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Large Eddy Simulation of Ignition and Combustion of Ethylene/Air Turbulent Jet Diffusion Flame with Reduced Kinetic Mechanism

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In this paper, unsteady process of ignition and combustion of turbulent plane-jet diffusion flame of ethylene/air at varied fuel/air ratios is numerically simulated with Large Eddy Simulation (LES) and a reduced kinetic mechanism of ethylene. The kinetic mechanism consisting of 25species and 131steps is reduced from a 71species/395steps detailed mechanism via the method of error-propagation-based directed relation graph (DRGEP) and sensitivity analysis. The LES results of height of flame lift-up and averaged temperature profiles at different downstream locations are compared with the DNS result of Yoo (2011) and satisfactory agreements are found. Unsteady processes of ignition and combustion of ethylene plane-jet diffusion flame are simulated with varied fuel injection velocities. Dynamic evolutions of temperature field as well as CH2 and OH radicals are obtained, which are found to be strongly related to turbulence eddies caused by jet/air mixing layer. The present numerical study shows that LES method with reduced mechanism of hydrocarbon fuels can effectively simulate temporal and spatial evolution of ignition and combustion process.

Nomenclature

H = jet width
C_s = Smagorinsky constant
$\delta_{1/2}$ = local jet half-width
ξ_{st} = stoichiometric mixture fraction
t = time

subscript

st = stoichiometric

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I. Introduction

In recent years, ethylene is being used as a surrogate fuel of conventional hydrocarbon fuels such as kerosene for air-breathing engines [1, 2]. Compared to hydrogen, ethylene has longer ignition delay time and lower flame speed. Its ignition reliability and combustion performance are significantly different from those of hydrogen. Therefore, it is very necessary to study ignition and combustion properties of ethylene/air diffusion flame.

Numerical simulation of combustion process of hydrogen or methane has been well conducted [3, 4]. For simulation of hydrocarbons with larger molecules than methane, the most critical issue is how to deal with complicated detailed kinetic mechanism of hydrocarbons, which includes hundreds or even thousands of species and reaction steps for accurate prediction of ignition, flame formation and propagation [5, 6]. Direct application of detailed mechanisms in numerical simulation becomes expensive, especially for turbulent combustion. At the same time, the so-called "stiffness" due to variations in characteristic times of elementary reactions leads to low efficiency in the temporal convergence of the solution, resulting in further increase in the computational cost. Therefore, reduction of detailed mechanism is critical for effective simulations of unsteady and turbulent combustions.

In recent years, Lu and Law [7] proposed the directed relation graph (DRG) method for efficient mechanism reduction. Pepiot-Desjardins and Pitsch [8] then improved the original DRG method and developed the directed relation graph with error propagation (DRGEP) method. Niemeyer et al. [9] proposed a method of DRGEP with sensitivity analysis (DRGEPSA), in which sensitivity analysis is applied for further reduction of certain remaining species after the DRGEP procedure. It was shown that DRGEPSA is able to produce more compact mechanisms for the same level of accuracy compared to DRG or DRGEP alone. Zhong et al. [10] reduced the detailed mechanisms of ethylene, n-dodecane and surrogate of kerosene using the DRGEP with sensitivity analysis and examined accuracy of the reduced mechanisms with varied species numbers.

Large eddy simulation (LES) methodology has emerged as an effective tool for simulation of turbulent flow and turbulent combustion [11, 12]. The LES directly computes the large scale eddy structures via filter function with sub-grid scale models for calculation of small scale structures. In the present work, the unsteady process of ignition and combustion of turbulent diffusion flame of ethylene/air is simulated with the large eddy simulation and reduced mechanism of ethylene. The reduced mechanism consists of 25 species and 131 elementary reactions that obtained from detailed mechanism, using the error-propagation-based direct relation graph (DRGEP) with sensitivity analysis. The reduced mechanism agrees well with detailed mechanism based on the comparisons of ignition delay time and laminar flame speed. The height of flame lift-up determined by the present results agrees quite well with that by DNS [13] with much larger mesh size and computational cost. Two cases with different fuel injection velocities (204m/s and 306m/s) are conducted. The simulations of turbulent combustion of ethylene/air provide a series of instantaneous temperature fields and distributions of species, which provides useful information of better understanding of combustion properties of hydrocarbon fuels.

II. Numerical Method and Validations

The spatially developing turbulent diffusion jet flame is simulated in a 2-dimensional slot-burner configuration as shown in Fig.1. The slot in the center is 2-millimeter wide. Fuel consisting of 18% ethylene and 82% nitrogen by volume is injected from the slot at a temperature of 550K. The heated air flows around the fuel at atmosphere pressure and an inlet temperature of 1550K. Two cases with fuel injection velocity of 204m/s and 306m/s are simulated in the paper.

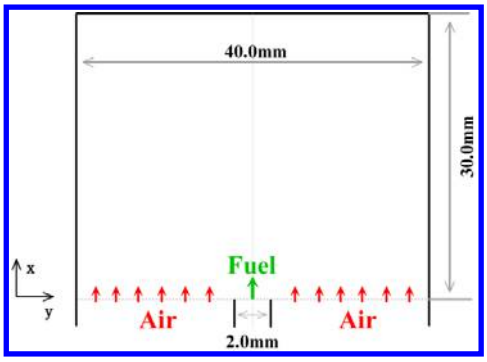


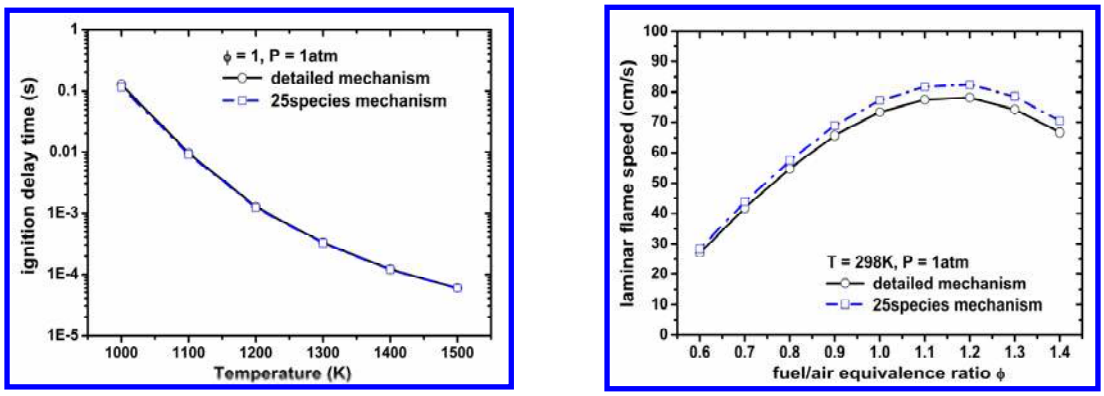
Fig.1 Sketch of the slot-burner with fuel injection in the center

Finite volume method is used to solve the Navier-Stokes equations and transport equations of species with AUSM flux splitting. The 2nd-order upwind scheme and 2nd-order center scheme are respectively applied to the convective flux terms and the viscous flux terms. The time advancement is calculated by the implicit Euler method. The Smagorinsky-Lilly model [14] with a pre-given model coefficient of C_s=0.1 is used for calculation the sub-grid scale stress. The perfect gas assumption is used and The NASA standard temperature polynomials have been used to determine the specific heat at constant pressure. Viscosity and thermal conductivity of species are calculated by kinetic theory with pre-given Lennard-Jones characteristic length and energy parameters. Fick's law governs mass diffusion, and the turbulent Schmidt number set to 0.7. The computational domain is $15H\times 20H$ in the streamwise x and transverse y, where H is the width of slot. A uniform grid is used in the streamwise, while stretched meshes are applied in the transverse direction. The total number of mesh is more than 300,000. The unsteady calculation is advanced at a constant time step of 1μs and the total simulation time is 10ms. The computation is performed with MPI parallel technique with 32 CPU cluster and approximately 8,000 CPU hours are required for one case. Compared to the computational cost of DNS for the same problem reported in reference [13], the LES method with reduced kinetic mechanism may greatly decrease the computation cost.

The turbulent/combustion interaction is modeled by the method of eddy dissipation concept (EDC) developed by Magnussen and Hjertager [15]. The key idea of EDC is that chemical reactions with finite rates typically occur in

vortices of turbulent flow and the reaction rates are controlled by characteristic times of both the kinetic mechanism and the turbulence. With EDC model, kinetic mechanism can be fully coupled to the flow and temperature solver.

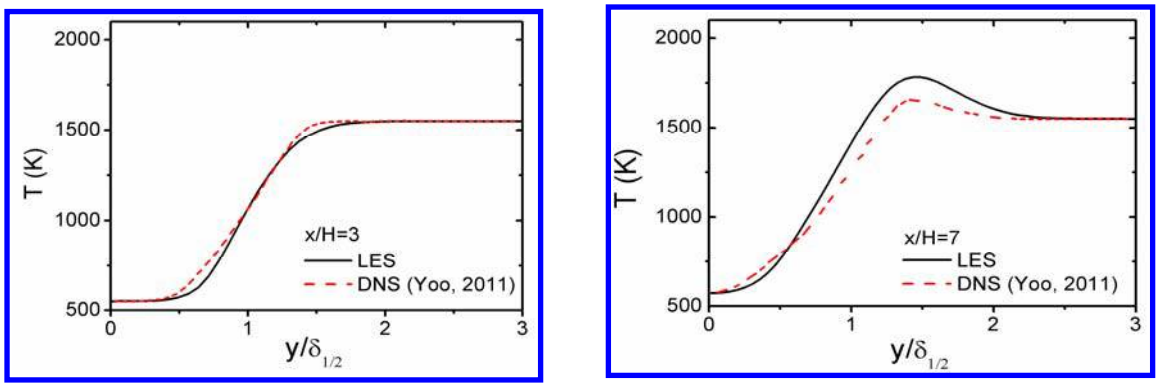
The reduced mechanism is obtained with reduction methods of error-propagation-based directed relation graph (DRGEP) and sensitivity analysis (SA) from a detailed mechanism (71 species and 395 reaction steps) proposed by H. Wang [16]. The reduced mechanism is comprised of 25 species (H2, H, O, O2, OH, H2O, HO2, H2O2, CH2, CH2*, CH3, CH4, CO, CO2, HCO, CH2O, CH3O, C2H2, C2H3, C2H4, C2H5, HCCO, CH2CO, C2H3O, N2) and 131 reaction steps. The accuracy of the reduced mechanism is examined by comparing laminar flame speed and ignition delay time predicted with the detailed and the reduced mechanisms. Fig.2 (a) gives the comparison of ignition delay time and Fig.2 (b) plots the result of laminar flame speed. As shown in the figures, good agreements between results of the two mechanisms are observed.



(a) **(b)**

Fig.2 Comparison of the detailed mechanism with the 25-species mechanism
(a): ignition delay time; (b): laminar flame speed

Fig.3 (a), (b) shows distribution of Favre-averaged mean temperature profile at two downstream locations of x=3H and x=7H for the case with a fuel injection velocity of 204m/s. The DNS results of temperature profiles are also plotted for comparison. In the figures, $\delta_{1/2}$ denotes the local jet half-width as defined in the reference of [17]. The profiles of LES agree well with the DNS result that proves accuracy of the present LES results. The height of flame lift-up is also compared and a discrepancy of only 3.4% is found between the present calculation (5.6H) and the DNS result (5.8H).



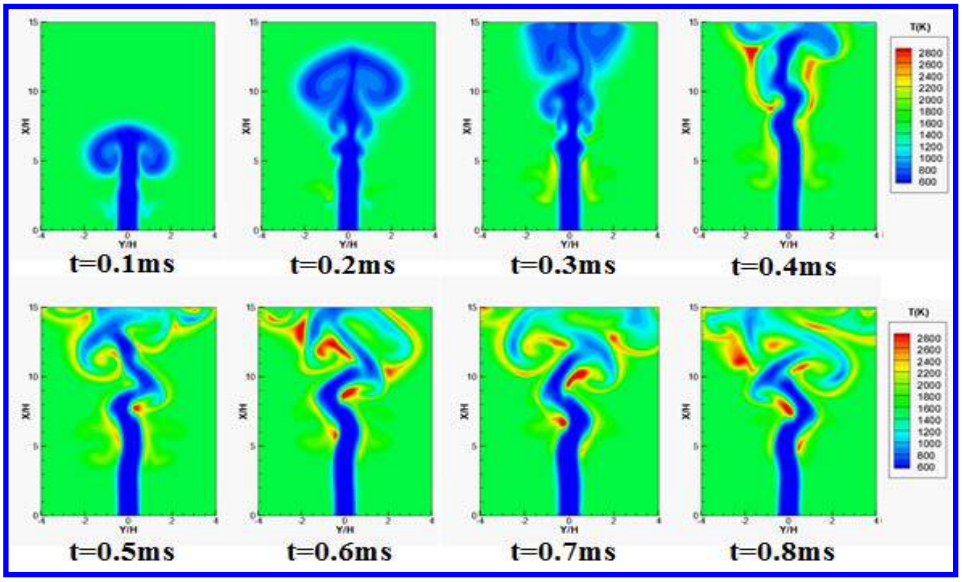
(a) **(b)**

Fig.3 Comparison of temperature profiles obtained with LES and DNS

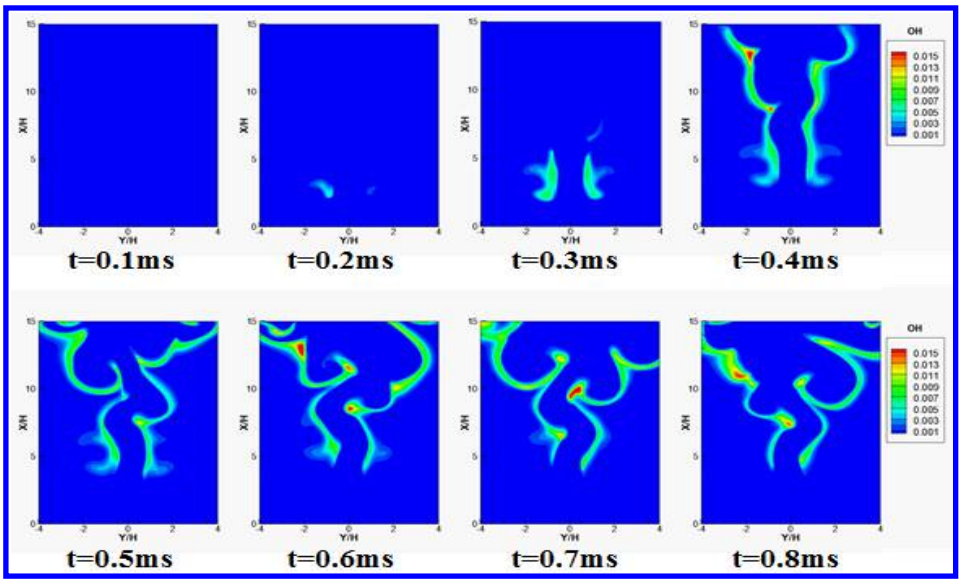
III. Results and Discussions

A. Injection speed of 204m/s

Fig.4 (a), (b), (c) shows time development of instantaneous temperature, mass fraction of OH and CH2 from *t*=0.1ms to *t*=0.8ms, during the ignition process. As shown in Fig. 4 (a), ignition of fuel occurs at approximately at *t*=0.3ms, indicating an ignition delay time of 0.3ms for the ethylene/air diffusion flame. As time increases, ignition process comes into completion and flame is formed and propagates. The time changes of CH2 and OH contours as given in Fig. 4 (b) and (c) indicate dynamic motion of flame, which is strongly related to turbulence eddies caused by the fuel/air mixing.



(a)



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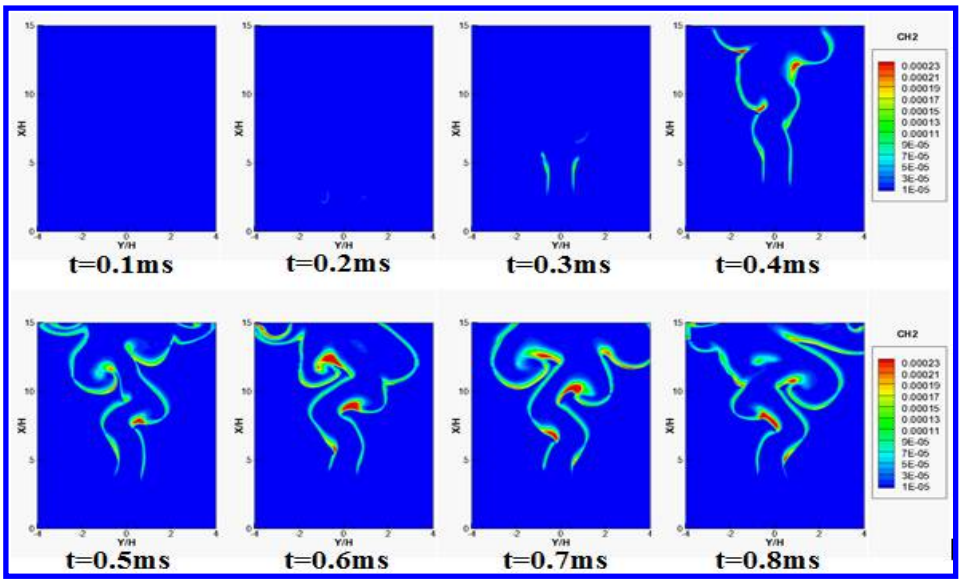


(c)

Fig. 4 Time development of contours of (a): instantaneous temperature, (b): mass fraction of OH, (c): mass fraction of CH2 for the case with injection velocity of 204m/s

Fig.5 (a), (b) shows the enlarged view of local flow field as indicated by the white rectangular box on the left figure. Instantaneous streamlines are plotted in the figures with backgrounds of contours of mass fraction of OH and CH2. Radical OH is often used to show the high-temperature region, while radical CH2 is an indicator of flame front. In the right two figures, the white curves indicates the stoichiometric mixture fraction (ξ_{st}=0.27) where generally,

combustion efficiency is highest for diffusion flames. It is readily observed that most of OH radical is formed and concentrated in a fuel-lean region and most of CH2 radical exists around the curve of stoichiometric mixture fraction. The vortices causes significant stretching and torsion of streamlines and enhances fuel/air mixing that accelerates the reaction rate. Based on the present results, it is believed that turbulent vortices due to fuel/air mixing are the primary factor for the formation and evolution of diffusion flame.

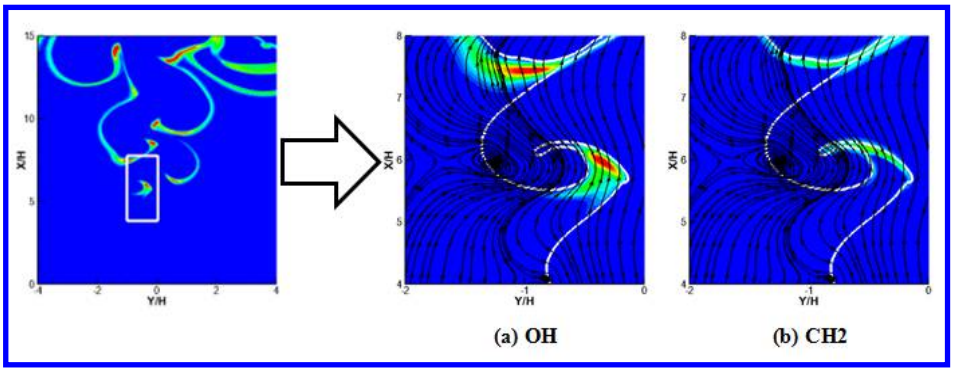
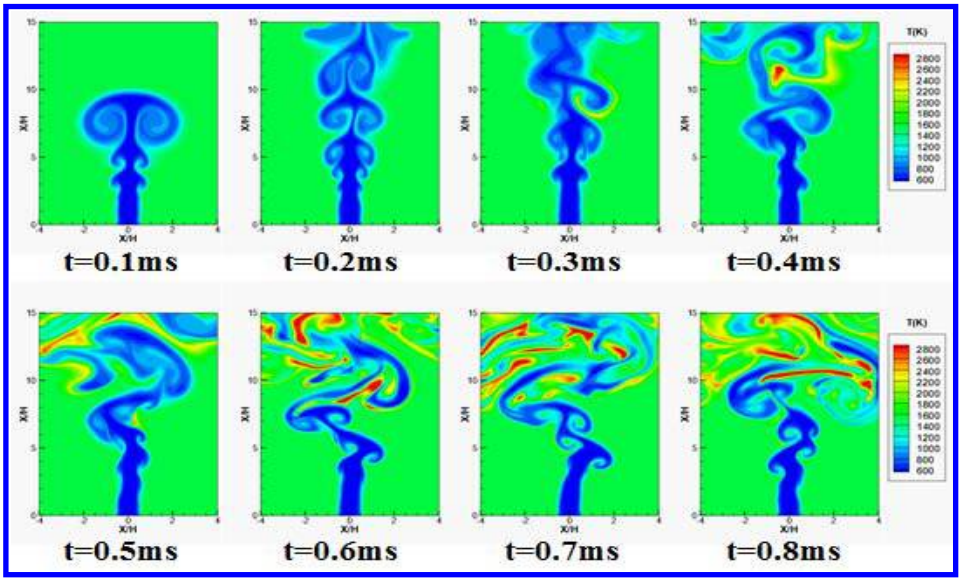


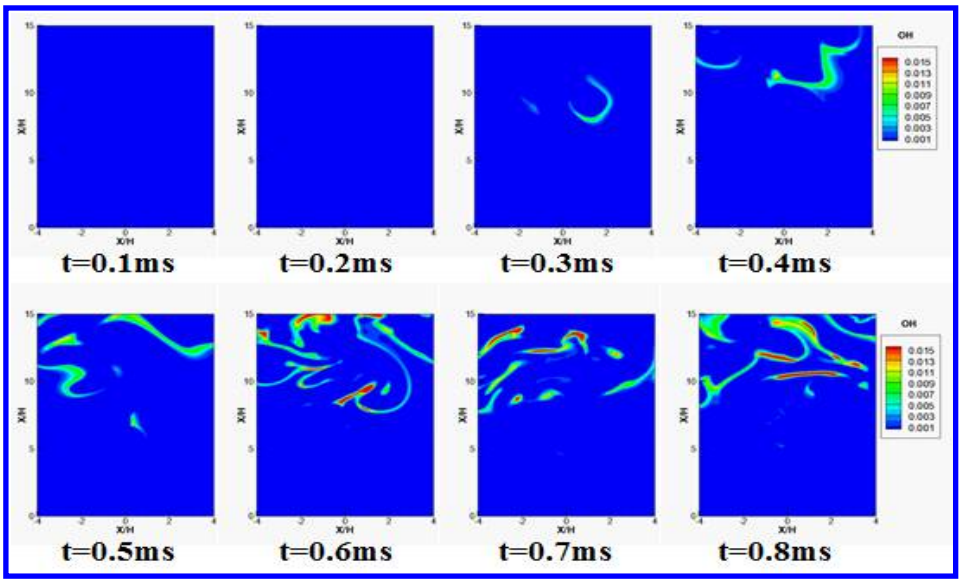
Fig. 5 Enlarged views of local fluid field with contours of mass fraction of OH and CH2

B. Injection speed of 306m/s

Fig.6 (a), (b), and (c) gives the contours of instantaneous temperature, mass fraction of OH and CH2 for the case with fuel injection velocity of 306m/s. Fig.6 (a), ignition occurs at a time of t=0.3ms. As the fuel injection velocity goes up, the dynamicity and instability of flame becomes more obvious and the height of flame lift-up increases significantly. For this case, the flame is nearly blown out since the injection velocity is considerably large.



(a)



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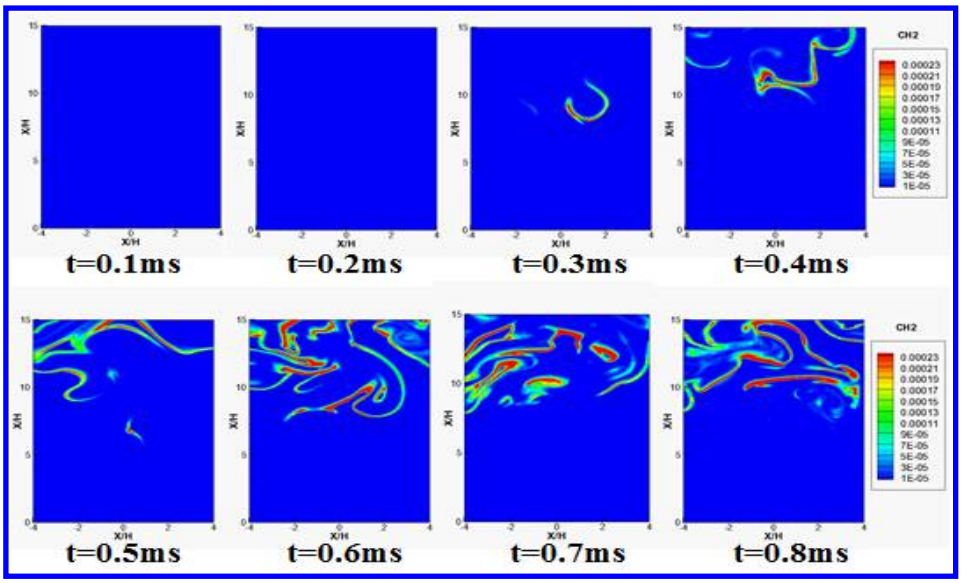

(c)

Fig. 6 Time development of contours of (a): instantaneous temperature, (b): mass fraction of OH, (c): mass fraction of CH2 for the case with injection velocity of 306m/s

V. Conclusions

In this paper, unsteady process of ignition and combustion of ethylene diffusion flame is numerically simulated with large eddy simulation and reduced mechanism of ethylene. The reduced mechanism of 25 species and 131

reactions, is reduced from a detailed mechanism via DRGEP and sensitivity analysis. The predicted laminar flame speed and ignition delay time by the reduced mechanism agrees well with those of the detailed mechanism. The distributions of Favre-averaged mean temperature profiles at different downstream locations are found to be in good agreement with the DNS results as well as the height of flame lift-up. Dynamic evolutions of temperature field as well as CH2 and OH radicals show strong effect of turbulence vortices on the flame formation and distortion. As fuel injection velocity increases, the instability of flame becomes more obvious and the height of lift-up increases significantly. Furthermore, the present work shows that LES method with a qualified reduced mechanism of hydrocarbons is able to simulate the unsteady process of ignition and combustion for non-premixed diffusion flames.

Acknowledgements

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References

[1] A. M. Storch, M. Bynum, J. Liu, M. Gruber., "Combustor operability and performance verification for HIFiRE flight 2." AIAA Paper 2249 (2011): 2011.

[2] F. Zhong, L. Chen, F. Li, X. Zhang, C. J. Sung. “Numerical Simulation of Ignition and Combustion of Ethylene in a Supersonic Model Combustor with a Reduced Kinetic Mechanism.” Combustion Science and Technology, 185(4) (2013): 548-563.

[3] L. M. Das., "Hydrogen-oxygen reaction mechanism and its implication to hydrogen engine combustion." International Journal of Hydrogen Energy 21.8 (1996): 703-715.

[4] J. B. Bell, S. D. Marcus, F. G. Joseph., "Numerical simulation of premixed turbulent methane combustion." Proceedings of the Combustion Institute 29.2 (2002): 1987-1993.

[5] H. J. Curran, P. Gaffuri, W. J. Pitz, C. K. Westbrook., "A comprehensive modeling study of n-heptane oxidation." Combustion and flame 114.1 (1998): 149-177.

[6] M. Mehl, W. J. Pitz, C. K. Westbrook, H. J. Curran., “Kinetic modeling of gasoline surrogate components and mixtures under engine conditions.” Proceedings of the Combustion Institute, 33(1) (2011): 193-200.

[7] T. Lu, C. K. Law., "A directed relation graph method for mechanism reduction." Proceedings of the Combustion Institute 30.1 (2005): 1333-1341.

[8] P. Pepiot-Desjardins, P. Heinz, "An efficient error-propagation-based reduction method for large chemical kinetic mechanisms." Combustion and Flame 154.1 (2008): 67-81.

[9] K.E. Niemeyer, C.-J. Sung, M.P. Raju, "Skeletal Mechanism Generation for Surrogate Fuels Using Directed Relation Graph with Error Propagation and Sensitivity Analysis", Combustion and Flame 157(2010): 1760-1770.

[10] F. Zhong, S. Ma, X. Zhang, C.J. Sung, K.E. Niemeyer, “Development of Efficient and Accurate Skeletal Mechanisms for Hydrocarbon Fuels and Kerosene Surrogate.” Acta Mechanica Sinica, 1 (2014).

[11] A. Kempf, R. A. Lindstedt, J. Janicka, “Large-eddy simulation of a bluff-body stabilized nonpremixed flame.” Combustion and flame, 144(1) (2006): 170-189.

[12] V. Raman, H. Pitsch, “Large-eddy simulation of a bluff-body-stabilized non-premixed flame using a recursive filter-refinement procedure.” Combustion and flame, 142(4) (2005): 329-347.

[13] C.S. Yoo, E.S. Richardson, R. Sankaran, J. H. Chen, "A DNS study on the stabilization mechanism of a turbulent lifted ethylene jet flame in highly-heated coflow", Proceedings of the Combustion Institute, 33(1) (2011): 1619-1627.

[14] J. Smagorinsky, "General circulation experiments with the primitive equations: I. the basic experiment*." Monthly weather review 91.3 (1963): 99-164.

[15] B.F. Magnussen, B.H. Hjertager, "On Mathematical Models of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion", Proceedings of the Combustion Institute, 16(1) (1976): 719-729.

[16] H. Wang, A. Laskin, "A Comprehensive Kinetic Model of Ethylene and Acetylene Oxidation at High Temperatures", Progress Report for an AFOSR New World Vista Program (1998).

[17] C.S. Yoo, R. Sankaran, J. H. Chen, “Three-dimensional direct numerical simulation of a turbulent lifted hydrogen jet flame in heated coflow: flame stabilization and structure.” Journal of Fluid Mechanics, 640 (2009): 453-481.