Comprehensive Analyses on the Influential Factors in Supersonic Combustion Simulation using Dynamic Adaptive Chemistry Method

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Abstract

To overcome the major challenge of reactive flow simulation for chemical kinetics dominated flame dynamics in supersonic combustion, on-the-fly mechanism reduction for high fidelity simulation of scramjet becomes mandatory. For dynamic adaptive chemistry (DAC) methodology, there are three major factors controlling the accuracy and efficiency of the overall simulation, namely the mechanism reduction method, error threshold value ε_{DAC}, and search initial species (SIS). In the present work, systematic investigations of the three influential factors were conducted for large eddy simulation of ethylene fueled supersonic combustion within a unified DAC framework. The results show that all the four mechanism reduction methods, i.e., DRG, DRGEP, PFA and DAC-L are adequate for the combustor's global performance prediction regarding the wall pressure, the stable combustion productions, and temperature. However, for intricate flame stabilization characteristics, the DRG, DRGEP and DAC-L methods yield comparable prediction accuracy in radical distributions, whereas the PFA method leads to relatively large discrepancies compared to direct integration with detailed mechanism. The DRGEP method obtains the best balance between the numerical accuracy and computational efficiency among the four methods, while the PFA method is the most computational demanding one. Regarding the mechanism reduction error threshold value, the relative errors in physical property predictions increase as the relaxation of the error threshold value. And the comparative study suggests that the ε_{DAC} should not exceeds 10^{-4} for high fidelity simulations of supersonic combustion. Furthermore, the stable species combination namely fuel, O_2 and N_2 incurs larger relative errors in radical mass fraction prediction than the combination including fuel and intermediate species HO_2 and CO. Nevertheless, the latter is less computational efficient than the former as it requires 15% more CPU time to solve the stiff ODE system of the resultant skeletal mechanism. It should be noted that the computational overheads for mechanism reduction under various ε_{DAC} values and SIS combinations are almost the same, and the overall computational efficiency is mainly determined by the CPU time for solving the size-reduced skeletal mechanisms.

Keywords:

Dynamic adaptive chemistry,

Mechanism reduction method

Error threshold

Search initial species

High-fidelity numerical simulation

1 Introduction

Hypersonic air-breathing propulsion technology has gained increasing attentions in the past few decades, and one of the enabling technologies is the development of a propulsion system capable of operating across an extended range of Mach number (Ma) [1]. Consequently, extending the limiting operation condition and enhancing the combustion efficiency of supersonic combustion ramjet engine (scramjet) raise challenges to the research of reliable ignition and robust flame stabilization in supersonic flow [2]. Theoretically, it’s undoubted that accurate prediction of transient flame dynamics requires appropriate modeling of detailed chemical kinetics as its prerequisite [3]. Nevertheless, comprehensive chemical kinetic mechanisms for realistic fuels often incorporate reaction pathways valid over a wide range of operating conditions and typically involve hundreds of species and thousands of elementary reactions, which is inhibitive for high fidelity simulations [4, 5].

However, for most practical combustion problems, a relatively smaller number of species and reactions dominate the pivotal combustion characteristics such as flame propagation and heat release. This observation leads to the mechanism reduction approach that eliminate redundant species and reactions from the full mechanisms [6]. Most methods reduce the full mechanism to a single skeletal mechanism, either by defining a problem specific merit function or generating reduced sub-mechanisms at a group of sampled conditions, which is also known as static skeletal mechanism. The static skeletal mechanism strategy has enjoyed its popularity for a long time in supersonic combustion simulations [7-9] owing to high computation efficiency.

However, recently Wu et al. [10] revealed that the static skeletal mechanism approach is insufficient for flame dynamics prediction in scramjet engines. As the static skeletal mechanisms are generated before reactive flow simulations, their feasibility ranges can hardly cover the diverse thermochemical conditions encountered for most transient problems. Essentially, this deficiency of the static skeletal mechanism approach is inherited from the separation of mechanism reduction and fluid dynamic simulation, since the entire thermochemical space is unknown a priori. To this end, Liang et al. [11] proposed the dynamic adaptive chemistry (DAC) methodology, in which the adaptively reduced mechanisms were rigorously valid for their local and instantaneous thermochemical conditions with only minor computational overheads. This procedure removes redundant species from the detailed mechanism and freezes their mass fractions in the subsequent calculation, resulting in a reduced ODE system thus accelerates the computation. Basically, the performance and accuracy of the DAC scheme depend on the reduction method utilized, the search initiating species (SIS) chosen, and the error threshold value specified.

To minimize the computational overhead for mechanism reduction during the running time, mechanism reduction methods that scale linearly with the problem size are typically used in the DAC scheme. Tosatto et al. [12] formulated a DRG-based [6] DAC scheme, which achieves speedup factor of 5 and 10 for steady JP-8 flame and a transient ethylene flame, respectively. Yang et al. [13] combined the DAC scheme with the DRG method in turbulent methane flame simulation and accurately reproduced the combustion process of a partially stirred reactor. Liang et al. paired a modified version of the DRGEP [14] in DAC (denoted as DAC-L hereinafter) for single cell HCCI (Homogeneous-Charge Compression Ignition) [11] and homogeneous auto-ignition simulations [15] to achieve more than 30-fold speedup with high accuracy. Contino et al. [16-18] also utilized the DRGEP-based DAC to investigate the nitric oxide effect on the ignition of iso-octane in a single cylinder HCCI engine, which gained a speed-up factor up to 1500 when coupled DAC with ISAT. Gou et al. [19] paired the PFA [20] method with the DAC scheme with error control, and obtained 5-100 fold speedup with high accuracy. By combining an element flux analysis (EFA) method with the DAC scheme, He et al. [21] achieved a 25-fold speedup in a simulation of *n*-pentane in a pairwise mixed stirred reactor, nonetheless the overhead of flux-based reduction method consumed nearly 20% of the total computational time. As a systematic assessment, Li et al. [22] demonstrated that the DRGEP, DAC-L and EFA models are more superior in performance compared to the DRG and PFA models in moderate or intense low-oxygen dilution (MILD) combustion.

To control the accuracy and efficiency of the DAC scheme, an appropriate error threshold value ε_{DAC} for mechanism reduction is generally determined by user knowledge or trial and error. However, this could be challenging since there is no direct relation between the model reduction threshold and the error of the resultant skeletal mechanism. To this end, Gou et al. [19] devised a PFA-based DAC scheme with error control, in which data tabulated from zero-dimensional calculations were combined with progress variables to automatically determine appropriate error thresholds during the simulation. Despite its high speedup factor (5-100 folds), the tabulated data and choice of reaction progress variables may lack generality in turbulent combustion simulations. Thus, a new DAC scheme that concerns solution error control was formulated by Oluwayemisi et al. [23], and proven to be as fast as DRG model in zero-dimensional auto-ignition and two-dimensional laminar flame calculations. Besides, Xie et al. [24] improved the accuracy in ignition delay time and composition calculation of DRG-based DAC by introducing a Jacobian-aided rate analysis to control the solution error.

Finally, apart from the mechanism reduction method and reduction error threshold, the other major factor controlling the performance and accuracy of DAC scheme is the selection of search initiating species. Traditionally, search initiating species are chosen based on their expected importance to key combustion process. Typical choices of SIS include the fuel, oxygen, combustion products (e.g. CO_2), and necessary radical or intermediate species (e.g. H, OH, CO, HO_2). The original DRG method [6] initiates the search with fuel or oxidizer, however Liang et al. [11] found that fuels fails to connect to any other species in the post-ignition stage in the DAC scheme, which necessitates the inclusion of CO and HO_2 in the SIS as [Fuel, CO, HO_2]. Meanwhile, for mechanism reduction with DRGEP method, Niemeyer et al. [25] using the hydrocarbon parent fuel, O_2, and N_2 as SIS [Fuel, O_2, N_2] worked well. In an attempt to follow the reaction progress, Shi et al. [26] proposed an extended DAC (E-DAC) scheme that switches between a small numbers of SIS sets based on local thermochemical state, yielding an additional 8-10% time saving in a three-dimensional simulation for *n*-heptane. However, the E-DAC scheme utilizes only a given number of SIS sets, hence its accuracy will suffer if combustion conditions are encountered where none of the SIS are appropriate. As such, Curtis et al. [27] developed a method to automatically determining appropriate SIS for DRGEP-based DAC scheme, which solely relies on the local thermochemical state, namely the relative important index.

Originated from the tackling of complex chemistries involved in internal combustion engines, the application of DAC scheme in scramjet engine is not straightforward and its efficacy is not sufficiently evaluated. This can be attributed to the fact that the convection and diffusion process are more significant due to heterogeneous combustion in scramjet engines. A DRGEP-based DAC scheme was exploited in our previous ethylene-fueled supersonic combustion simulation and just preliminarily demonstrated the balanced capability in accurate prediction of flame stabilization and computation efficiency [28]. The goal of the present work is to provide a further assessment of the DAC scheme under supersonic combustion conditions, covering all the aforementioned performance-affecting factors such as the mechanism reduction method, the reduction error threshold, and search initiating species.

Large eddy simulation will be conducted with four different mechanism reduction methods against a benchmark case using a detailed ethylene oxidation mechanism (57-species, 269-reactions) [29]. To assess the capability of the DAC under various configurations, comprehensive comparisons will be given regarding fluid flow characteristics, combustor's global efficiencies and flame dynamics. The paper is outlined as follows. First, Section 2 outlines the formulation and framework of the dynamic adaptive chemistry method in more details. Then the experimental configuration, numerical methodology and associated simulation setup for the supersonic combustion baseline are elaborated in Section 3. Influences of the mechanism reduction method, error threshold value and search initiating species on the numerical accuracy and computational efficiency of the dynamic adaptive chemistry simulations are systematically discussed in Section 4. Finally, conclusions are given in Section 5.

2 Dynamic Adaptive Chemistry Algorithm

2.1 Framework of the dynamic adaptive chemistry scheme

In finite-rate chemistry framework, each computational cell is treated as an individual chemistry problem with pressure, temperature and species mass fraction comprised in a thermochemical state vector $\boldsymbol{\phi} = \boldsymbol{\phi}(p, T, Y_1, Y_2 \ldots Y_{Ns})$. Most reacting flow solvers rely on an operator splitting method: transport term and chemical source term are solved sequentially. Generally, the computational effort for solving these stiff ODEs scales at least with the square of the number of species, which becomes remarkable for large-scale combustion simulation with complex hydrocarbon fuels. As for the simulations with DAC scheme, the full chemistry mechanism is first reduced to a skeletal mechanism with N_{asp} active species (superscript a), and N_{isp} inactive species (superscript i). As a result, the chemical source terms are formulated by a set of stiff ODEs:

$$\begin{bmatrix} \dot{y}_1^a \\ \vdots \\ \dot{y}_{N_{asp}}^a \\ \dot{T} \end{bmatrix} = \begin{bmatrix} f_1\left(p, T, \dot{y}_1^a \dots \dot{y}_{N_{asp}}^a, \dot{y}_1^i \dots \dot{y}_{N_i}^i sp\right) \\ \vdots \\ f_{N_a}\left(p, T, \dot{y}_1^a \dots \dot{y}_{N_{asp}}^a, \dot{y}_1^i \dots \dot{y}_{N_{isp}}^i\right) \\ f_{N_a+1}\left(p, T, \dot{y}_1^a \dots \dot{y}_{N_{asp}}^a, \dot{y}_1^i \dots \dot{y}_{N_{isp}}^i\right) \end{bmatrix} \tag{1}$$

where p denotes the pressure, T the temperature, $\dot{y}_k^a$ the mass fraction of the kth of the active species, and $\dot{y}_m^i$ the mass fraction of the mth of the inactive species, respectively. To minimize the size of the ODE system while accounting for the third-body and pressure-dependent reactions, the concentrations of the inactive species are still considered when evaluating the chemical source terms [17]. The DAC scheme does this reduction on the fly for each local and instantaneous thermochemical condition encountered, and expedite the simulation by solving a downsized stiff ODE system.

2.2 Mechanism reduction methods

To assess various chemical mechanism reduction methods within the on-the-fly reduction framework, four approaches including the DAC-L [11], DRG [6], DRGEP [14], and PFA [20] are considered in the present work. Among all these methods, the DRG method serves as the backbone, which is based on a graph representation of the reaction network and establishes the linkage between various species with weighted factors. As schematized in Fig.1, each vertex represents a species in the full mechanism and each directed edge denotes the immediate dependence of one species to another. The interaction coefficient r_{AB} quantities the contribution of species B to the production rate of species A:

$$\varepsilon = r_{AB} = \frac{\sum_{i=1,n_R} \left| \upsilon_{A,i} \omega_i \delta_{Bi} \right|}{\sum_{i=1,n_R} \left| \upsilon_{A,i} \omega_i \right|} \tag{2}$$

where $\upsilon_{A,i}$ is the stoichiometric coefficient of species A in reaction i, ω_i denotes the production rate of reaction i, n_R the total number of reactions and δ_{Bi} is defined as:

$$\delta_{Bi} = \begin{cases} 1, & \text{if the } i\text{th reaction involves species B} \\ 0, & \text{otherwise} \end{cases} \tag{3}$$

Obviously, r_{AB} measures the normalized error of the production rate of species *A* incurred by the elimination of all the reactions that involve species *B*. Then a directed relation graph is constructed by a search procedure in which there is a directed edge from *A* to *B* if and only if r_{AB} exceeds or equal to a certain threshold value as displayed in Fig. 1(b).

Regarding the definition of dependencies between species, Pepiot-Desjardins and Pitsch [14] argued that a more accurate way is to use the net contribution instead of evaluating production and consumption separately, as in the directed relation graph with error propagation method (DRGEP):

$$r_{AB} = \frac{\left|\sum_{i=1,n_R} \upsilon_{A,i}\omega_i\delta_{Bi}\right|}{\max(P_A, C_A)} \tag{4}$$

in which P_A and C_A represent the production and consumption of species *A* respectively, which are expressed with:

$$P_A = \sum_{i=1,n_R} \max\,(0, \upsilon_{A,i}\omega_i) \tag{5}$$

and

$$C_A = \sum_{i=1,n_R} \max\,(0, -\upsilon_{A,i}\omega_i) \tag{6}$$

In the DRGEP method, the effect of removing species group is also included, since the previously removed species are considered recursively. In contrast to the DRG method, the DRGEP incorporates the notion of error propagation in evaluating the error r_{AB} which takes the length of the path the error has to propagate into account:

$$r_{AB,p} = \prod_{i=1}^{n-1} r_{S_i S_{i+1}} \tag{7}$$

where $S_1 = A$, $S_2 = B$ and p denotes a certain path that links species A and B while the overall error ε can be calculated as:

$$\varepsilon = r_{AB} = \max_{\text{all path p}} r_{AB,p} \tag{8}$$

The DAC-L method employed in the present study was first proposed by Liang et al. [11] based on a modified DRGEP method by neglecting the influence of removing a species group. As for the PFA method, it is based on the DRG and DRGEP methods, while contributions from both the directly and indirectly linked species are evaluated, leading to the r_{AB} with information from multiple generations [20].

2.3 Search-initiating species

In DRG-like method, species deemed of primary importance are selected as search initiating species and a search is performed to identify the set of species on which these initiating species depend. The mechanism reduction procedure is equivalent to identifying vertices to which there exist strong paths connecting them to a vertex in the search initial species set. The union of the subsidiary sets form the active species set of the resultant reduced mechanism.

Typically, reactions in oxidation mechanism of large hydrocarbon fuels can be classified into three interacting groups (1) hydrocarbon decomposition, (2) H_2-O_2 reaction system, and (3) CO oxidation reaction system. Correspondingly, search-initiating species have been chosen based on their expected importance to these chemical reaction groups. Typical choices of target species include the fuel, oxygen, combustion products (e.g., CO_2 and H_2O), and certain key radicals and intermediate known to be good indicator species (e.g., HO_2 and CO). Therefore, to demonstrate the effect of search initiating species on the performance of dynamic adaptive chemistry, two commonly used combinations: (1) SIS involving only stable species as fuel, O_2, and N_2 (denoted as Stable-SIS), (2) SIS consisting of fuel, intermediate species HO_2, and CO (denoted as Inter-SIS).

3 Simulation Configuration and Numerical Methodology

3.1 Description of the experiment configuration

The validation benchmark is taken from the experiment conducted by Situ et al. [30] in a directly connected pipe test rig. The quasi two-dimensional combustor is 1100 mm in length with a rectangle inlet of 65 mm in height ad 40 mm in width. As shown in Fig.2, a 370 mm long mixing section is followed by a 3.6° unilateral expansion section till the combustor exit. The incoming vitiated air supplied by burning hydrogen in air with oxygen replenishment, has a raised stagnation pressure of 0.09977 MPa and temperature of 1700 K. The vitiated air is composed of 71.5% N_2, 23.3% O_2 and 5.2% H_2O in mass fraction. The fuel stream is supplied with the hot products of kerosene/air combustion at Ma 1.25 in an upstream subsonic combustor. Since the products' exact composition is not available, thereby it is determined based on a simplified chemistry model [30]. Gaseous ethylene is considered as the surrogate to represent the main product of the kerosene pyrolysis after initial endothermic reactions [31]. Then the composition of the hot fuel-rich products is obtained based on a one-step global reaction by matching the combustion efficiency derived from measured total temperature and pressure at the upstream subsonic combustor exit. In the experiment, both air and fuel streams were axially injected into the supersonic combustor which was separated by a 6-mm-high plate. The experimental operation condition specifying the compositions of both the vitiated air and fuel streams are summarized in Table 1. During the experiment, static wall pressures were measured by 23 pressure taps on the lower wall and 13 taps on the upper wall, respectively.

Table 1. Experimental operating conditions for both vitiated air and fuel streams.

Parameter	P [MPa]	Ma	T [K]	Y_{N2}	Y_{O2}	Y_{C2H4}	Y_{H2O}	Y_{CO2}
Air	0.0977	2.15	491.9	0.7150	0.2330	0.0	0.0520	0.0
Fuel	0.1731	1.25	1771.9	0.6067	0.0103	0.1059	0.1566	0.1205

3.2 Numerical models and algorithm

To assess the effect of various influential factors in dynamic adaptive chemistry simulation of flame stabilization phenomenon, it is necessary to leverage the large eddy simulation to capture the fluid dynamics and mixing on the small-scale vortices. In this section, only a brief summary will be given regarding the physical models and numerical algorithms used in the present study, and more details can be found in our previous works [32, 33]. The Favre filtered conservation equations for mass, momentum, energy and species are solved. The laminar viscosity is obtained by Sutherland’s law, while the thermal and mass diffusion coefficients are calculated by assuming constant Prandtl and Schmidt numbers. The subgrid turbulent viscosity is obtained via the one-equation turbulence model, in which a transport equation of the subgrid kinetic energy is solved [34]. The filtered reaction rates, resulted from the turbulence-chemistry interaction, are modeled using a multi-scale subgrid turbulent combustion model, namely partially stirred reactor model (PaSR) [35].

The time discretization was handled with the second-order Crank-Nicholson scheme and second-order TVD (total variation diminishing) scheme was used for spatial discretization. The resultant equation system was solved by an in-house solver developed based on the OpenFOAM platform [10, 28, 29, 32, 33].

3.3 Numerical setup

The computational model is shown in Fig.2, where the streamwise and transverse coordinates $\hat{x}$ and $\hat{y}$ are normalized by the combustor length L and height H, respectively. The computational model spans one twentieth (2 mm) of its real width in the spanwise direction resembling the quasi two-dimensional characteristics. The computational grid was generated with block-structured hexahedral cells and local refinements were clustered around the shear layer emanating from the split plate. The shear layer where flame stabilizes is resolved by 61 transverse grid points to capture the turbulent mixing and combustion. The mean and maximum grid sizes in the mixing zone are 0.2 mm and 0.35 mm, respectively. Since the main reaction zone under the present combustor configuration is far away from the combustor walls, it is therefore modelled by slip condition to alleviate the grid resolution requirement near the wall. The grid convergence study has been conducted in our previous work based on three levels of grid refinement [10], and the present study employs the 0.28 million one as a balance between numerical accuracy and computation cost.

Regarding the boundary conditions, fixed pressure, temperature and species composition are specified according to those in Table 1 at both air and fuel inlets.

Turbulent-like inlet is imposed for the velocity inlet boundary in which the mean profile is modulated by white noise perturbation with 5% of its magnitude. Supersonic outflow boundary condition is applied to the combustor exit for all variables. The computational time step is constrained by a maximum Courant number of 0.3 to ensure numerical stability. A typical simulation takes 12 flow-through times ($t_f = L/U_\infty$), among which $8t_f$ are needed to reach the quasi-steady state followed by another $4t_f$ for data sampling and statistics.

4 Results and Discussion

4.1 Influence of the error threshold for DAC

In this section, we will demonstrate the influence of mechanism reduction error threshold value ε_{DAC} on the performance of DAC expedited supersonic combustion simulation using DRGEP mechanism reduction method. Fig. 3 presents the time-averaged pressure field predicted by DAC simulations with various threshold values for a qualitative comparison.

In consideration of the uncertainty in experiment measurement, simulation with the corresponding detailed ethylene chemical mechanism was conducted and serves as the baseline in the present work to offer the exhaustive thermochemical details. As shown in Fig. 3(e), the fuel and air streams undergo expansion and compression respectively after impinging upon each other. The subsequent expansion wave and oblique wave reflect from the upper and bottom walls and then interact at location around $\hat{x} = 0.105$. With combustion heat release, the shock wave is strengthened and impinges on the upper wall at around $\hat{x} = 0.282$ leading to a local high-pressure region. Generally, the other four simulations with various error threshold values faithfully reproduced the pressure contour and associated wave pattern.

Wall pressure predictions with various error threshold values ε_{DAC} are compared against the experimental data in Fig. 4. It is shown that the pressure on the upper wall promptly decreases at the combustor inlet, whereas incidence oblique shock wave on the lower wall increases the local pressure abruptly. After several times of inflections and wave-wave interactions, the strength of the oblique shock wave gradually attenuates as approaching the combustor exit. Quantitatively, pressure distribution on both upper and bottom walls predicted by four levels of ε_{DAC} are indiscernible, and the average relative errors compared to that predicted by detailed mechanism are within 0.2%. Especially, the four simulations with a wide range of ε_{DAC} all faithfully capture the slight pressure decline at $\hat{x} = 0.3$.

To evaluate the accuracy of various ε_{DAC} in predicting the combustor global combustion efficiency, mass fraction profiles of H_2O, CO_2 and CO as well as the temperature profile are probed at the combustor exit. Overall, numerical simulations with various ε_{DAC} values reproduce similar tendency as the detailed mechanism approach for both species and temperature distributions. However, it can be observed that with relative large ε_{DAC} values, the DAC simulations over predicts the peak value of CO mass fraction compared with that by DI calculation in the reacting shear layer as indicated in Fig. 5(b). Further, with the refinement of the error threshold values, the relative error incurred by DAC simulation decreases.

Since the discrepancies amongst various mechanism reduction methods are relatively small, the relative errors in predicting the maximum value for each individual physical property are quantified and summarized in Table 2. It can be found that the relative errors incurred by DAC simulations with various manifest a non-monotonic behavior regarding the ε_{DAC}, and the relative error exceeds 15% when ε_{DAC} is greater than 10^{-4}. This indicates that, for practical scramjet engine simulations with dynamic adaptive chemistry, it is more appropriate to keep the error threshold value ε_{DAC} within 10^{-4}.

Table 2. Relative errors for maximum value prediction by DAC simulation with DRGEP method under various error threshold values..

	$\varepsilon_{DAC} = 10^{-2}$	$\varepsilon_{DAC} = 10^{-3}$	$\varepsilon_{DAC} = 10^{-4}$	$\varepsilon_{DAC} = 10^{-5}$
ε_{H2O}^{max}	0.000	0.000	0.000	0.000
ε_{CO}^{max}	0.018	0.055	0.003	0.018
ε_{CO2}^{max}	0.022	0.012	0.011	0.021
ε_{T}^{max}	0.014	0.005	0.005	0.017

In our previous study [28], it was suggested that the static skeletal mechanism was incapable to accurately reproduce the flame stabilization location even with elaborately devised skeletal mechanism. After coupling the mechanism reduction with fluid flow simulation, the dynamic adaptive chemistry method manifested its superiority in flame dynamic prediction. As shown in Fig. 6 (a-c) two local regions with higher OH concentrations reside around $\hat{x} = 0.31$ and 0.41, which are almost identical to that predicted by the detailed mechanism in Fig. 6 (e). The simulation with the coarsest error threshold value of $\varepsilon_{DAC} = 10^{-2}$ also well reproduces the streamwise locations of these two regions, nevertheless with higher OH concentration quantitatively in the upstream location.

To further scrutinize the prediction accuracy of various mechanism reduction error threshold values, mass fraction of OH are sampled and compared to that simulated with detailed mechanism. The sampling locations are $\hat{x}_A = 0.1$, $\hat{x}_B = 0.2$, $\hat{x}_C = 0.3$ and $\hat{x}_D = 0.4$ along the combustor centerline respectively, which are denoted in Fig. 1. Fig. 7 displays the time-averaged profiles of OH mass fraction predicted under various ε_{DAC} at different streamwise locations. At location A where chemical reactions initiate, the DAC simulations with various levels of ε_{DAC} produce almost identical Y_{OH} distribution. At locations B, the discrepancies among each prediction become noticeable, wherein DAC simulations with $\varepsilon_{DAC} = 10^{-2}$ and $\varepsilon_{DAC} = 10^{-4}$ under predict the peak value of Y_{OH}. Further downstream, the discrepancies between DAC simulations with various error threshold values gradually fade away, while the simulation with $\varepsilon_{DAC} = 10^{-4}$ still attains favorable agreement with the DI calculation.

To assess the accuracy of various ε_{DAC} values in scramjet engine performance evaluation, quasi one-dimensional analyses were performed based on the simulation results. The one-dimensional distributions of physical properties are calculated by mass-weighted averaging on cross-section at each streamwise location. From Fig. 8, simulations with four various error threshold values yield indistinguishable streamwise distributions regarding mass fraction of representative species. It is worth noting that the heat release distribution is decisive for pressure distribution and in turn the propulsion performance of the scramjet engine. As can be observed from Fig. 8(d) that the simulations with dynamic adaptive chemistry method compare favorably with the direct integration of detailed chemistry regardless of when relatively small ε_{DAC} is employed, while large discrepancy will occur under coarse ε_{DAC} values. This again confirms that to accurately predict the engine performance, the ε_{DAC} value should not exceed 10^{-4}.

The aforementioned discussions concern more on the prediction accuracy with various error threshold values within the framework of dynamic adaptive chemistry, however for high-fidelity simulation, the computational efficiency is equally important. Fig. 9 displays the instantaneous number contours of active species obtained using various mechanism reduction methods. Fig. 9 (a) exemplifies the spatial distribution of local reactivity in the combustor, which is characterized by the number of active species obtained by DRGEP method based on local and instantaneous thermochemical conditions. Based on the distribution of N_{asp}, the entire combustor can be roughly divided into three regions, the fuel-rich region (mainly the fuel stream) near the upper wall, the fuel-lean region (mainly the air stream) near the bottom wall, and the reacting shear layer between these two streams. In the fuel-rich region, the chemical reactivity is predominately controlled by the fuel pyrolysis reaction under intermediate temperature, wherein the fuel converts into smaller hydrocarbons or radicals and involves many more reactions than in the combustion stage [36]. On the contrary, chemical reactions in the fuel-lean region can be faithfully represented by a small number of active species as the reaction can hardly occur in the vitiated air stream. In the shear layer, the mixing between mixtures and subsequent reaction occurs around a favorable local equivalence ratio, which yields high combustion temperature and can be characterized by active species in a number of 10 to 20. Regarding the spatial distribution of the active species, the DAC simulation with $\varepsilon_{DAC} = 10^{-4}$ resembles that with $\varepsilon_{DAC} = 10^{-5}$ both qualitatively and quantitatively. However, when increases the ε_{DAC} value, the number of active species in fuel rich stream decreases remarkably whereas decrease of N_{asp} in the vitiated air stream is relatively small.

For qualitative comparison, the domain averaged number of active species N_{asp} is exhibited in Fig.10 which is a direct representative of the overall computational load. It is shown that with tighter error threshold ε_{DAC}, the more active species are retained in the on-the-fly reduced chemical mechanisms. With the moderate ε_{DAC} value (10^{-3}), the number of active species is around 24, which achieves a remarkable reduction in species number compared to the detailed one (54 species). We also note that, for each ε_{DAC} value, fluctuation in active species number is always discernable. This indicates that, even in the steady state, the flame stabilization is a highly dynamical process being closely coupled with complex chemical kinetics.

The corresponding computational efficiency comparisons are displayed in Fig. 11. The computational speedup factor is calculated as

$$\chi_{su} = \frac{\tau_{DI}}{\tau_{DAC}} \tag{9}$$

where τ_{DI} and τ_{DAC} are the mean CPU times over simulations with detailed mechanism and dynamic adaptive method, respectively.

Regarding the computational efficiency, Fig. 11 shows the CPU times for each DAC simulation with various ε_{DAC}. Specifically, the CPU time consumption in chemical reaction calculation for dynamic adaptive chemistry approach can be divided into two main components, including the time for mechanism reduction and the time for solution of the subsequent ODE of the skeletal mechanism. It is interesting to find that the computational overhead incurred by the mechanism reduction process is almost unchanged under a wide range of ε_{DAC}. The computational speedup is more likely to be squeezed from the computational time for a size-reduced stiff ODE system. The simulation with DRGEP and $\varepsilon_{DAC} = 10^{-3}$ achieves a computational speedup factor $\chi_{su} = 3.17$, while 4.33 and 3.19 folds of speedup factors are obtained with coarser and tighter error threshold values of 10^{-2} and 10^{-4}, respectively.

Based on the above discussion, the DAC simulation with $\varepsilon_{DAC} = 10^{-4}$ performs favorably regarding both the numerical accuracy and computational efficiency. Thus, the investigation of other influential factors including the mechanism reduction method and the search initiating species will retain this configuration.

4.2 Synergetic influence of mechanism reduction method and error threshold

In this section, we will demonstrate the influence of mechanism reduction methods under error threshold value $\varepsilon_{DAC} = 10^{-4}$ on the performance of DAC expedited supersonic combustion simulation. Fig. 12 presents DAC synergized simulations with four mechanism reduction methods including DRG, DRGEP, DAC-L and PFA. This proves the efficacy of various mechanism reduction methods in dynamically adjusting the local representative skeletal mechanism based on instantaneous and local thermochemical properties, wherein all the DAC simulation could qualitatively reproduce the species' and temperature' distributions at the combustor exit with reasonable accuracy.

Table 3. Relative errors for maximum value prediction with various mechanism reduction methods.

	DRG	DRGEP	DAC-L	PFA
ε_{H2O}^{max}	0.000	0.000	0.000	0.000
ε_{CO}^{max}	0.080	0.003	0.012	0.022
ε_{CO2}^{max}	0.026	0.011	0.000	0.026
ε_{T}^{max}	0.015	0.005	0.006	0.012

Table 4 summarizes the relative errors for maximum value prediction by DAC simulation with various mechanism reduction methods. It can be found that the DAC-L method attains the best prediction accuracy in both temperature and species concentrations. Despite it considers formation and consumption fluxes of species at multiple generations in species dependency calculation, the PFA method incurs the largest relative error in predicting species mass fractions of CO and CO_2.

In Fig. 13(a), OH species mainly concentrate around the shear layer between two streams, however in very low mass fraction ($Y_{OH}{\sim}10^{-5}$), which indicates the initiation of oxidation reactions. At location B as shown in Fig. 13(b), the mass fraction of OH increases significantly and reaction zone becomes wider. Among the four mechanism reduction methods, DAC-L and DRGEP methods show reasonable good agreement with the detailed mechanism, while DRG and PFA methods slightly underpredict the peak value of OH mass fraction. At location C, all mechanism reduction methods produce similar results as the detailed mechanism method. Further downstream, at location D, OH mass fraction calculated by DRGEP method again shows good agreement with that by detailed mechanism. However, the PFA method overshoots the peak value in OH mass fraction at the fuel lean side.

Regarding the spatial distribution of the active species in Fig.14, the DRGEP method resembles the DRG method both qualitatively and quantitatively. In the simulation with the DAC-L method, the number of active species in the fuel-lean region and the reacting shear layer is slightly larger than that in the DRG and DRGEP methods. However, a remarkable difference can be found in the PFA method when compared to the other three counterparts, as the fuel rich region possesses around 44 active species, while the number of active species approximates the detailed mechanism (54 species) in the reacting shear layer. For qualitative comparison, the temporal evolution of the domain averaged active species number is exhibited in Fig. 15. The DRGEP method produces the least number of active species, which is consistent with the observation in Fig 14. In the simulation with the DAC-L method, the resultant N_{asp} is around 33.5, which is relatively larger than that produced by DRG and DRGEP method. This should be attributed to the fact that the influence of removing a species group is neglected in the DAC-L method compared to DRGEP method. The dynamic adaptive chemistry simulation employing the PFA method results in a much larger N_{asp} compared to the other three methods. This phenomenon can be reasonable explained by that the mechanism reduction in PFA method involves chemical information from multi generations, hence renders a larger reaction network

As for the overall computational efficiency, as shown in Fig. 16, the CPU time for solving the ODE on a reduced-scale system consumes just a quarter of the original calculation with the detailed chemistry (DI case), while the mechanism reduction incurs overhead which is about 30% of the total computational load. Therefore, the overall computational speed-up factor achieves 2.82 to 3.72 depending on the adopted mechanism reduction method.

It is worth noting that the definition of the threshold is different for the different mechanism reduction methods. So it isn't fair to compare them keeping the same threshold values. Thus, we conducted as sweep across all possible combinations of mechanism reduction methods and error threshold values to investigate their synergetic effect. As present in Fig. 17, the DAC simulation with DRGEP and $\varepsilon_{DAC} = 10^{-4}$ yields the best balance between the computational cost and numerical accuracy.

4.3 Influence of the search initiating species

Further, from the essence of the DRG-based mechanism reduction method, the search initiating species is decisive to the resultant reaction network as the related relation graph is constructed starting from the SIS set. In the present work, two typical SIS sets including the stable reactant combination as C_2H_4, O_2 and N_2 denoted as Stable-SIS, and C_2H_4 as well as intermediate species such as CO, HO_2 which is denoted as Inter-SIS. It should be noted that, the DRGEP-based DAC simulations in this section are conducted under a relative tight error threshold of 10^{-4}.

Fig. 18 demonstrates the influence of the SIS on the prediction of species mass fractions and temperature at the combustor exit. Analogous to those in Fig. 5 and 12, the most notable discrepancy is again found in the CO mass distribution. As summarized in Table 4, the Stable-SIS induces 0.8% relative error in CO prediction, which is nearly 0.5% higher than that by Inter-SIS simulation. Furthermore, the simulation with Inter-SIS achieves much lower relative errors compared to those predicted by Stable-SIS regarding CO_2 mass fraction and temperature distributions.

Table 4. Relative errors for maximum value prediction by DAC simulation with DRGEP method and various SIS combinations.

	ε_{H2O}^{max}	ε_{CO}^{max}	ε_{CO2}^{max}	ε_{T}^{max}
Stable-SIS	0.000	0.008	0.024	0.018
Inter-SIS	0.000	0.003	0.011	0.005

As can be seen from Fig. 19 (a), (b) and (c), the influences of SIS at upstream locations are marginal compared to that induced by mechanism reduction method and error threshold value. However, the effect of SIS becomes more pronounced at downstream location D, where the Stable-SIS simulation significantly overpredicts the maximum value of OH mass fraction. By parsing through the directed relation graph constructed at this location, it is recognized that two elementary reactions $\mathrm{R25{:}\ OH + CO \rightleftharpoons CO_2 + H}$ and $\mathrm{R14{:}\ OH + HO_2 \rightleftharpoons H_2O + O}$ are excluded from the local skeletal mechanism built based on the Stable-SIS. Hence, the consumption rate of the OH radical at location D is attenuated compared to that based on Inter-SIS.

The contours of active species number N_{asp} obtained with Inter-SIS and Stable-SIS are displayed in Fig. 20. It is obvious that the N_{asp} of Stable-SIS is smaller than that obtained by Inter-SIS in the entire combustor including both the fuel-rich and the fuel-lean streams. Especially, in the fuel-rich stream, the DAC simulation with Stable-SIS needs 30-40 active species while that with Inter-SIS requires another 10 more species. This tendency is further quantified in Fig. 21, which shows that the DAC simulation with Inter-SIS overall requires around 29 species, and the Stable-SIS simulation needs 24 active species. Correspondingly, the Inter-SIS combination is more computational demanding than the Stable-SIS as displayed in Fig. 22. It is worth noting that the computational overhead for mechanism reduction is comparable for both SIS combinations, while the Inter-SIS needs 15% more CPU time to solve the resultant stiff-ODE.

5 Concluding remarks

The dynamic adaptive chemistry (DAC) augmented large eddy simulation of supersonic combustion in ramjet engine was realized in this study. The influences of mechanism reduction method, mechanism reduction threshold value and search initiating species were systematically evaluated in a unified framework. Numerical validation was first conducted against experimental measurement and the simulation results obtained by direct integration of detailed mechanism were employed to assess the accuracy and computational efficiency of DAC simulations with various configurations.

Based on our comprehensive assessment, four mechanism reduction methods are all found to be adequate for wall pressure and combustor's global metrics predictions. However, for detailed flame stabilization characteristics, the DRG, DEGEP and DAC-L methods attain comparable prediction accuracy in radical's distribution, while the prediction by PFA method shows relatively large relative error. Among all these four mechanism reduction methods, the DRGEP method obtains relatively better balance between the numerical accuracy and computational efficiency, whereas the PFA is the most computational demanding one.

As the mechanism reduction error threshold value increases, the relative errors in predicting intermediate species also increase. It is found that the computational overheads for mechanism reduction under various error threshold values remain almost unchanged, and the overall computational efficiency is mainly determined by the CPU time for solving the size-reduced skeletal mechanisms. And for high fidelity simulation of supersonic combustion, it is necessary to keep the ε_{DAC} within 10^{-4} to ensure that the relative error in radical mass fraction prediction does not exceed 15%. Regarding the search initiating species, the stable species combination including fuel, O_2 and N_2 produces larger relative error in radicals' concentration prediction than the combination including fuel and intermediate species HO_2 and CO. However, the latter is less computational efficient than the former as it needs 15% more CPU time to solve the stiff ODE system of the resultant skeletal mechanism.

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7 Reference

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