

Combustion Mechanism Modelling of Ethylene and Its Application in Numerical Study of High Speed Turbulent Combustion *

GONG Chun-ming, LIU Jian-wen, GUO Jin-xin, ZHANG Bo

(Science and Technology on Scramjet Laboratory, Beijing Power Machinery Institute, Beijing 100074, China)

Abstract: In order to obtain a combustion mechanism suitable for modelling high-speed turbulent combustion of ethylene, detailed combustion mechanism construction, mechanism reduction and turbulent combustion simulation were performed in the present work. The detailed combustion mechanism of ethylene considering pressure-dependent reactions was first developed based on the hierarchical method. A 24-species reduced kinetic mechanism for ethylene combustion was then systematically developed from the detailed mechanism through mechanism reduction with a directed relation graph (DRG) and time scale reduction based on quasi-steady state assumptions (QSSA). Error of the worst-case for auto-ignition with the reduced mechanism is 17%, while the average error is less than 7%. Three-dimensional simulations were carried out for cavity-stabilized flames covering fuel-lean and fuel-rich conditions by implementing the reduced mechanism in the commercial software, Fluent. The numerical results showed that the reduced mechanism obtained in the present work can accurately compute heat release of ethylene combustion and well reproduce the static pressure profile for different equivalence ratios with an average error less than 10%. The reduced mechanism developed with high chemical fidelity can be adopted for high speed turbulent combustion simulations in propulsion systems.

Key words: Detailed mechanism; Skeletal mechanism; Reduced mechanism; Numerical simulation; Turbulent combustion

CLC number: V312+.1 **Document code:** A **Article number:** 1001-4055 (2020) 03-0582-13

DOI: 10.13675/j.cnki.tjjs.190479

乙烯燃烧反应机理建模及其在高速湍流燃烧仿真中的应用

巩春明, 刘建文, 郭金鑫, 张 波

(北京动力机械研究所 高超声速冲压发动机技术重点实验室, 北京 100074)

摘 要: 为了得到一个适用于高速湍流燃烧数值模拟的乙烯燃烧机理, 开展了乙烯燃烧详细机理构建、简化及高速湍流燃烧数值模拟工作。基于分层方法并考虑压强相关反应, 首先构建了乙烯的燃烧详细反应机理。通过采用直接关系图法 (DRG) 以及准稳态假设法 (QSSA) 的简化方法, 从详细反应机理系统简化得到了24物种的简化机理。由简化机理计算的点火延迟时间跟详细机理相比最大误差17%, 平均误差小于7%。将简化机理耦合到商业软件Fluent, 开展了覆盖贫油和富油条件下凹槽构型燃烧室

* 收稿日期: 2019-07-09; 修订日期: 2019-09-07。

作者简介: 巩春明, 博士, 工程师, 研究领域为燃烧反应机理构建及超声速燃烧数值模拟。E-mail: 154552485@qq.com

通讯作者: 张 波, 博士, 研究员, 研究领域为先进发动机设计及数值模拟。E-mail: zhangbo31s@qq.com

引用格式: 巩春明, 刘建文, 郭金鑫, 等. 乙烯燃烧反应机理建模及其在高速湍流燃烧仿真中的应用[J]. 推进技术, 2020, 41(3): 582-594. (GONG Chun-ming, LIU Jian-wen, GUO Jin-xin, et al. Combustion Mechanism Modelling of Ethylene and Its Application in Numerical Study of High Speed Turbulent Combustion [J]. *Journal of Propulsion Technology*, 2020, 41(3):582-594.)

的三维数值模拟。数值模拟结果表明,所构建的简化机理能够准确地预测乙烯燃烧释热,可以很好地再现不同当量比条件下静压曲线,平均误差小于10%。该简化机理具有较高的化学保真度,可以应用于推进系统中的高速湍流燃烧模拟。

关键词: 详细机理; 骨架机理; 简化机理; 数值模拟; 湍流燃烧

1 Introduction

Hydrocarbon fuels are usually used as main propellant in propulsion systems for its high volumetric energy content as well as convenient storage and ease of transportation, though ignition delay time of a hydrocarbon fuel is longer than that of hydrogen. As a gaseous hydrocarbon fuel, ethylene has both great energy per unit volume (59.4MJ/m^3) and the advantage of easier storage and handling. Moreover, ethylene is also one of the most abundant thermal decomposition products of aviation kerosene^[1]. Therefore, much attention has been paid to turbulent combustion process of ethylene fueled engines. Up to now, many experimental studies have been carried out for ethylene combustion in high-speed turbulent flow. These studies include ignition and sustained combustion characteristic, combustion and flame dynamics, and vitiation effects on ethylene turbulent combustion characteristics.

Except experimental studies, due to the rapid development of computational fluid dynamics (CFD), numerical simulations on turbulent combustion process of ethylene in advanced aeroengines are also performed. The numerical results of turbulent reactive flows are highly related to the turbulent model, the turbulent combustion model and the chemical reaction model, etc. Generally, the so called “stiff problem” will be caused when incorporating the detailed chemical mechanism in CFD simulation. Thus, one-step^[2-3] or multi-step^[4] overall reaction models of ethylene are often used in large-scale numerical simulations. However, these overall reaction models can't be used to describe the unsteady process such as ignition and extinction. Moreover, as a result of ignoring important radicals and intermediate forming from fuel combustion, the heat release and temperature computed by the overall reaction models are usually higher. Though the kinetic parameters and reaction order of these overall reaction models are generally fitted from experimental results, they are highly dependent on specific experimental conditions and

thus with severely restricted applicability. Thus, the importance of incorporating more complex chemical kinetic models in turbulent reactive flows has been recognized and the reduced reaction models developed from detailed kinetic models are gradually used in numerical simulations of large-scale turbulent reactive flows^[5].

For kinetic modelling study of ethylene combustion to compute ignition delay time and laminar flame speed, two detailed kinetic mechanisms AramcoMech 1.3^[6] and USC Mech 2.0^[7] are widely used. Moreover, these two mechanisms are also used as the core mechanism for developing detailed combustion mechanisms for large-molecular-weight hydrocarbon fuels. Compared to USC Mech 2.0^[7], AramcoMech 1.3^[6] has considered much more pressure-dependent rate constants and chemical-activated reaction pathways. However, many more theoretical studies on pressure-dependent rate coefficients with high-accuracy have been reported in the literature. And these rate coefficients aren't considered in AramcoMech 1.3^[6]. Thus, the reaction channels and rate coefficients obtained from these theoretical studies can further improve the computation of ignition delay time and laminar flame speed of ethylene combustion under a wide range of temperatures and pressures.

In general, the detailed mechanism of hydrocarbon fuel contains a large number of species and reactions involving different time scales which will cause the stiff problem. In order to reduce the computation cost and the stiff problem in numerical simulation of turbulent reactive flows, the detailed mechanism has to be reduced by eliminating unimportant species and reactions. As shown in the review of Lu et al.^[8], the process of detailed mechanism reduction mainly includes skeletal reduction, isomers lumping and time-scale analysis. Skeletal mechanism reduction methods include directed relation graph (DRG)^[9], DRG EP^[10], path flux analysis (PFA)^[11], principal component analysis (PCA)^[12], computational singular perturbation (CSP)^[13], level of importance (LOI)^[14], level of connection (LOC)^[15], global pathway selection (GPS)^[16], flux projection tree

(FPT)^[17], approximate trajectory optimization algorithm (ATOA)^[18], sensitivity analysis (SA)^[19] and so on. Time-scale analysis reduction approaches include rate-controlled constrained-equilibrium (RCCE)^[20], intrinsic low dimensional manifold (ILDM)^[21], quasi-steady-state assumptions (QSSA)^[22] and so on. For ethylene combustion mechanism reduction, PFA, PCA and ATOA are applied to obtain skeletal mechanism by Yu et al.^[23], Esposito et al.^[12] and Liu et al.^[18], respectively. Li et al.^[24] systematically reduce ethylene combustion mechanism by combining DRGEP^[10], PFA, SA and QSSA methods, and the final reduced mechanism reproduce satisfactory auto-ignition delay times. Jiang et al.^[15] apply LOC and QSSA to reduce ethylene combustion mechanism and choose a premixed flame structure as targets to verify the skeletal and reduced mechanism. The results show that calculations from the skeletal and reduced mechanism agree well with those from the detailed mechanism. It should be mentioned that the skeletal mechanism obtained is still based on elementary reaction steps after eliminating unimportant species and reactions by skeletal reduction, whereas the final reduced mechanism obtained after isomers lumping and QSSA is in the overall reaction form. In numerical simulations of turbulent reactive flows in high speed, the turbulent combustion model like flamelet models^[25] can incorporate the skeletal mechanism to simulate turbulent combustion, while the more time consuming model eddy dissipation concept (EDC)^[26] can incorporate the reduced mechanism in the overall reaction form to improve computational efficiency.

In the present study, a detailed kinetic model consisting of 153 species and 1435 reactions for ethylene combustion under a wide range of pressures and temperatures is developed based on USC Mech 2.0^[7], AramcoMech 1.3^[6] and recent quantum chemical studies at first. Then, mechanism reduction is performed by combining DRG, SA and FPT to derive a skeletal mechanism, which consists of 42 species and 207 reactions. After further reduced by QSSA, a 24-species reduced mechanism with 20 lumped global reactions is obtained. Finally, the 24-species mechanism is implemented into commercial software Fluent 13.0 to perform numerical simulations of ethylene combustion at different equivalence

ratios in a model combustor. The purpose of the present study is to develop a reduced mechanism of ethylene combustion and incorporate it in large-scale turbulent combustion simulations.

2 Detailed mechanism development and reduction

2.1 Detailed mechanism development

The detailed kinetic mechanism of ethylene is developed based on the hierarchical method^[27], which consists of C₀~C₄ chemistry. The hierarchical structure of the mechanism is mainly based on the specific potential energy surface (PES) as shown in Figure 1. CH₂, C₂H₄, C₂H₃O₂ and so on do not represent chemical compounds, each of them represents the specific PES that is determined by the number of carbon, hydrogen and oxygen atoms involved in the reaction. The PESs with same carbon number are clarified into C_x chemistry (x=0, 1, 2, 3, 4). Each PES consists of several reaction channels, through considering important reaction channels on each PES and combining different PESs, the final reaction network is obtained. The rate coefficients of pressure-dependent reactions of important reaction channels are mainly from high-accuracy quantum chemical calculations and theoretical kinetic studies in literature. It should be mentioned that no rate coefficients are tuned to make the computed results agree well with experiments. The thermochemical properties of species involved on the PESs come mainly from high-accuracy *ab initio* calculation results of Goldsmith et al.^[28], and transport data are taken from AramcoMech 1.3^[6]. At this point, the detailed kinetic model of ethylene combustion consisting of 153 species and 1435 reactions is obtained. It is not feasible to discuss each reaction contained within the mechanism, the reactions considered can be simplified into four main reaction classes: (1) isomerization, (2) dissociation/recombination, (3) chemical activated reactions and (4) hydrogen abstraction. The first three reaction classes are pressure-dependent and the fall-off of the rate constants for these reactions are considered.

The detailed kinetic model of ethylene combustion consisting of 153 species and 1435 reactions is first validated against experimental results. Laminar flame

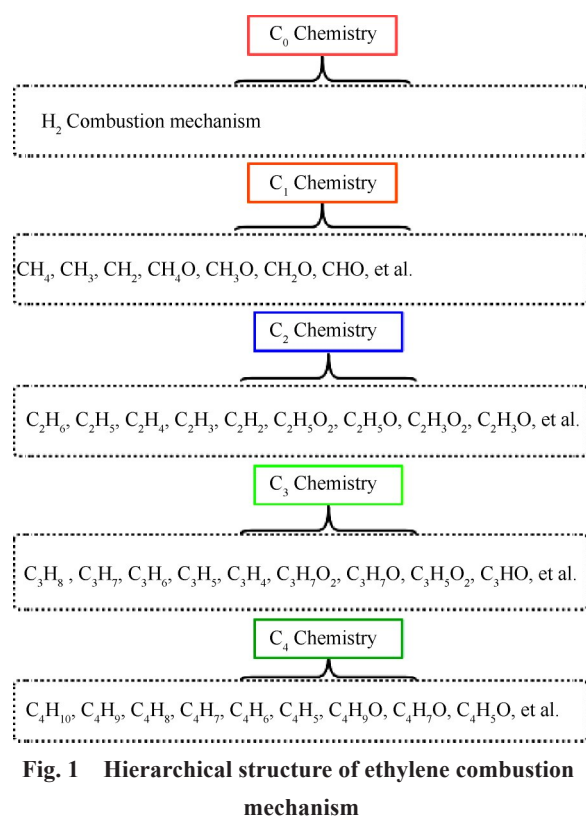


Fig. 1 Hierarchical structure of ethylene combustion mechanism

speeds, ignition delay times, species profiles and premixed flame structures are chosen as targets for validation. Numerical modelling of ignition delay time and species profile are performed using 0-D (zero-dimensional) reactor, while laminar flame speed and flame structure are simulated by the flame speed calculator from Chemkin-Pro. There have been many experimental studies covering different types about ethylene combustion and oxidation in literature, and only some represented results are used to validate the kinetic model in the present work.

The experimental results^[29-31] of laminar flame speed over a wide range of equivalence ratios from 0.6 to 1.8 are applied to validate the mechanism. Here, the equivalence ratio, φ is defined as the ratio of the actual fuel/oxidizer ratio to the fuel/oxidizer ratio in the stoichiometric equation. During the simulation of laminar flame speed, the thermo-diffusion (Soret effect) is taken into account, and multicomponent transport properties and trace species approximation are used. Figure 2 depicts experimental and computed laminar flame speeds. It can be found that the computed results are in good agreement with all the three experimental results at fuel-lean conditions. At fuel-rich conditions, the com-

puted results are higher than the experimental results of Ravi et al.^[29] and Park et al.^[30], but close to those of Hirasawa et al.^[31]. The experimental results are obtained in counterflow flame by Park et al.^[30] and Hirasawa et al.^[31], and in outwardly propagating spherical flame by Ravi et al.^[29], respectively. Given the uncertainty in experimental measurements and the rate constants in the mechanism, the computed results are acceptable.

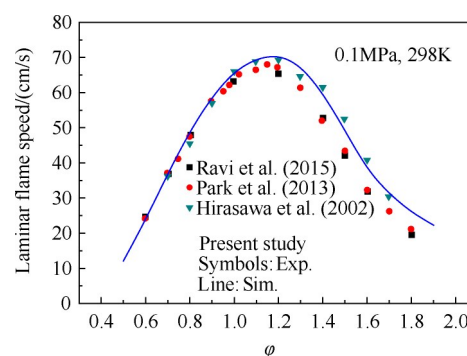


Fig. 2 Comparison of experimental and computed laminar flame speeds

In order to validate the mechanism over different equivalence ratios, auto-ignition simulations are performed for $\varphi=0.5$, 1.0 and 2.0. The shock-tube measurements of ethylene/air mixtures by Penyazkov et al.^[32] in the temperature range of 1060K~1520K, pressures of 0.59MPa~1.65MPa, and equivalence ratios of $\varphi=0.5$, 1.0, and 2.0 are taken for validation. In the present study, ignition delay time is defined by the location of the maximum OH concentration gradient. Comparisons between the experimental data and the simulation results are shown in Figure 3. It can be found that the scatter of the ignition delay time characterized by CH, C₂ and pressure from experimental measurements is obvious especially at high temperatures. And there are some errors for fuel-lean conditions especially at low temperatures and the errors decrease with the equivalence ratio increasing. Overall, the present mechanism accurately reproduces the ignition delay times of ethylene over the experimental temperature range and captures the pressure dependence of ignition delay time.

The experimental species profile used for validation are from Hidaka et al.^[33], who studied the oxidation of ethylene behind reflected shock waves in the tempera-

ture range 1100K~2100K at pressures 0.15MPa~0.45MPa with reaction times varying between 1.39ms and 2.66ms. The initial reactant composition is 0.6% C_2H_4 , 0.3% O_2 and 99.1% Ar. Figure 4 shows the comparison between computed results and experimental measurements. $[M]$ is the concentration of reactant or products at the specific time. $[C_2H_4]_0$ is the initial ethylene concentration. As can be seen, the computed results reproduce concentration of the major products and ethylene as a function of temperature satisfactorily.

The flame structure of ethylene combustion is validated over two equivalence ratios. The experimental results for fuel-lean ($\phi=0.5$) and fuel-rich ($\phi=1.7$) premixed ethylene flame at atmospheric pressure studied by Delfau et al.^[34] and Gerasimov et al.^[35] are taken for validation, respectively. Figure 5 depicts comparisons

between experimental data and computed results. As seen, the mechanism reproduces well reactants consumption and main products formation of the lean ethylene flames. Measured and simulated mole fraction profiles of reactants and major products (CO , CO_2 , H_2 , H_2O) for fuel-rich are shown in Figure 6. One can conclude that the reaction mechanism well reproduces the mole fraction profiles of reactants, as well as H_2 , H_2O and CO_2 in the flame, except for the mole fraction of CO . In the determination of the carbon material balance in the post-flame zone, carbon-containing products other CO and CO_2 were not taken into account by Gerasimov et al.^[35]. Thus, the experimental measurement of CO and H_2O is higher than those of calculations.

Overall, from the above validations of laminar flame speed, ignition delay time and flame structure, it

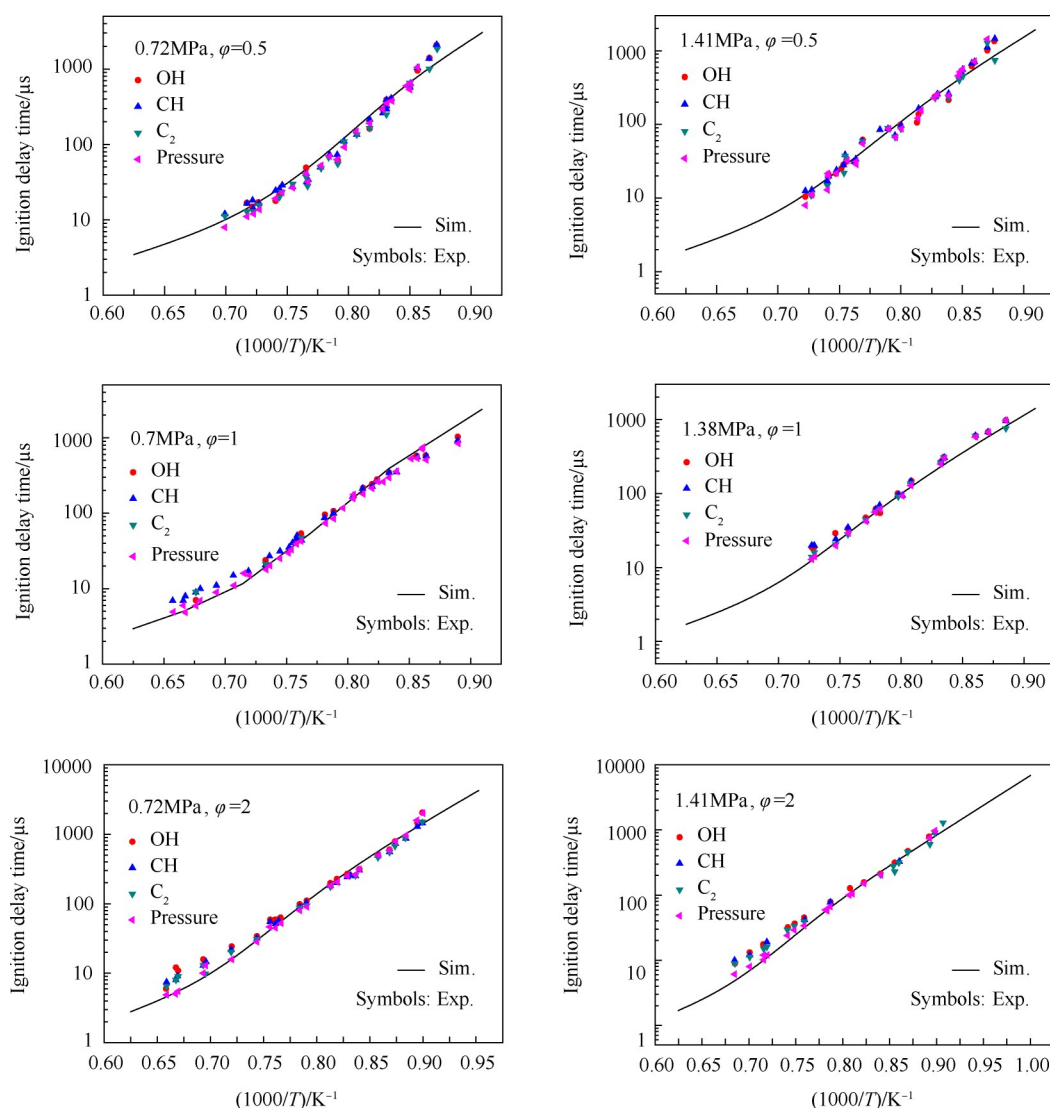


Fig. 3 Comparisons of computed and experimental ignition delay times of ethylene in air

can be concluded that the mechanism developed in the present work is capable of computing combustion characteristics of ethylene for a wide range of temperatures and equivalence ratios. Thus, the detailed mechanism is used for mechanism reduction in the following.

2.2 Mechanism reduction

The mechanism reduction for ethylene is performed using the DRG method^[9], which is often used as the first step in the generation of a skeletal mechanism. The conditions of DRG reduction are performed at equivalence ratios 0.5, 1.0 and 1.5, pressures 0.1MPa, 0.5MPa and 1.0MPa, temperatures 900K to 2000K. The

starting species of DRG reduction are selected as C_2H_4 , O_2 , CO_2 , H_2O , CO . In order to further remove species and reactions, the FPT method^[17] is utilized. A sequence of threshold values from 0.1 to 0.45 with a step of 0.05 are adopted for DRG reduction, and another sequence of threshold values from 0.01 to 0.03 with a step of 0.005 are chosen for FPT. Finally, the SA method^[19] is used to further delete unimportant reactions and a threshold value of 0.05 is found proper to obtain a skeletal with good fidelity. The final skeletal mechanism consists of 42 species and 207 reactions. The computed results by the skeletal and reduced mechanism are given in Fig-

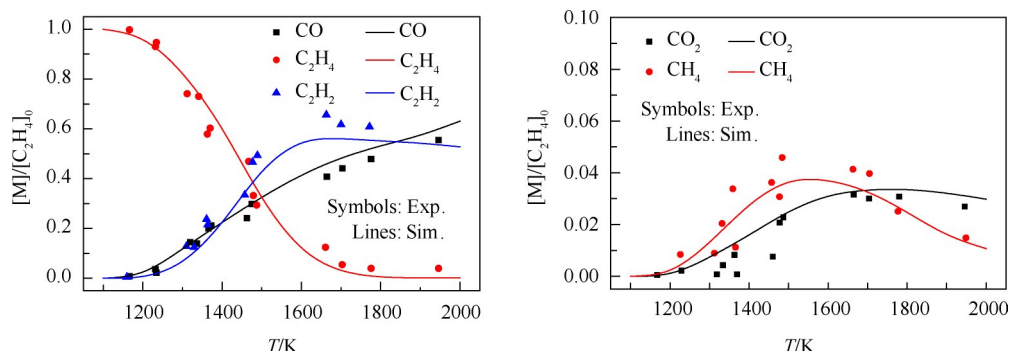


Fig. 4 Comparison of experimental and computed species profile

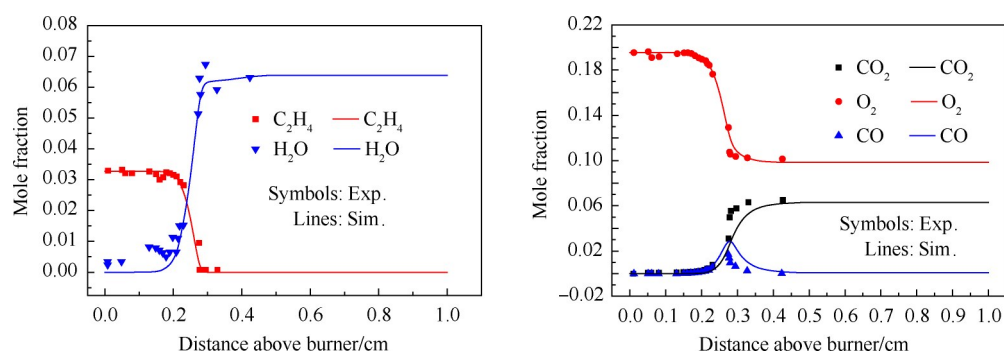


Fig. 5 Mole fractions of reactants and major products in ethylene flames ($\phi=0.5$)

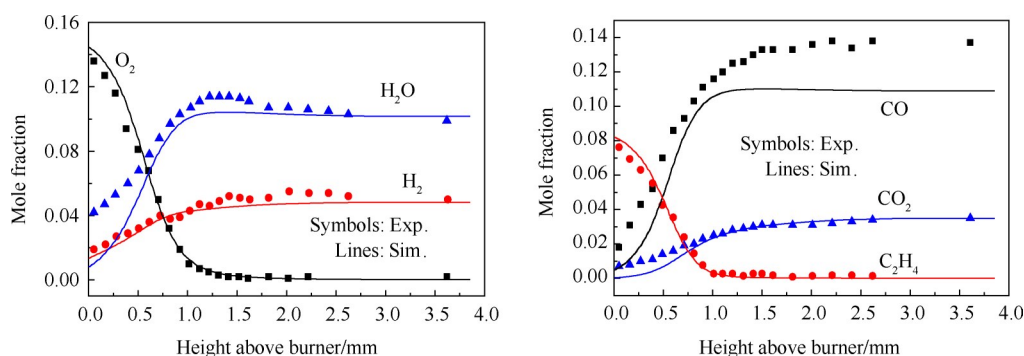


Fig. 6 Mole fractions of reactants and major products in ethylene flames ($\phi=1.7$)

ure 7 and 8. The species concentration profiles and ignition delay time calculated by the skeletal mechanism are closed to those calculated by the detailed mechanism. This indicates that the important species and reaction pathway are retained in the skeletal mechanism. Thus, the skeletal mechanism with 42 species and 207 reactions are used for further reduction by QSSA^[22].

After validation of skeletal mechanism, we have performed global reduction. Based on the skeletal mechanism, CSP method^[13] is used to obtain QSS species from simulation results at pressure 0.1MPa and 0.5MPa, equivalence ratios 0.5, 1.0 and 1.5, temperatures 1200K and 1600K. QSSA is applied to 18 species, resulting in a 24-species reduced mechanism with 20 global reactions shown in Table 1.

The reduced mechanism is validated for flame structure and auto-ignition, as shown in Figure 7 and 8. The validation covers fuel-lean and fuel-rich conditions that used in large scale simulation in the next section. As seen in Figure 7, two equivalence ratios 0.8 and 1.2 are validated and the flame structure computed by the reduced mechanism is closed to that by the skeletal and detailed mechanism. The maximum error is CO concentration computed at equivalence ratio 1.2 and the overall results computed by the reduced mechanism are acceptable. The ignition delay times are validated in the temperature range of 1000K to 1800K and a pressure of 0.25MPa, which corresponds to the static pressure in the model combustor used in the present study. As

seen, except for the maximum error appearing at the low temperature of 1100K, the ignition delay times computed by both the reduced mechanism and the skeletal mechanism are very close to those by the detailed mechanism. Error of the worst-case for auto-ignition with the reduced mechanism is 17%, while the average error is less than 7%. Thus, the reduced mechanism is utilized in large-scale numerical study of ethylene combustion in the model combustor.

3 Numerical simulation and discussion

The model combustor considered in the present work is taken from the model experimentally studied by Zhong et al.^[36] and is shown in Figure 9. It consists of four sections, a nearly constant area section of 674mm followed by three expansion sections (I, II and III). The length of three expansion sections is 480mm, 702mm and 344mm, respectively. Two parallel cavities located in section I and the section of the combustor is 54.5mm × 75mm at the entry. The present calculation has been carried out on a half geometry based on symmetry consideration, ethylene is injected from one and a half orifice located both on the upper and lower side-wall. The inlet stagnation conditions and equivalence ratios are given in Table 2. Vitiated air with mass fractions of 23.3% O₂, 5.9% H₂O, 9.6% CO₂ and 61.2 % N₂ is considered in the calculation.

The computations are performed using the commercial software Fluent 13.0. Two-equation, shear stress

Table 1 24-species reduced mechanism of ethylene

Species	H, H ₂ , O, O ₂ , OH, H ₂ O, HO ₂ , H ₂ O ₂ , CH ₃ , CH ₄ , CO, CO ₂ , CH ₂ O, CH ₂ CO, CH ₂ CHO, CH ₃ CHO, C ₂ H ₃ OH, cC ₂ H ₄ O, C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₅ , aC ₃ H ₅ , C ₃ H ₆ , N ₂		
Reactions	H+O ₂ =O+OH	2H+2CO=O ₂ +C ₂ H ₂	H ₂ +O=H+OH
	H+OH=H ₂ O	H ₂ +OH+CO=O ₂ +CH ₃	H+CH ₃ =CH ₄
	OH+CO=H+CO ₂	H+O ₂ +C ₂ H ₂ =O+CH ₂ CHO	CH ₃ CHO=H+CH ₃ +CO
	H+C ₂ H ₄ =C ₂ H ₅	O ₂ +C ₂ H ₄ =2H+H ₂ +2CO	cC ₂ H ₄ O=CH ₃ CHO
	2HO ₂ =O ₂ +H ₂ O ₂	O+CH ₂ O=H+OH+CO	C ₂ H ₃ OH=H+CH ₃ +CO
	H ₂ +OH=H+H ₂ O	H+OH+2CO=O ₂ +CH ₂ CO	C ₃ H ₆ =H+aC ₃ H ₅
	H+O ₂ =HO ₂	O ₂ +C ₃ H ₆ =O+CH ₃ +CH ₂ CHO	

Table 2 Inlet conditions used in numerical simulations

<i>Ma</i>	<i>T</i> ₀ /K	<i>p</i> ₀ /MPa	Mass flow rate (air)/(kg/s)	<i>T</i> _{fuel} /K	Equivalence ratio
3.46	1430	3.6	1.71	300	0.62, 0.76, 0.86, 1.07

transport (SST) $k-\omega$ model developed by Menter^[37] is implemented with default values. The EDC model^[26] is used to model the turbulence-chemistry interaction which takes into account the influence of both the kinetic model and turbulence on the reaction rates. The species and reaction rates of the final reduced mechanism are defined in user-defined function (UDF) in order to

be utilized in Fluent 13.0. The in situ adaptive tabulation (ISAT) algorithm proposed by Pope^[38] is adopted to accelerate integrations to reduce the computational cost. The total nodes of the grid are 3million. Moreover, in order to improve local numerical precision, the mesh is refined in areas such as wall, cavity, and shear layer.

In the present numerical simulation, four equiva-

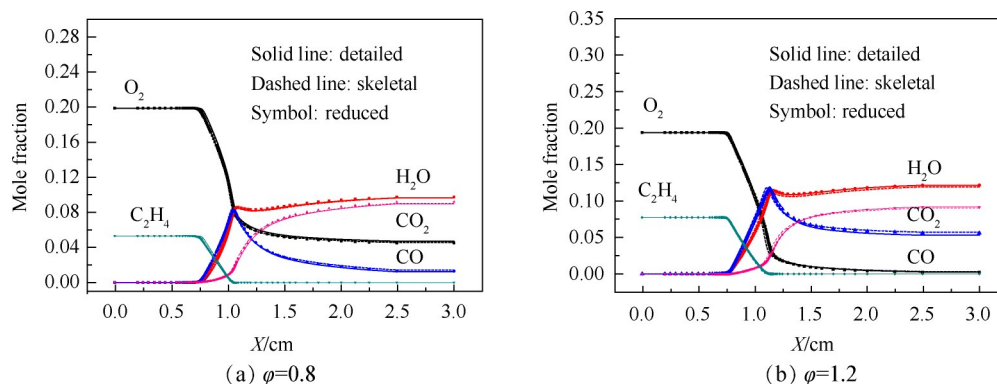


Fig. 7 Comparisons of flame structure computed by detailed mechanism, skeletal mechanism and reduced mechanism

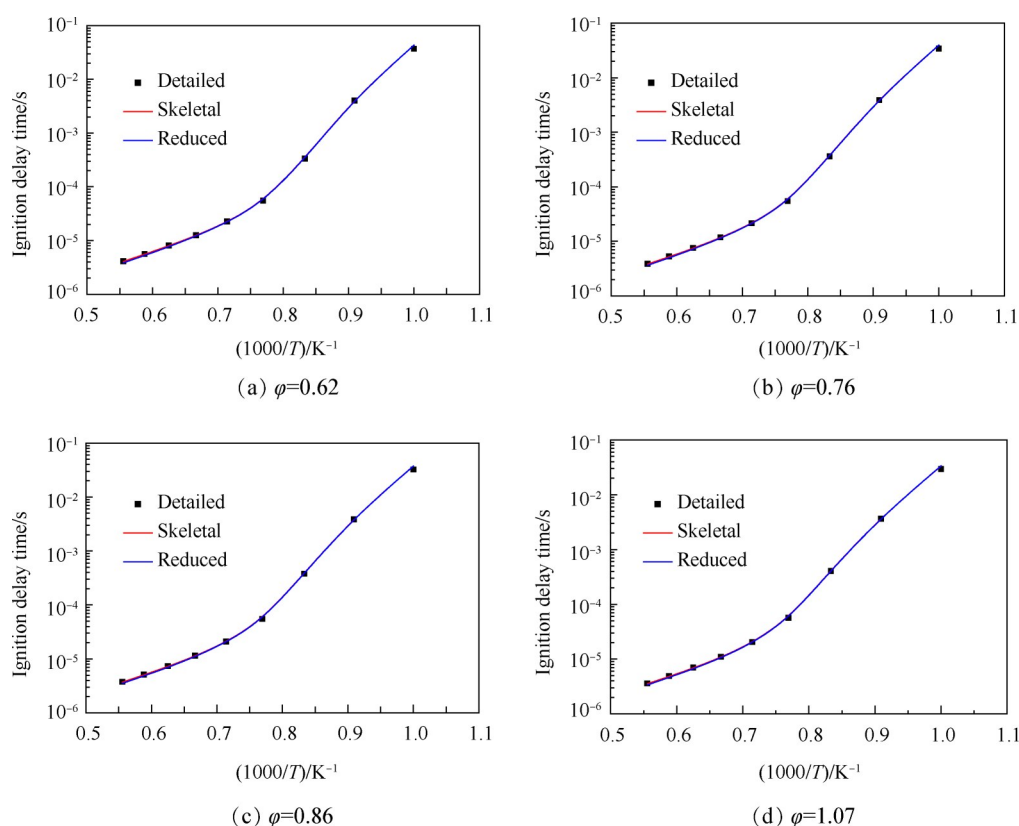


Fig. 8 Comparisons of ignition delay times computed by detailed mechanism, skeletal mechanism and reduced mechanism

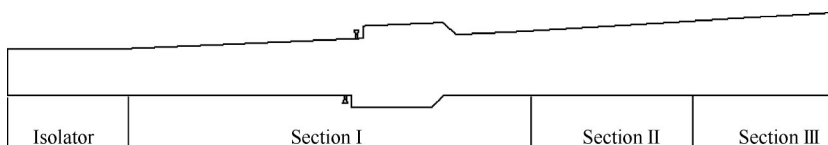


Fig. 9 Schematic of model combustor geometry

lence ratios covering fuel-lean and fuel-rich conditions are calculated in order to study its influence on turbulent reactive flow field of ethylene combustion. Figure 10 shows the comparisons of static pressure profiles obtained by the present calculation with those measured from experiments. The calculated results accurately reproduce the trend of static pressure variation along the streamwise direction, and the computed peak value of static pressure also agrees well with experimental measurements. Moreover, the locations of initial pressure rise near the combustor entrance are well simulated. The peak pressure locating at the cavity and the peak value of static pressure increasing with equivalence ratio increasing are also captured by the present calculation. Thus, it can be concluded that the present reduced mechanism can accurately describe heat release of ethylene combustion in high-speed flow conditions.

Figure 11 shows the simulated counters of Ma for equivalence ratio 0.76 and 1.07. As one can see, the subsonic regions are mainly distributed in two cavities and near wall regions around the lower cavity. The subsonic regions around the lower cavity are larger than those around the upper cavity, and the subsonic regions increase with increasing equivalence ratio. Moreover,

the shock train moves towards upstream for the higher equivalence ratio as a result of more heat releasing by combustion. Due to the very low Ma in the two cavities, the residence time is long enough for steady combustion and flame propagation, and thus resulting high temperatures in the cavities as shown in Figure 12. The upper and lower cavity is in different flame stabilization mode, the former is in cavity shear layer mode while the latter is in jet-wake mode. Moreover, one can also find that the penetration height of ethylene from the lower injector is larger than that from the upper injector. The temperature in the lower cavity is obviously lower than that in the upper cavity. With increasing equivalence ratio, the upper high temperature region thickens gradually. Figure 13 shows the static pressure counters simulated for $\varphi = 0.76$ and 1.07 at side wall. High pressure mainly appears at the parallel cavities and the pressure rise due to combustion moves towards upstream of the main flow with increasing equivalence ratio. It should be mentioned that the combustion flame of ethylene in the present condition may oscillate and lead to different flame stabilization mode. In order to capture dynamic process of flame stabilizing, unsteady simulation of combustion flow field by high-accuracy turbulent model such as

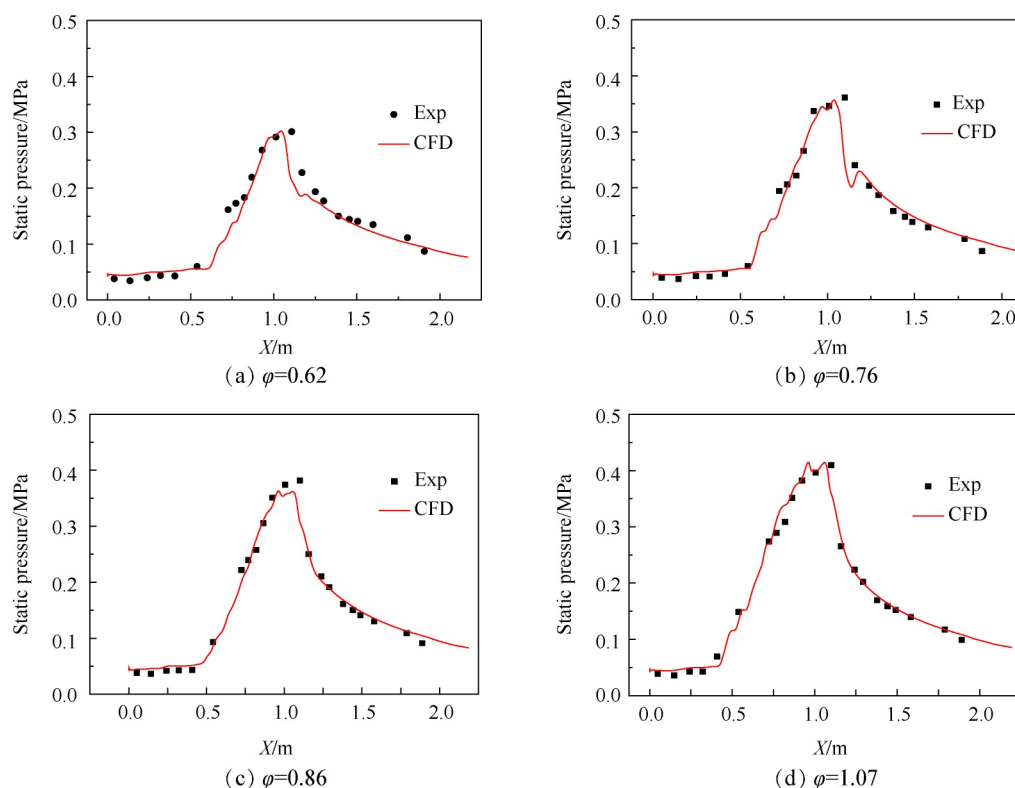


Fig. 10 Comparison of measured and calculated static pressures of side wall along the streamwise direction

large eddy simulation (LES) is proposed to accurately calculate the separation region. However, the high-accuracy study of capturing the details of combustion flow field is beyond the present work, which focuses on developing reduced combustion mechanism for CFD simulation, and unsteady simulation by LES will be performed in the future.

Figure 14 shows the mass fraction distributions of several important species. CO is mainly formed in the cavity and much more CO formation in the lower cavity than that in the upper cavity for these two equivalence ratios. For the higher equivalence ratio, much more CO and H₂O are formed in the expansion section. The total temperature counters show that combustion in the upper

cavity is more complete than that in the lower cavity, so more CO₂ is formed in the upper cavity. H₂O is mainly formed in the cavities, the layer near the upper and lower wall at the low equivalence. These mass fraction counters describe the distribution of important species forming in steady combustion process of ethylene, and these counters are in accordance with the reactive flow counters of Ma , total temperature and static pressure.

From the above discussion, it can be concluded that the reduced mechanism combining the turbulent combustion model EDC is efficient for numerical study of ethylene combustion in the high-speed flow. The reduced mechanism is preferred for large-scale numerical simulations of ethylene combustion.

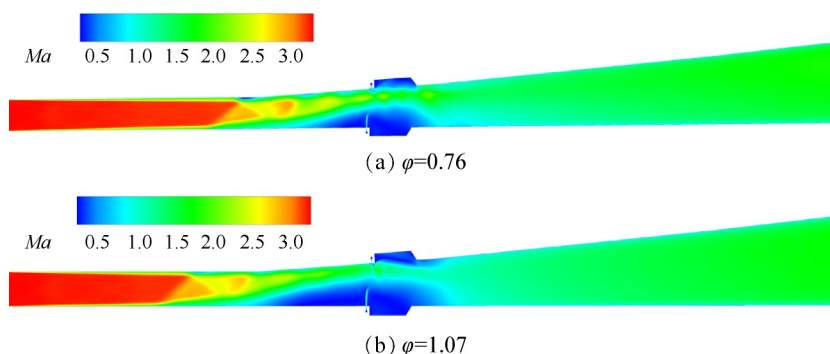


Fig. 11 Counters of Ma number at spanwise center plane

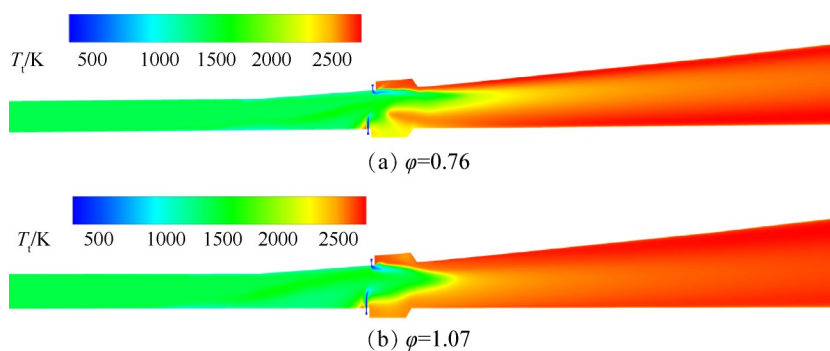


Fig. 12 Counters of total temperature at spanwise center plane

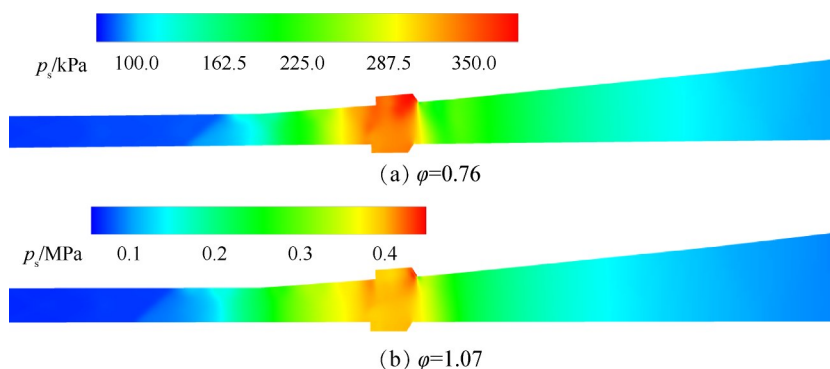


Fig. 13 Counters of static pressure at sidewall

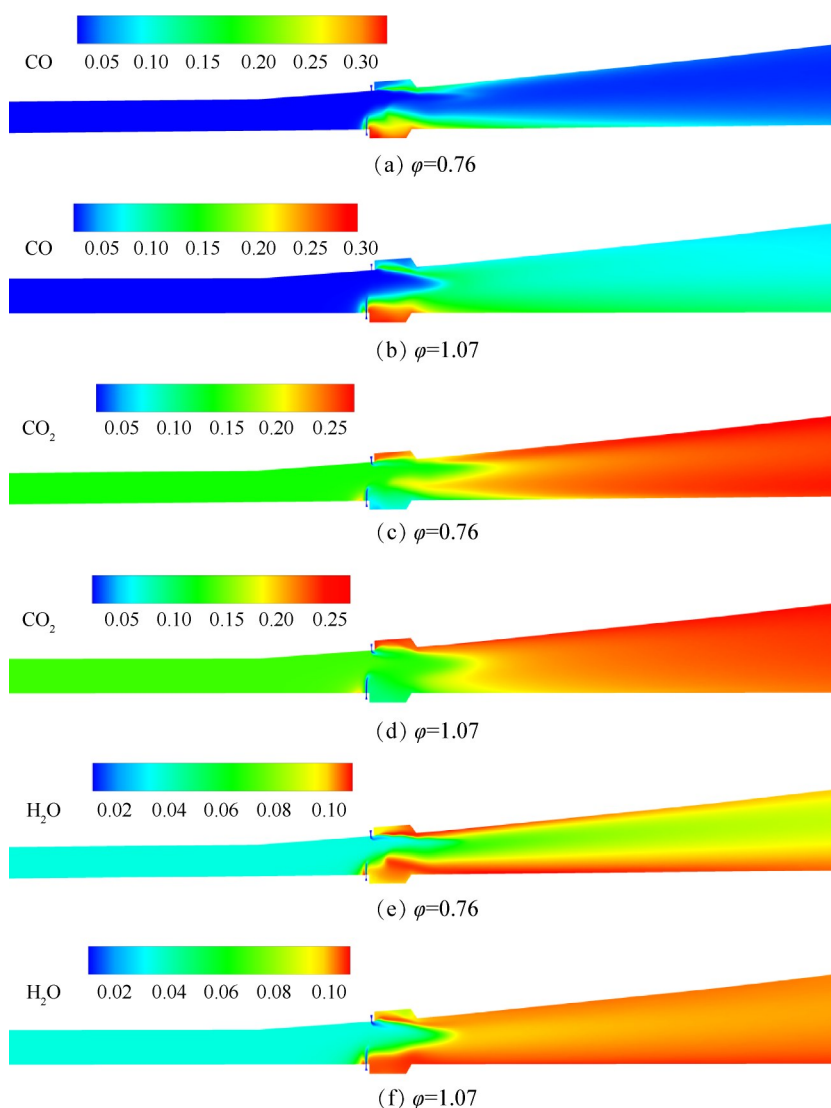


Fig. 14 Mass fraction of important species counters at spanwise center plane

4 Conclusions

Based on the hierarchical method, a detailed mechanism consisting of 153 species and 1435 reactions for ethylene combustion considering pressure-dependent rate constants is developed. The comparisons between modelling and experimental results show that the detailed mechanism can describe ignition delay time, laminar flame speed and product distributions of ethylene combustion satisfactorily. A reduced mechanism consisting of 24 species and 20 reactions is obtained from detailed mechanism reduction by combining DRG, FPT, SA and QSSA method. Error of the worst-case for auto-ignition with the reduced mechanism is 17%, while the average error is less than 7%.

3D simulations are carried out for cavity-stabilized

flames at different equivalence ratios by implementing the reduced mechanism in Fluent. The numerical results well reproduce the static pressure profile and the average error is less than 10%. It is concluded that the reduced mechanism can accurately describe heat release of ethylene combustion at different equivalence ratios in turbulent combustion. Thus, the reduced mechanism is considered to be proper for large-scale numerical study in turbulent combustion by CFD with high chemical fidelity.

Acknowledgment: This work is supported by the National Key R&D Program of China (Nos. 2017YFB0202405).

References

- [1] Xu K, Meng H. Modelling and Simulation of Supercritical-Pressure Turbulent Heat Transfer of Aviation Kero-

- sene with Detailed Pyrolytic Chemical Reactions[J]. *Energy and Fuels*, 2015, 29 (7): 4137–4149.
- [2] Dharavath M, Manna P, Chakraborty D. Numerical Exploration of Mixing and Combustion in Ethylene Fueled Scramjet Combustor[J]. *Acta Astronautica*, 2015, 117 (1): 305–318.
- [3] Dharavath M, Manna P, Chakraborty D. Tip-to-Tail Numerical Simulation of a Hypersonic Air-Breathing Engine with Ethylene Fuel[J]. *Acta Astronautica*, 2016, 128 (1): 107–118.
- [4] Cai Z, Wang Z, Sun M, et al. Investigation of the Flow Field Characteristics in a Scramjet Combustor with the Rearwall-Expansion Cavity [R]. *AIAA* 2017–2148.
- [5] Liu X, Cai Z, Tong Y. Investigation of Transient Ignition Process in a Cavity Based Scramjet Combustor Using Combined Ethylene Injectors [J]. *Acta Astronautica*. 2017, 137(1): 1–7.
- [6] Metcalfe W K, Burke S M, Ahmed S S, et al. A Hierarchical and Comparative Kinetic Modelling Study of C_1 – C_2 Hydrocarbon and Oxygenated Fuels [J]. *International Journal of Chemical Kinetics*, 2013, 45(10): 638–675.
- [7] Wang H, You X, Joshi A V, et al. High-Temperature Combustion Reaction Model of $H_2/CO/C_1$ – C_4 Compounds (USC Mech Version II) [EB/OL]. http://ignis.usc.edu/USC_Mech_II.htm, 2007.
- [8] Lu T, Law C K. Toward Accommodating Realistic Fuel Chemistry in Large-Scale Computations [J]. *Progress in Energy and Combustion Science*, 2009, 35(2): 192–215.
- [9] Lu T, Law C K. A Directed Relation Graph Method for Mechanism Reduction [J]. *Proceedings of the Combustion Institute*, 2005, 30(1): 1333–1341.
- [10] Pepiot-Desjardins P, Pitsch H. An Efficient Error-Propagation Based Reduction Method for Large Chemical Kinetic Mechanisms [J]. *Combustion and Flame*, 2008, 154(1): 67–81.
- [11] Sun W, Chen Z, Gou X, et al. A Path Flux Analysis Method for the Reduction of Detailed Chemical Kinetic Mechanisms [J]. *Combustion and Flame*, 2010, 157 (7): 1298–1307.
- [12] Esposito G, Chelliah H K. Skeletal Reaction Models Based on Principal Component Analysis: Application to Ethylene-Air Ignition, Propagation, and Extinction Phenomena [J]. *Combustion and Flame*, 2011, 158(3): 477–489.
- [13] Valorani M, Creta F, Goussis D A, et al. An Automatic Procedure for the Simplification of Chemical Kinetic Mechanisms Based on CSP[J]. *Combustion and Flame*, 2006, 146(1): 29–51.
- [14] Lovas T. Automatic Generation of Skeletal Mechanisms for Ignition Combustion Based on Level of Importance Analysis [J]. *Combustion and Flame*, 2009, 156(7): 1348–1358.
- [15] 蒋 勇, 邱 榕. 复杂化学机理简化的关联水平法 [J]. *化学学报*, 2010, 68(5): 403–412.
- [16] Gao X, Yang S, Sun W. A Global Pathway Selection Algorithm for the Reduction of Detailed Chemical Kinetic Mechanisms [J]. *Combustion and Flame*, 2016, 167 (1): 238–247.
- [17] Liu A K, Jiao Y, Li S H, et al. Flux Projection Tree Method for Mechanism Reduction [J]. *Energy and Fuels*, 2014, 28(8): 5426–5433.
- [18] 刘爱科, 李书豪, 王 繁, 等. 乙烯氧化动力学机理简化 [J]. *推进技术*, 2015, 36 (1): 142–148. (LIU Ai-ke, LI Shu-hao, WANG Fan, et al. Reduction of Ethylene Combustion Kinetic Mechanism [J]. *Journal of Propulsion Technology*, 2015, 36(1): 142–148.)
- [19] Whitehouse L E, Tomlin A S, Pilling M J. Systematic Reduction of Complex Tropospheric Chemical Mechanisms, Part I: Sensitivity and Time-Scale Analyses [J]. *Atmospheric Chemistry and Physics*, 2004, 4(7): 2025–2056.
- [20] Jones W P, Rigopoulos S. Reduced Chemistry for Hydrogen and Methanol Premixed Flames via RCCE [J]. *Combustion Theory and Modelling*, 2007, 11(5): 755–780.
- [21] Maas U, Pope S B. Simplifying Chemical Kinetics: Intrinsic Low-Dimensional Manifolds in Composition Space [J]. *Combustion and Flame*, 1992, 88(3): 239–264.
- [22] Turanyi T, Tomlin A S, Pilling M J, et al. On the Error of the Quasi-Steady-State Approximation [J]. *Journal of Physical Chemistry*, 1993, 97(1): 163–172.
- [23] 于 浩, 陈 正, 苟小龙. 乙烯氧化机理的简化 [J]. *工程热物理学报*, 2013, 34(2): 376–379.
- [24] 李 瑞, 何国强, 秦 飞, 等. 乙烯燃烧化学动力学机理的简化与分析 [J]. *航空动力学报*, 2018, 33(9): 2074–2083.
- [25] Peters N. Laminar Diffusion Flamelet Models in Non-Premixed Turbulent Combustion [J]. *Progress in Energy and Combustion Science*, 1984, 10(3): 319–339.
- [26] Ertesvag I S, Magnussen B F. The Eddy Dissipation Turbulence Energy Cascade Model [J]. *Combustion Science and Technology*, 2000, 159(1): 213–235.
- [27] Westbrook C K, Mizobuchi Y, Poinot T J, et al. Computational Combustion [J]. *Proceedings of the Combustion Institute*, 2005, 30(1): 125–157.
- [28] Goldsmith C F, Magoon G. Green W H, Database of Small Molecule Thermochemistry for Combustion [J] *Journal of Physical Chemistry A*, 2012, 116(36): 9033–9057.
- [29] Ravi S, Sikes T G, Morones A, et al. Comparative Study on the Laminar Flame Speed Enhancement of Methane with Ethane and Ethylene Addition [J]. *Proceedings of*

- the Combustion Institute*, 2015, 35(1): 679–686.
- [30] Park O, Veloo P S, Egolfopoulos F N. Flame Studies of C_2 Hydrocarbons[J]. *Proceedings of the Combustion Institute*, 2013, 34(1): 711–718.
- [31] Hirasawa T, Sung C, Joshi A, et al. Determination of Laminar Flame Speeds Using Digital Particle Image Velocimetry: Binary Fuel Blends of Ethylene, N-Butane, and Toluene[J]. *Proceedings of the Combustion Institute*, 2002, 29(2): 1427–1434.
- [32] Penyazkov O G, Sevrout K L, Tangirala V, et al. High-Pressure Ethylene Oxidation Behind Reflected Shock Waves [J]. *Proceedings of the Combustion Institute*, 2009, 32(2): 2421–2428.
- [33] Hidaka Y, Nishimori T, Sato K, et al. Shock-Tube and Modelling Study of Ethylene Pyrolysis and Oxidation[J]. *Combustion and Flame*, 1999, 117(4): 755–776.
- [34] Delfau J L, Biet J, Idir M, et al. Experimental and Numerical Study of Premixed, Lean Ethylene Flames [J]. *Proceedings of the Combustion Institute*, 2007, 31(1): 357–365.
- [35] Gerasimov I E, Knyazkov D A, Yakimov S A, et al. Structure of Atmospheric-Pressure Fuel-Rich Premixed Ethylene Flame with and Without Ethanol [J]. *Combustion and Flame*, 2012, 159(5): 1840–1850.
- [36] Zhong Z, Wang Z, Sun M. Effects of Fuel Cracking on Combustion Characteristics of a Supersonic Model Combustor[J]. *Acta Astronautica*, 2015, 110(1): 1–8.
- [37] Menter F R. Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications[J]. *AIAA Journal*, 1994, 32(8): 1598–1605.
- [38] Pope S B. Computationally Efficient Implementation of Combustion Chemistry Using In-Situ Adaptive Tabulation [J]. *Combustion Theory and Modelling*, 1997, 1(1): 41–63.

(编辑:刘萝威)