INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 40 (2015) 683–691

Available online at www.sciencedirect.com

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IDDES simulation of hydrogen-fueled supersonic combustion using flamelet modeling

Haosu Wang, Fanli Shan, Ying Piao, Lingyun Hou*, Jian Niu

School of Aerospace, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 25 June 2014
Received in revised form
24 September 2014
Accepted 16 October 2014
Available online 22 November 2014

Keywords:
Hydrogen
Supersonic combustion
Flamelet/progress variable model
Improved delayed detached eddy simulation

ABSTRACT

A turbulent combustion modeling method combining the improved delayed detached eddy simulation (IDDES) model and the flamelet/progress variable (FPV) model is developed and then applied in the hybrid RANS/LES simulation of two canonical configurations for hydrogen-fueled supersonic combustors, namely the DLR supersonic combustor and Gamba model combustor. Results of both cases show good agreement with experiment, validating the accuracy of this method in both two- and three-dimensional combustion simulations. Moreover, the results suggest that the IDDES model is capable of capturing large scale vortex structures, and verify that the FPV model is applicable under supersonic conditions. Meanwhile, the k-ω SST model combined with the FPV model is applied in both cases. It is found that the application of the k-ω SST model leads to larger deviations compared with that of the IDDES model. Further analysis indicates that large scale vortex structures can influence the distribution of control variables of the FPV model, which further affects the species mixing and reaction progress. Therefore, the simulation of turbulent transport process has a significant effect on the performance of the FPV model.

Introduction

Supersonic combustion is considered as one of the fundamental issues in the study of hypersonic air-breathing propulsion systems. Hydrogen, with superior ignitability and reactivity compared with hydrocarbon fuels, is an important choice for the fuel of supersonic combustors [1]. Existing hydrogen-fueled supersonic combustors consist of configurations like a strut injector and transverse jet to improve the fuel/air mixing process, involving complex interactions between turbulence and combustion [2,3]. Therefore, the implementation of an accurate turbulent combustion modeling method is critical for the simulation of supersonic combustion [4].

In combustion modeling, the basic issue is the closure of the chemical source term in species transport equations [5]. As a widely applied approach to solve this problem, the flamelet model allows the computation of chemistry to be performed independently of the combustor simulation, and generates a lookup table called flamelet library to store the results. These results, such as species mass fractions, are stored in the table as functions of certain scalars, thus can be read and interpolated during actual combustor simulation. This approach noticeably reduces the computational cost, allowing the use of detailed chemical mechanisms [6]. Conventional steady laminar flamelet (SLF) model [7] introduces mixture fraction Z to feature the mixing process of fuel and oxidizer, assuming the temperature and species mass fractions only depend on Z and its dissipation rate. However, the

* *Corresponding author*. Tel./fax: +86 10 62772157.
E-mail address: lyhou@tsinghua.edu.cn (L. Hou).
http://dx.doi.org/10.1016/j.ijhydene.2014.10.124

Nomenclature

C_p	specific heat coefficient at pressure constant, J kg^{-1} K^{-1}
C	progress variable
D	diffusion coefficient
h	specific enthalpy, J kg^{-1}
k	turbulent kinetic energy, m^2 s^{-2}
P	pressure, Pa
Pr	Prandtl number
Sc	Schmidt number
T	temperature, K
t	time, s
Y	mass fraction
Z	mixture fraction

Greek letters

ε	dissipation rate of turbulent kinetic energy, m^2 s^{-3}
μ	dynamic viscosity, kg m^{-1} s^{-1}
ρ	density, kg m^{-3}
χ	scalar dissipation rate, s^{-1}
ω	turbulent eddy frequency, s^{-1}
$\dot{\omega}$	mass production rate, kg m^{-3} s^{-1}

Subscripts

0	stagnation property
i	species
st	stoichiometric
t	turbulent

Superscripts

~	Favre-averaged
—	Reynolds-averaged
″	fluctualtions

mixture fraction includes no information about chemical reactions, so combustion simulated by this model is solely determined by the mixing degree. In order to overcome this issue, the flamelet/progress variable (FPV) model is proposed by Pierce [8]. This approach replaces the scalar dissipation rate in the SLF model with progress variable C to quantify the reaction process, and is becoming a more applicable approach for combustion modeling [9].

In the flamelet library of low speed flow fields, the temperature variation is dominated by chemical reactions. Therefore, the local temperature values can be obtained directly by reading from the flamelet library [10]. Nevertheless, in supersonic combustors, the kinetic energy is comparable to the chemical energy [11], so the temperature is affected not only by the chemistry, but also by strong compressibility effects which result in noticeable changes in the kinetic energy [12]. In this situation, reading temperature values from the flamelet library only reflects the influence of the chemical energy, but cannot account for that of the kinetic energy. To address this issue, a concise modification method has been introduced by Oevermann [2], in which temperature is no longer obtained by the flamelet library, but is calculated by solving the energy equation. Since this method takes compressibility effects into consideration, it is adopted in several supersonic combustion studies [2,13].

Accurate simulation of turbulent combustion problems not only depends on appropriate combustion models, but also relies on reasonable turbulence models. The improved delayed detached eddy simulation (IDDES) model is a recently developed hybrid RANS/LES model by Shur [14]. The IDDES model adopted in this paper is constructed based on the k-ω SST model [15], and it is a combination of delayed detached eddy simulation (DDES) with a hybrid model aimed at wall-modeled LES (WMLES). This approach features several intricate blending and shielding functions, making a smooth and fast transition between LES and RANS regions so that large scale vortex structures in the boundary layer and free shear layer are better predicted [16]. There have not been many applications of the IDDES model. The method combining the IDDES model and FPV model to simulate turbulent combustion has not been proposed and applied before.

As for the verification of simulation methods, the DLR supersonic combustor [2] and Gamba model combustor [3] are both suitable since they were designed to include main features of a realistic system: the former combustor includes a strut-based injector, and the latter is composed of a transverse jet.

In this paper, a method combining the IDDES model and a modified FPV model is developed using an in-house code and then applied in a two-dimensional simulation of DLR supersonic combustor and a three-dimensional simulation of Gamba model combustor. The result of DLR supersonic combustor is in good agreement with experiment, and the simulation of Gamba model combustor successfully predicts the reaction in the recirculation and near-wall regions. Meanwhile, the k-ω SST model is combined with the FPV model and applied in both cases. Results of these two modeling methods are compared to analyze the influence of turbulent flows on chemical reactions. Then, the influence of turbulent transport prediction on the accuracy of FPV model is addressed according to the results of both cases.

Physical models and numerical methods

Flamelet library of the FPV model

In the counterflow diffusion flame, by coordinate transformation of species transport equations and the energy equation from physical space to mixture fraction Z space, and assuming that the Lewis number is equal to unity, the flamelet equations can be derived as:

$$\begin{aligned} \rho \frac{\partial Y_i}{\partial t} &= \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i \\ \rho \frac{\partial T}{\partial t} &= \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \frac{1}{C_p} \sum_{i=1}^{NS} h_i \dot{\omega}_i \end{aligned} \tag{1}$$

where χ is the scalar dissipation rate, measuring the decay of mixture fraction fluctuations. Given a set of stoichiometric scalar dissipation rates χ_{st}, the flamelet equations can be solved and the results are then stored in the laminar flamelet