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Large eddy simulation of flame structure and combustion mode in a hydrogen fueled supersonic combustor

Zhi-wei Huang, Guo-qiang He, Fei Qin, Xiang-geng Wei*

Science and Technology on Combustion, Internal Flow and Thermal-structure Laboratory, Northwestern Polytechnical University, Xi'an Shaanxi 710072, PR China

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ABSTRACT

In this study, Large Eddy Simulation (LES) of supersonic turbulent mixing and combustion adopting a Partially Stirred Reactor (PaSR) sub-grid combustion model is performed for a hydrogen fueled model scramjet combustor. The compressible LES solver, which adopts a skeleton of 27 steps and 9 species hydrogen chemical kinetics model, is used to simulate the flowing and combustion processes based on structured hexahedral grids. The code is implemented in an Open Source Field Operation and Manipulation (OpenFOAM) solver, and validated against experimental data in terms of mean axial velocity and static temperature at different cross-sections, all show good predictions. An analysis of the flow field is carried out to investigate the supersonic turbulent flame structure and combustion mode in the combustor. Mixture fraction is extracted to indicate the reaction progress at different sites, which donates the most likely flame locations when at stoichiometric. Comparison of combustion parameters including OH mass fraction, scalar dissipation rate, flame index and heat release rate spatial distribution reveals that the supersonic combustion has the characteristics of a turbulent diffusion flame, where combustion is held at non-premixed mode controlled by turbulent mixing in the shear layers. A time scale analysis, the Damköhler Number is performed to examine these reactive zones in more detail. The role of auto-ignition in flame stabilization and lift-off is revealed.

Introduction

The development of reliable hypersonic air-breathing engines such as Supersonic Combustion Ramjets (Scramjets) and Combined-Cycle Engines (CCEs) requires the appropriate solutions for many technical challenges. Such examples are hypersonic and high temperature gas dynamics, flame stabilization of supersonic combustion, thermal protection both internally and externally, the integration of propulsion systems with the flight vehicles, endothermic hydrocarbon fuel technologies and the development of ground-based test facilities and flight experiments [1,2]. One of the most essential issues among these leading edge technical challenges is the turbulent mixing and combustion in the engine combustors [3]. For a scramjet, the main flow throughout the

* *Corresponding author*. Tel.: +86 029 88460327; fax: +86 29 88493406.
E-mail address: qinfei@nwpu.edu.cn (F. Qin).
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combustor remains supersonic, thus due to the high flow speed and the consequent short residence time of fuel in a limited combustor length, the adequate mixing and combustion between the fuel and air must take place at a time scale of the order of milliseconds. What makes things worse is that supersonic combustion experiments are complicated and only a few limited-runtime ground test facilities are available, while flight experiments are far too expensive to conduct for fundamental research. Thus, one of the most cost-effective ways to investigate turbulent mixing and combustion processes in a scramjet lies in the use of Computational Fluids Dynamics (CFD), provided that proper models and accurate boundary conditions are specified [4].

Large eddy simulation, in which large energetic flow scales are resolved directly on the grid while the small scale ones are modeled, has achieved significant progress in modeling both non-reactive and reactive turbulent flows. It is considered to be a promising tool for the large scale engineering applications of turbulent mixing and combustion simulations [5]. The continuously rapid growth in computational power and fast progress in Sub-Grid Models (SGM) in recent decades have made it possible for numerical analysis of such systems. Nevertheless, the interaction of turbulence with other physical processes such as chemical kinetics remains a great challenge. The traditional Reynolds-Averaged Navier–Stokes (RANS) models together with flame-let and Eddy Break-Up (EBU) models have long been successfully applied in many engineering problems, mainly due to their fast turn-around time and abundant success in providing design guidance for matching exit temperature profile requirements [6]. Whereas, it is not the case for high-speed flows and scramjet-like engines due to the inherent time variant characters under such conditions. A better understanding and predicting capability of mixing and combustion features in a scramjet combustor is desired for the large scale practical use of such air-breathing engines.

The LES-LEM (Linear Eddy Mixing) model [7] and the localized dynamic sub-grid closure [8] were adopted for compressible turbulent mixing and combustion in the German Aerospace Center (DLR) model scramjet combustor. Results indicated the potential applicability of LES in the studies of supersonic flow and combustion. Fundamental physics of mixing, combustion and vorticity generation as well as the interaction between shock waves, boundary layer and heat release are analyzed by means of 3D LES using detailed chemistry, with the Fractal Model (FM) to close all the sub-grid terms in a scramjet [9]. Result confirms that burning hydrogen is efficient and feasible in supersonic flows and therefore is a good candidate for hypersonic air-breathing applications. A hybrid RANS/LES method is used to investigate the combustion oscillations in a supersonic combustor with hydrogen injection upstream of a cavity flame-holder [10]. Two mechanisms, i.e. unsteady flame spreading from the cavity shear layer to the main stream and the auto-ignition of the combustible fluid packets formed around the fuel jet accompanied by the generation of the hairpin-like vortices, are found to be attributed to combustion oscillations. The flame-let and PaSR sub-grid combustion models were adopted for LES studies of supersonic combustion in the ONERA [11], DLR [4,12] and HyShot II [13] scramjet combustors based on the open source platform of OpenFOAM [14]. The Eddy Dissipation Concept (EDC) model under the framework of OpenFOAM is applied to a gas turbine, and handles turbulent-chemistry interactions well in the low-speed flow regime [15]. A RANS simulation along with SST k-ω turbulence model based on OpenFOAM CFD toolbox is also report in Ref. [16]. It was proved that OpenFOAM is a promising tool for the designs of scramjets, and its applicability in the studies of supersonic combustion mechanisms was validated.

The objective of this paper is to study the supersonic turbulent flame structure and flame stabilization mechanism in a model combustor, and to deepen understandings of complex physical–chemical processes occurring under scramjet-like conditions. The PaSR sub-grid combustion model is described in detail, so is the LES solver and its governing equations. LES results are analyzed and main features and structures of the flow field are discussed.

Mathematical descriptions and numerical models

Governing equations

The governing equations employed for LES studies of turbulent reacting flows are obtained by applying a local grid size Δ based spatial filter to reactive Navier–Stokes Equations (NSEs) for mass, momentum, energy and species conservation laws [17], describing the convective motions of the fluid, the diffusive transport processes and chemical reactions. And after Favre filtering, can be expressed as [18]:

$$\begin{cases} \partial_t(\bar{\rho}) + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{v}}) = 0 \\ \partial_t(\bar{\rho}\tilde{\boldsymbol{v}}) + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{v}}\otimes\tilde{\boldsymbol{v}}) = -\nabla p + \nabla\cdot\left(\bar{\mathbf{S}} - \mathbf{B}\right) + \bar{\rho}\tilde{\boldsymbol{f}} \\ \partial_t\left(\bar{\rho}\tilde{h}_s\right) + \nabla\cdot\left(\bar{\rho}\tilde{\boldsymbol{v}}\tilde{h}_s\right) = \partial_t(\bar{p}) + \tilde{\mathbf{S}}\cdot\nabla\tilde{\boldsymbol{v}} + \nabla\cdot\left(\bar{\boldsymbol{h}} - \boldsymbol{b}_h\right) + \bar{\rho}\tilde{\sigma} - \sum_{i=1}^{N}\left(\overline{\dot{\omega}_i}h_{f,i}^{\theta}\right) \\ \partial_t(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{v}}\tilde{Y}_i) = \nabla\cdot\left(\bar{\boldsymbol{j}}_i - \boldsymbol{b}_i\right) + \overline{\dot{\omega}_i} \end{cases} \quad (1)$$

Here, ρ is the density, $\boldsymbol{v}$ the velocity, p the pressure, $\mathbf{S}$ the viscous stress tensor, $\boldsymbol{f}$ the body force, $h_s = \sum_i Y_i \int_{T_0}^{T} C_{p,i}(T)dT$ the sensible enthalpy, T the temperature, $\boldsymbol{h}$ the heat flux vector, Y_i the species mass fraction, $\dot{\omega}_i$ the species reaction rate and $\boldsymbol{j}_i$ the species mass flux, $h_{f,i}^{\theta}$ the species standard formation enthalpy and σ the radiative heat loss which is neglected here.

Sub-grid flow and combustion models

The unresolved sub-grid flow physics is concealed in the sub-grid stress tensor $\mathbf{B} = \bar{\rho}(\widetilde{\boldsymbol{v}\otimes\boldsymbol{v}} - \tilde{\boldsymbol{v}}\otimes\tilde{\boldsymbol{v}})$ and flux vectors $\boldsymbol{b}_i = \bar{\rho}(\widetilde{\boldsymbol{v}Y_i} - \tilde{\boldsymbol{v}}\tilde{Y}_i)$ and $\boldsymbol{b}_h = \bar{\rho}(\widetilde{\boldsymbol{v}h} - \tilde{\boldsymbol{v}}\tilde{h})$, which results from the filtered non-linear terms. According to [15], under the assumption that the gas mixture to be linearly viscous and optically thin with Fourier heat conduction and Fickian species diffusion law applicable, and disregard the sub-grid contributions to the constitutive equations, these terms can be modeled by the Mixed Model, in which they are approximately expressed as [19]: