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Direct numerical simulation of a supersonic lifted hydrogen jet flame: A priori study on combustion models

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ABSTRACT

In this study, a systematic assessment of turbulent combustion submodels of conditional moment closure (CMC) has been conducted using DNS data of a three-dimensional spatially-developing supersonic lifted hydrogen flame with a Mach number of 1.2 at the jet injection. It has been found that Beta pdf of mixture fraction can well capture the mixing space of the high speed reacting flow. The linear model exhibits a good performance for the axial velocity predictions. Girimaji's model for scalar dissipation rate performs well at upstream, while the AMC model presents better further downstream. The first order closure for the conditional reaction rate deviates a lot from the DNS extracted results. Second-order corrections made to temperature only or to the two rate-limiting reaction steps induce improvement, still with much discrepancy. Second order closure considering fluctuations of all the reacting species and temperature can accurately reproduce the DNS results.

1. Introduction

Renewed interests in hypersonic flight vehicles both for terrestrial travel and space exploration and transport have greatly motivated research effort towards supersonic combustors [1–4]. One of the critical issues for a scramjet combustor is the realization of efficient fuel–air mixing and combustion within a short flow residence time, which is typically of the order of milliseconds associated with supersonic flight speeds. Within such a limited time span, fuel should be mixed with air and burned completely to reduce the combustor length and weight. Detailed understanding of the fuel–air mixing and combustion mechanism in a supersonic flow field is vital to the successful design of supersonic propulsive devices [5].

The recent development of highly resolved techniques in optical measurement enabled us to examine the structure of the supersonic flowfields [6–9]. Ben-Yakar et al. [6] conducted experimental investigations on time evolution and mixing characteristics of hydrogen and ethylene transverse jets in supersonic cross flows and revealed significant differences in the near-flow field properties of the two jets, while OH planar laser-induced fluorescence (PLIF) was performed to verify the molecular mixing in the combustible gaseous jets. Takahashi et al. [9] examined the availability and benefits of using acetone PLIF in the supersonic mixing flow field produced by a normal sonic jet injected into a supersonic cross-flow. However, the difficulties in measuring complex high-speed unsteady flow fields restrict the availability of experimental data, which are as yet insufficient to account for the underlying mechanisms. Moreover, reliable quantitative measurement is difficult and the simultaneously obtainable quantities of the three dimensional features under supersonic conditions are very limited. Numerical approaches are an

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Nomenclature

ρ	density (kg/m^3)
u_i	velocity in the i direction (m/s)
Y_k	mass fraction of species k
$V_{k,i}$	the i component of the diffusion velocity of species k (m/s)
$\dot{\omega}_k$	mass production reaction rate ($kg/m^3/s$)
W	the mixture molecular weight (kg/mol)
σ_{ij}	stress tensor ($kg/m/s^2$)
$f_{k,j}$	the body force (m/s^2)
T	temperature (K)
e_t	specific total energy (J/kg)
q_i	the heat flux ($J/m^2/s$)
R_u	universe gas constant (J/mol/K)
$\dot{Q}$	the external heat source ($J/m^3/s$)
D	jet core diameter (m)
ξ	mixture fraction
η	sample of mixture fraction
Q	conditional mean mass fraction of species i
$\mathbf{v}$	conditional mean velocity vector
N	scalar dissipation rate (1/s)
w	conditional mean reaction rates ($kg/m^3/s$)
P	possibility density function

attractive alternative for supplementing insights into unsteady features for supersonic mixing and combustion flow fields.

Modeling of scramjet combustion is a formidable task, due to the complex aerothermodynamics. Conventional Reynolds Averaged Navier–Stokes (RANS) models, with simplified combustion models, are obviously insufficient for capturing the features of unsteady flow, owing to their intrinsic dissipative and time-averaging characteristics. Large eddy simulation (LES) methods have the potential to reduce the modeling sensitivity inherent to RANS approaches, because the intent of LES is to resolve the large-scale turbulent structures while modeling only the small scales. However, to predict the salient features of scramjet combustion, improved reaction mechanisms and turbulence-chemistry interaction models must be incorporated. Wang et al. [10,11] have conducted a series of LES of mixing and combustion characteristic of supersonic combustors with cavity flame-holders, where an assumed sub-grid PDF closure model is used for turbulence combustion interaction.

Various combustion models have been devised for the RANS or LES simulations of reacting flows, such as flamelet models [12], the transported probability density function (PDF) [13] and conditional moment closure (CMC) [14]. CMC has been recognized as a promising method with sound theoretical background and accuracy at a reasonable cost in diverse engineering problems. CMC solves the transportation equations for the conditional Favre means of species i's mass fraction $Q_i = \langle \rho Y_i | \xi = \eta \rangle / \langle \rho | \xi = \eta \rangle$ and conditional temperature Q_T, where angled brackets denote ensemble averaging and η is the sample space variable for mixture fraction ξ. According to Bilger's [14] closure derivation, the transport equation for Q_i is given as,

$$\frac{\partial Q_i}{\partial t} = -\langle \mathbf{v}|\eta\rangle \cdot \nabla Q_i + \langle D_i \nabla\xi \nabla\xi|\eta\rangle \frac{\partial^2 Q_i}{\partial \eta^2} - \frac{\nabla \cdot \left(\langle \mathbf{v}'' Y_i'' |\eta\rangle P(\eta) \langle \rho|\eta\rangle \right)}{P(\eta)\langle \rho|\eta\rangle} + \langle w_i|\eta\rangle \quad (1)$$

where $\mathbf{v}$ is velocity, D_i is diffusivity, $P(\eta)$ is the mixture fraction PDF, $\mathbf{v}''$, Y_i'' are fluctuations $Y_i = Q_i + Y_i''$. The terms on the right-hand side are referred to convective term, diffusion term, turbulent flux term and reaction source term, respectively. The underlying advantage of the CMC method is that the fluctuations about the conditional averages on mixture fraction (ξ) are much smaller than fluctuations about unconditional averages. The closure of nonlinear chemical reaction rates can be resolved using the conditional moments of reactive scalars Q_i, $\langle w_i(\mathbf{Y})|\eta \rangle = w_i(\mathbf{Q})$, leading to the first order CMC. However, simulations of turbulent methane–air diffusion flames with local extinction and reignition [15], show some discrepancies between predictions and measurements. In this case, temperature fluctuations around its conditional mean become significant and neglecting these fluctuations in the closure of the chemical reaction rate terms seems unacceptable. It is expected that a higher order closure will be needed to represent the effect of conditional fluctuations of reactive scalars for relevant species or reaction steps more accurately.

Direct numerical simulation (DNS) is a powerful tool for the priori and posteriori testing of combustion models. DNS has a unique advantage to resolve all length and time scales of turbulence and chemistry compared to other methods, without any turbulence and combustion models. DNS of a three-dimensional spatially-developing supersonic turbulent jet hydrogen flame with a Mach number of 1.2 has been conducted with detailed chemical mechanisms. The global characteristics of the flame such as instantaneous flame topology, stabilization mechanism, scalar mixing and dissipation, have been discussed in our previous work [16–18]. In the present work, conditional statistics of the supersonic jet flame are analyzed within the framework of CMC models. The main objective is to provide a systematic assessment of the conditional moment closure submodels for the right-hand side terms in Eq. (1) using DNS data of the supersonic jet flame.

2. DNS database

2.1. Fully compressible DNS solver for supersonic combustion

A fully compressible solver for direct numerical simulation (DNS) of supersonic combustion has been developed in our group. The solver has been well validated and then adopted to simulate a three-dimensional supersonic turbulent jet flame. The numerical algorithm has been demonstrated in detail in our previous work [17]. For completeness