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A passive scalar-based method for numerical combustion

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ABSTRACT

A passive scalar-based method for analyzing unsteady combustion processes has been proposed. Transport equations for passive scalars have been derived based on mixture fraction concept widely used for the description of nonpremixed combustion. These equations can be solved together with the conventional computational fluid dynamics (CFD) governing equations so that these passive scalars are readily utilized to trace the mass transport in simulations of complicated reacting flows, regardless of turbulence and chemistry models. The approach is used together with large eddy simulation to study the cavity-stabilized H_2 jet combustion in a supersonic combustor, where characteristics of the mass transfer into and out of the cavity are captured and cavity residence time is obtained for the first time under reacting flow conditions.

Introduction

Numerical simulation has now become a very useful research tool for complex combustion processes since reliable methods [1] and models [2] have been developed in the recent past. On the one hand, knowledge of the physical processes of combustion and related analysis of experimental data provide a necessary platform for development and validation of numerical methods and models. On the other hand, flow and combustion details obtained from numerical simulations facilitate a better understanding of combustion physics and experimental observations. In particular, numerical simulation tends to exert more and more impacts on combustion research due to the rapid progress in computer technology.

A great variety of flows in practical engineering applications are turbulent and inherently unsteady, where unsteady methods are necessary to appropriately capture the dynamics of such complex flows. Direct numerical simulation (DNS) allows one to resolve all scale structures, but is computationally time consuming and remain limited to low Reynolds numbers, thus unsteady RANS (URANS) and large eddy simulation (LES) become the realistic alternatives in the foreseeable future [3]. Especially, LES has emerged as a viable and powerful tool for the simulation of various complex combustion problems [4–6].

LES can provide abundant information of reacting flows with high resolutions in both time and space and many previous studies have focused on improving the performance of LES. Actually, how to extract as much useful information as possible from the simulations is equivalently important,

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which therefore serves as a key motivator for the present study. Considering that mass transfer plays a central role in complex combustion processes, a passive scalar-based approach is proposed to trace mass transport in numerical combustion. Then, this method is applied in the framework of LES to preliminarily analyze cavity-stabilized H_2 jet combustion in a supersonic combustor.

A passive scalar-based approach for mass tracing

Mass transfer is a key process in characterizing combustion stabilization in high-speed flows where recirculation regions are usually involved. Due to the difficulty in measuring this complex unsteady process experimentally, numerical simulation appears as a powerful complementary tool. Non-reacting cavity [7] and jet-cavity flows [8] have been studied numerically regarding the cavity/mainstream mass exchange characteristics for scramjet applications. In these non-reacting cases, each species was divided into two nominal species (in or out of the cavity) when the flow reached a periodic steady state, and the transport equations for all nominal species were solved simultaneously. However, this procedure may cause problems in reacting cases because too many nominal species appear. Considering the H_2/air reacting system with 9 chemical species (O_2, H_2O, H_2, OH, O, H, HO_2, H_2O_2, N_2), for example, the number of nominal species becomes as many as 37 due to the decomposition and recombination of the chemical species since each chemical element might show as two nominal elements. Thus the computational cost and complexity would rise up rapidly. In an effort to solve this problem, a passive scalar-based approach for analyzing reacting flows is proposed, borrowing ideas from the mixture fracture concept widely used for the description of nonpremixed combustion [9].

Considering a mixture including N_s chemically reacting species and N_e elements, if a binary diffusion flux is adopted and if all diffusivities are equal, i.e. $D_i = D$, the balance equation for the element mass fraction Z_j is [9].

$$\frac{\partial \rho Z_j}{\partial t} + \nabla \cdot \left(\rho \vec{v} Z_j\right) = -\nabla \cdot \left(\rho D \nabla Z_j\right) \tag{1}$$

where $j = 1,2,\ldots,N_e$. The underlying idea is that though the atoms may move from one compound to another during reactions, they themselves are conserved. Denoting a_{ij} as the number of atoms of element j in a molecule of species i, the mass fraction of species i is

$$Y_i = \sum_{j=1}^{N_e} \left(\frac{W_i}{a_{ij} W_j} Z_j \right) \Bigg|_{a_{ij} \neq 0} \quad i = 1, 2, \ldots, N_s \tag{2}$$

where W_k denotes the corresponding molar mass. Denoting f_k as the mass fraction of the material concerned, it can be written as

$$f_k = \sum_{i=1}^{N_s} b_{ki} Y_i \tag{3}$$

where b_{ki} is one if species i is concerned, and zero otherwise. Substitution of Eq. (2) into Eq. (3) yields

$$f_k = \sum_{j=1}^{N_e} \sum_{i=1}^{N_s} \left(\frac{b_{ki} W_i}{a_{ij} W_j} Z_j \right) \Bigg|_{a_{ij} \neq 0} \tag{4}$$

Combing Eq. (1) and Eq. (4), one obtains

$$\frac{\partial \rho f_k}{\partial t} + \nabla \cdot \left(\rho \vec{v} f_k\right) = -\nabla \cdot \left(\rho D \nabla f_k\right) \tag{5}$$

These equations are sources free such that f_k are passive (conserved) scalars. From the mass conservation law, although the mass of reacting species change in combustion, the total sum of the material originated from a specified region does not change during chemical reactions. These equations can be solved together with the conventional computational fluid dynamics (CFD) governing equations to trace the mass transport in simulations of complicated reacting flows, regardless of turbulence and chemistry models. Notably, these scalars are simply transported by the fluid particles and diffused by molecular effects without any action on the flow dynamics, and can be used to trace an arbitrary portion of mass in the system.

Application to LES of cavity-stabilized H_2 jet combustion

Computational configuration

As an example, the passive scalar-based approach is integrated into LES to analyze cavity-stabilized H_2 jet combustion in a supersonic combustor, where we adopt the passive scalar f_in to trace the mass transport processes of cavity fluid (mixture of reactants and products within the cavity). The physical models and numerical schemes for the combustion LES have been detailed and validated in Refs. [10–12].

The calculation simulates a model scramjet combustor [13] designed at National University of Defense Technology. The airstream entering the combustor has a total temperature of 1486 K, total pressure of 1.6 MPa and Mach number of 2.52. Schematic of the computational domain is shown in Fig. 1, which has a width of 20 mm and height of 40 mm. A cavity with a depth of $D = 8$ mm, a length-to-depth ratio of $L/D = 7$ and an aft angle of 45° is mounted on the bottom wall. Gaseous hydrogen which has a total temperature of 300 K, total pressure of 1.2 MPa and Mach number of 1.0 is transversely injected into the mainstream through a 2-mm orifice located 10 mm upstream of the cavity. The boundary-layer thickness at the combustor entrance is $\delta_{inf} = 2.5\ mm$, resulting in a Reynolds number of $Re_{\delta_{inf}} = 37539$. Total number of grid points for the LES is about 16 million.

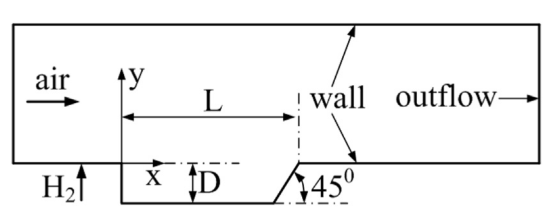

Fig. 1 – Schematic of computational domain.