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On the application of tabulated dynamic adaptive chemistry in ethylene-fueled supersonic combustion

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ABSTRACT

The demands for extending the limiting operation conditions and enhancing the combustion efficiency of scramjets raise new challenges to the research of reliable robust and controllable flame stabilization in supersonic flows. In the present study, Large Eddy Simulation of flame stabilization in a realistic supersonic combustor, employing the tabulation of dynamic adaptive chemistry (TDAC) method were conducted, in comparisons with other relevant chemistry treatment methods, i.e., dynamic adaptive chemistry (DAC), global skeletal mechanism, and detailed mechanism. The wall pressures, the pseudo one-dimensional metrics, combustor global performance and flame structures are all well reproduced by the DAC/TDAC methods compared with the experimental measurements and the benchmark predictions by the detailed mechanism, while the global skeletal mechanism fails to predict the flame stabilization characteristics. The reason for the discrepancy induced by the skeletal mechanism in the flame stabilization simulation was further illustrated through reaction path analyses. Regarding the computational efficiency, the DAC method shows high efficiency for complex reaction systems, with an almost linear increasing speedup factor with the increase of species number. The TDAC method almost doubly further improves the DAC efficiency. The DAC/TDAC methods show great potential of alleviating the huge computational cost while improving the chemistry fidelity for supersonic combustion especially for flame stabilization modeling.

1. Introduction

Hypersonic air-birthing propulsion systems capable of sustained operation in flight have received renewed research interest during the past decade [1]. Although considerable achievements have been made in understanding the flow physics in scramjet combustors [2], there still remains significant challenges including efficient mixing and stabilized combustion within limited flow residence time. More importantly, with regard to the extension of the operating envelops and enhancement of combustion efficiency, robust flame stabilization was proved to be one of the most intractable challenges. Three different flame stabilization modes in hydrogen fueled dual-mode scramjet were first observed by Micka and Driscoll [3] via flame luminosity experimentally. More comprehensive experiments by Yuan et al. [4] using time-resolved CH* chemiluminescence found four distinct modes in an ethylene-fueled supersonic combustor in which a weak combustion mode is absent in Micak and Driscoll. Wang et al. [2] summarized the state-of-the art about the fundamental problems and recent advances regarding cavity-stabilized scramjet combustor but the lack of comprehensive experimental measurements renders this challenge still unsolved.

However, due to the prohibitive cost of ground test, the difficulties in measuring reacting flow quantities in supersonic flow as well as the complexity of the aerothermodynamics, high-fidelity numerical simulation is not only complementary but is absolutely necessary for understanding and then optimizing the supersonic combustion in scramjets [5,6]. To achieve accurate predictions on the essential physical and chemical properties of the turbulent reacting flow, great efforts have been devoted to the development of high-resolution numerical schemes [7] and turbulent–combustion interaction models [8–10] for supersonic combustion simulation, whereas the importance of the comprehensive chemical mechanism is prominently overlooked. In consideration of this, Wu et al. [11] thoroughly analyzed the influence of chemistry mechanisms in faithfully reproduction the flame stabilization mode in the strut injection scramjet engine. They also realized that various elementary reactions control the flame stabilization mechanism in different reaction zones. In addition, the deficiency of the skeletal mechanism in well reproducing the flame stabilization structure in an

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Nomenclature

Symbols

p	pressure
ρ	density
T	temperature
Y_k	mass fraction of species k
c_k	mole concentration of species k
dQ	heat release rate
$\dot{\omega}$	chemical source term
υ	kinematic viscosity
υ_t	turbulent viscosity
υ_{eff}	effective kinematic viscosity
ε	turbulence dissipation rate
S_{ij}	strain rate tensor
τ_c	characteristic time scale of chemical reaction
τ_m	characteristic time scale of turbulent mixing
κ	reacting volume fraction in PaSR model
Cp	constant pressure specific heat
L	characteristic length of the combustor
H	height of the combustor
t_f	flow through time, $t_f = L/U_\infty$
ψ^q	query composition vector $\psi^q = \{p, T, Y_1, Y_2, \ldots Y_N\}$
ψ_a^q	query composition vector with active species
$\boldsymbol{R}$	reaction mapping
$\mathbf{R}^I$	linearized reaction mapping
ϕ	equivalence ratio
N_{sp}	number of active species
N_{cell}	number of computational cells
η_p	total pressure loss
η_c	global combustion efficiency
dA	incremental area projection in the streamwise direction
ε_{DAC}	threshold value for DAC module
ε_{ISAT}	threshold value for ISAT module
τ_{ing}	ignition delay time
δ_{ing}	relative error of ignition delay time
S_u	laminar flame speed
δ_{su}	relative error of laminar flame speed
Ma	Mach number

sub- and super-scripts

∞	physical properties of the air inflow
^	normalized form of the corresponding physical quantity
$-$	spatial filtering
$\sim$	favre filtering

Abbreviations

DAC	dynamic adaptive chemistry method
ISAT	in-situ adaptive tabulation method
TDAC	tabulation of dynamic adaptive chemistry method
ODE	ordinary differential equation
EOA	ellipsoid of accuracy
DRGEP	directed relation graph with error propagation
DI	direct integration

ethylene-fueled model scramjet was elaborated by comparing with experimental data and results obtained with detail mechanism in Wu et al. [12]. After reviewed plentiful available simulated scenarios, Gonzalez-Juez et al. [6] speculated that an appropriate chemical mechanism is more important, if no remarkable improvement in the treatment of turbulent–combustion interaction can be anticipated.

Improving the accuracy of the chemical mechanisms while minimizing their sizes are both required for the numerical modeling. Usually, adopting reduced or skeletal mechanisms in turbulent combustion modeling is a tradeoff to the formidable computational cost especially in hydrocarbon-fueled propulsion systems [13]. For instance, Potturi and Edwards [14] utilized a 22-species reduced ethylene mechanism in a cavity-stabilized scramjet engine, while Zettervall et al. [15] used a skeletal mechanism of 19 species with 57 reversible reactions to mimic the kerosene combustion chemistry in a multi-burner annular aero-engine combustor. Therefore, exploit the accuracy of the comprehensive chemical mechanism, based on the concept of multiple sets of chemical mechanisms for different reaction zones and different reaction stages, dynamic adaptive chemistry (DAC) method [16] provides a promising approach to retain the mechanism accuracy while minimizing its size spatiotemporally.

In this work, the main objective is to illustrate and analyses the seamless process of utilizing DAC method in supersonic combustion simulation while enhance its efficiency through coupling of the mechanism reduction method with the tabulation algorithm. This strategy, also called tabulation of dynamic adaptive chemistry (TDAC), overcomes the two sources of computational overhead in simulations, i.e. number of cells and chemical species. In the present study, the TDAC method of Contino et al. [17–20] is briefly introduced before the descriptions of the experimental case and the numerical details. The DAC/TDAC methods are firstly applied in simulating auto-ignition and one-dimensional laminar flame propagation to validate their accuracy and efficiency against the direct integration. Then supersonic combustion modelings employing different chemistry treatment methods, i.e., DAC, TDAC and global skeletal mechanism, are compared with those by the detailed mechanism, to further verify their capabilities in flame stabilization prediction.

2. Tabulation of dynamic adaptive chemistry methodology

The computational cost required by reactive flow simulation depends on both the number of grid cells and the complexity of the fuel oxidation mechanisms. Under the framework of direct integration, the total times to solve the system of species evolving equations are proportional to the number of cells. The size of fuel oxidation mechanism determines the workload of the stiff nonlinear solver to integrate the ordinary differential equation (ODE) system. Reduction of computational efforts for these two aspects is achieved by the TDAC method [17] which is briefly illustrated in Fig. 1. The TDAC method is composed of two elementary layers: a tabulation layer and a mechanism reduction layer.

The tabulation layer employs the in situ adaptive tabulation (ISAT) method [21]. During the integration of the species-evolving ODE system over the current time-step, a query composition vector ψ^q is firstly provided to the tabulation layer. The ISAT module will try to retrieve a previously stored result of reaction mapping $\mathbf{R}(\psi^0)$ within the local error threshold ε_{ISAT} and linearly estimates the current reaction mapping as $\mathbf{R}^I(\psi^0)$. If the query is not retrievable within the current ellipsoid of accuracy (EOA), direct integration of the stiff ODE system will be applied and the binary tabulation tree will be expanded by adding a new leaf or growing the current leaf depending on whether the local error exceeds the ε_{ISAT}. The pressure as a status variable is also stored in the ISAT table since the constant pressure assumption is no longer valid for transient supersonic flows with high compressibility. Although similar to the treatment in the internal combustion engine simulation [17], the setup is much more challenging. In the previous engine simulations, pressure changed widely over the entire simulation but without dramatic change within the computational domain, mostly because it was homogeneous charge compression ignition. In su-