, relative to RANS, is the computational cost.

The special section on advanced simulation of scramjet combustion and mixing in this issue of the *AIAA Journal* was motivated by the need to assess the current state of the art in this important technological area. The genesis of the efforts originates from the Fluid Dynamics Technical Committee of AIAA, in which a Discussion Group was formed to address the issue. This was followed by a highly successful invited session on the topic at 2009 AIAA Aerospace Sciences Meeting (ASM) in Orlando, Florida. Eight experts on high-speed-combustion modeling were invited to present their work and provide an assessment of the state of the art of scramjet combustion and mixing. The *AIAA Journal* Editorial Board agreed to allow the special section on the subject based on its evaluation of the significance. The presenters at the ASM meeting were invited to contribute, and additional international contributors were also brought in to participate. The various contributions went through the normal *AIAA Journal* review process, the outcome of which is the five papers in this special section of this issue.

The first paper is by Ingenito and Bruno, who address some fundamental aspects of supersonic combustion ramjet, with a focus on the physics, as a way to reverse what the authors see as an undue emphasis on numerics over physics. The paper provides a fairly detailed discussion of the effects of compressibility (Mach number) on turbulence, reaction rate, and flame regime. Helicity (the projection of the vorticity vector onto the velocity vector), or streamwise vorticity, is discussed as a way of characterizing the effects of compressibility on turbulent supersonic internal flows. The authors remind the reader that, unlike in subsonic flows, vorticity transport is not exclusively driven by vortex stretching, but also by compressibility and baroclinic effects. They report higher growth rates in high-Mach-number, fully-three-dimensional shear layers compared with incompressible flows, and they consider this to be a source of enhanced mixing at the molecular level, potentially leading to short flames and efficient combustion. One important result from their work is the derivation, on simple dimensional grounds (as in the original $-5/3$ law), of the decay of turbulence energy with wave number to the power of $-8/3$, and the consequent observations that the dissipative eddies in supersonic flows are larger than those in subsonic flows. Experiments have supported this observation. Thus, in supersonic flows, the smallest eddies might only be able to wrinkle flames, without thickening them.

Concerning the effects of compressibility on reaction rate, the authors show that compressibility effects on collision frequency could become very important in supersonic flows and that the reaction rate is enhanced by high speed: an effect that should be taken into account when modeling chemical kinetics for supersonic combustion.

Compressibility effects are shown to alter the boundaries of the flame regimes relative to Borghi's diagram or Kilmov-William's. The authors suggest that large Mach numbers raise the possibility of flamelets in eddies. The simulation of hydrogen/air combustion in NASA Langley Research Center experiments under the SCHOLAR program is used to demonstrate some of the theoretical results.

The second paper is by Génin and Menon, who address a solution to two of the major problems that confront high-speed computational fluid dynamics (CFD): 1) the development of schemes that maintain their integrity (accuracy, robustness, etc.) in regions of high discontinuities, as well as in the smooth part of the flow, and 2) the development of versatile turbulence closures that are valid for a wide range of aerospace engineering applications. Génin and Menon address these issues from the perspective of LES, with a focus on adaptable numerical algorithms (via the Harten–Lax–van Leer contact and Harten–Lax–van Leer–Einfeldt hybrid), and dynamically obtain turbulence parameters and subgrid-scale closures that do not have adjustable constants. These approaches are particularly welcome for high-speed flows, in which the development of LES closures is more limited, and the issues of dilatational and solenoidal contribution to dissipation has not been fully resolved. In Génin and Menon's paper, the compressible part of the turbulent field (or turbulent Mach number) is considered to be small in the high-speed boundary and shear layers, with possible significant contributions in situations in which shock waves interact with boundary or shear layers, as in scramjet combustion flows. The application of the numerical work was based on the facility used in experimental studies at the DLR, German Aerospace Center, which also produced the validation data for the simulations.

For the high-speed-combustion problem, a large number of subgrid-scale terms arise that require modeling: subgrid kinetic energy, subgrid gas constant-temperature correlation, subgrid stress, subgrid viscous work, subgrid enthalpy flux, subgrid diffusion of energy, subgrid species flux, subgrid species diffusion–velocity correlation, subgrid mixture-gas constant-temperature correlation, and subgrid mass-fraction–internal-energy correlation. The subgrid-scale kinetic energy, obtainable via a transport equation, requires that additional terms (triple-velocity correlations, production, dissipation, and pressure dilatation) be modeled. Génin and Menon provide models for the foregoing subgrid-scale terms, except the last four, which are neglected. Note that DNS results in realistic geometries are not yet available for these terms, and so they represent part of the unresolved problem in high-speed-combustion flow simulation. Agreement with experimental data is reported to be fairly good, with discrepancies that are probably due to the use of velocity slip conditions at the walls in the transverse direction. The closure of the

LES and subgrid kinetic-energy equations gives rise to five parameters, including the turbulence Prandtl number and turbulence Schmidt number, which are dynamically evaluated in the paper by Génin and Menon.

The third paper, by Berglund et al., also presents LES simulations of supersonic mixing and combustion, but for the National Aerospace Laboratory of Japan supersonic combustor, equipped with the two-stage strut injector and connected to ONERA's vitiated air heater. An explicit eddy-dissipation-concept, finite-rate-chemistry LES model is used in conjunction with a 1-, 2-, and 7-step reaction mechanism, the induction times of which are compared with a 19-step mechanism. The authors note that the flame in the system is outside of the flamelet regime in the Borghi diagram, justifying their use of the finite-rate-chemistry models. This observation should be contrasted with the suggestion by Ingenito and Bruno that the flamelet regime was valid for their system.

Compared with the paper by Génin and Menon, both of which are based on LES, although to different levels of fidelity, the paper by Berglund et al. is heavier on reaction modeling. Whereas Génin and Menon modeled six subgrid-scale terms and dynamically evaluated five parameters, including the turbulence Schmidt and Prandtl numbers, Berglund et al. model three subgrid-scale terms (stress tensor, energy flux, and species flux), using the mixed model for this purpose and assuming constant values for most of the parameters. (Turbulence Schmidt and Prandtl numbers are kept constant at 0.9 and 0.7, respectively.) Like Génin and Menon, a transport equation is solved for the subgrid kinetic energy, although, unlike the former, the models for the enclosed terms in this equation are not presented. Wall-modeled LES is used in order to reduce grid requirement, the same motive that made Génin and Menon use slip conditions on the horizontal walls. Berglund et al. investigate both the partially stirred reactor (PaSR) and the quasi-laminar (QL) approaches for modeling the reaction rate. Their PaSR approach assumes a zero spatial gradient for the species in a cell, so that the time derivative term balances the reaction-rate term in the species transport equations. Here, each LES cell is divided into a (temporal) fine scale, in which mixing and reaction take place, and a (temporal) surrounding that is dominated by (temporal) large-scale flow structures. The difference between the mass fractions at the two time levels divided by the characteristic time difference is used to estimate the filtered reaction rate. A subgrid mixing time (harmonic mean of the Kolmogorov time scale and the time scale from subgrid length and velocity scales) and a reaction volume-fraction parameter are introduced. QL approaches use the resolved scales to directly estimate the reaction rate. That is, the model does not account for the effects of the subgrid-scale turbulence–chemistry interaction.

In general, the seven-step mechanism gives the best comparison with experimental data for many results and yields the highest combustion efficiency. This indicates the need for detailed chemistry and the importance of differential species diffusion. The studies show that the influence of the subgrid combustion model is virtually negligible, consistent with a couple of cited prior studies.

In the fourth paper, Baurle and Edwards present an assessment of the state of the art a for RANS and RANS/LES hybrid in connection with scramjet-combustion-motivated supersonic mixing of coaxial free jets. The experiments for the jets have been carried out at NASA Langley Research Center and provide invaluable data for validating supersonic-mixing calculations. The differential behavior of argon and helium (as the inner jet nozzle fluid, with air being the outer) was investigated in relation to the values of the turbulence Schmidt number and the prediction of supersonic-mixing-layer spreading rates. The significantly superior computational efficiency of RANS-based approaches relative to LES or DNS has encouraged the use of RANS for realistic aerospace systems. However, the high sensitivity of the approach to model parameters seriously undermines its utility and mandates the need to calibrate the procedure for every class of problem. Combining the standard approach with the more expensive LES procedure, which is known to be fairly universal in some aspects, appears to be an effort in the right direction.

The RANS simulations displayed a strong sensitivity to the choice of the turbulence Schmidt number, with observations that were not consistent between argon and helium. The hybrid approach was found to overpredict the mixing-layer spreading rate for the helium case, while underpredicting the rate of mixing when argon was used as the injectant. The calculations by Baurle and Edwards used the VULCAN code.

The fifth and last paper in the special section is by Faure et al. This paper investigates the effects of inlet velocity distortion and the fidelity of the modeling of unsteady turbulence on mixing and supersonic combustion in a generic circular cross section at a flight Mach number 6 and an altitude of approximately 24.2 km. Various injector locations are investigated. The inlet distortion studies consider velocities from three types of inlet profile: two streamline-traced inlets, referred to as Scoop and Jaws, and a baseline uniform inflow boundary condition. Frozen and finite rate chemistries are investigated for each inlet profile type and the calculations assume steady state. The unsteady-turbulence model-fidelity studies focus on the combustion region and compare the performance of unsteady RANS (URANS) and LES for the case of combusting flow with finite chemistry.

A uniform airflow to the combustor at Mach 2.2 and a stagnation temperature of 960 K are assumed, and the fuel (ethene) is injected at the rate of 400 m/s. The domain for model fidelity is restricted to a one-eighth section of the circumference. A 20-step reduced-kinetic mechanism for ethene–air combustion is used.

The steady RANS and URANS models are based on the k-ω model, together with laminar conservation species equations. Although the LES methods are not as advanced as in Génin and Menon, the authors do use a similar locally dynamic kinetic-energy model procedure for the subgrid kinetic energy, including the dynamic evaluation of the coefficient in the determination of the eddy viscosity in terms of the square root of the subgrid-scale kinetic energy and the local grid size. An assumed product of probability density functions is used for the subgrid chemistry, and the transport equations for the mixture fraction and progress variable (change of mass fraction over time) are solved.

The greater distortion pattern in Jaws's inflow profile resulted in higher levels of mixing, combustion efficiency, and thrust ratio, compared with Scoop's. As expected, high levels of compression at the upstream of the cavity affect the development of the shear layers and downstream combustion. Concerning unsteady-turbulence model fidelity, URANS does not resolve the small structures, and it displays higher levels of diffusion (large scales in the flow structure). The chemical reaction time is observed to be lower in URANS than in LES, perhaps because of the higher level of diffusion in URANS. This leads to a reduction in the ignition time (Damköhler number).

Collectively, these papers provide the state of the art of the simulation of scramjet combustion and mixing, as well as some identification of the major scramjet experimental facilities worldwide.

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