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Numerical Investigation on PDEs with Mixed Fuels

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Summary

Pulse detonation turbine engines (PDTEs), which are used as power generation, are desirable to use hydrocarbon from the aspect of infrastructure of fuels. In the present study, we investigate the performance of PDEs using mixed hydrocarbon fuels. With the detailed 42-species and 168-step mechanism, numerical simulations on mixed-fuel-and-air PDEs are conducted. We use CH_4-C_3H_8, CH_4-H_2, and C_3H_8-H_2 as fuels, and examine characteristic features of detonations with different blend ratios. We perform calculations on the Chapman-Jouguet detonation speeds and chemical reaction lengths, and investigate ZND profiles of chemical reactions. Then we evaluate PDEs performances by changing blend ratios. These results show good agreements with theoretical results. In CH_4-C_3H_8 case, specific impulses do not depend on the mixing ratio very much, while in other cases, they depend on the mole fraction of hydrogen.

Introduction

Pulse detonation engines (PDEs) have gathered widely attention as next-generation aerospace engines [1, 2]. PDEs are internal combustion engines which extract power by cyclic detonation waves. The potential of PDEs makes the engine smaller and lighter than current jet engines, because detonation waves compress a mixture instead of a compressor. PDEs will be acceptable for a flight at a hyper sonic speed, Mach 5, so it is expected to be used at SST and space planes. The system of PDEs with a turbine is also promising as power generation, called Pulse Detonation Turbine Engines (PDTEs) [3, 4]. PDTEs have several advantages over existent engines: high heat efficiency, small scaling, light weight, simple structure, and so on. PDTEs are one of the best systems to use natural gas as fuels for economical and ecological reasons. A main component of natural gas is CH_4 but the detonability of CH_4 is extremely small. Therefore we must modify the CH_4 mixture by adding some detonable components to adopt the mixture as PDEs fuels. In the present study, the detonation features and PDE performance are numerically examined with various blend ratio of mixed hydrocarbon fuels by 42-species and 168-step detailed mechanism (Westbrook, 1984) [5].

Numerical Setup

In a present paper, 1-D numerical simulations are conducted for steady and

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unsteady detonations with mixed hydrocarbon fuels. The steady detonation characteristics of D_{CJ} and L_{OH} are calculated by the software, AISTJAN [6] and ZND [7].D_{CJ} is the frontal shock speed of Chapman-Jouguet (CJ) detonation and L_{OH} is the reaction length determined as the distance between the shock front and the location of peak mole fraction of OH. We utilize C_3H_8-CH_4(Case A), CH_4-H_2(Case B), and C_3H_8-H_2(Case C) as fuels. For all fuels, stoichiometric air (O_2-3.76N_2) is provided as oxidizer. The initial gas conditions are 0.1013 MPa at the static pressure and 298.15 K at the static temperature. The computational domain for PDEs is 40 L_{OH}. Grid resolution for this study is 5 points/L_{OH}. We employ high-pressure and high-temperature driver gas region on the thrust wall (1.0L_{OH} in thickness) to initiate detonation wave. The driver gas conditions are 7.5 MPa and 2000 K. The mixture conditions for unsteady 1-D simulations are listed in Table 1.

Table 1: Stoichiometric mixed fuel and air conditions.

Case	Mole fraction of gas mixture					D_{CJ}	M_{CJ}	γ_1	$\overline{\gamma_2}$	L_{OH}
	CH_4	C_3H_8	H_2	O_2	N_2	m/s				mm
A	0.8	0.2	-	2.6	9.78	1803.2	5.166	1.391	1.159	3.933
	0.6	0.4	-	3.2	12.03	1802.6	5.199	1.394	1.167	2.852
	0.4	0.6	-	3.8	14.29	1802.1	5.222	1.396	1.166	2.411
	0.2	0.8	-	4.4	16.54	1801.8	5.239	1.398	1.166	2.144
	0	1	-	5	18.80	1801.5	5.252	1.399	1.166	2.018
B	0.8	-	0.2	1.7	6.39	1814.1	5.094	1.388	1.160	7.641
	0.6	-	0.4	1.4	5.26	1828.1	5.066	1.390	1.160	4.030
	0.4	-	0.6	1.1	4.14	1849.9	5.024	1.392	1.159	2.232
	0.2	-	0.8	0.8	3.01	1887.9	4.959	1.395	1.166	1.070
C	-	0.8	0.2	4.1	15.42	1805.6	5.238	1.399	1.166	1.908
	-	0.6	0.4	3.2	12.03	1812.0	5.218	1.399	1.166	1.763
	-	0.4	0.6	2.3	8.65	1823.3	5.182	1.399	1.165	1.526
	-	0.2	0.8	1.4	5.26	1849.5	5.107	1.400	1.157	1.143

Results and discussion

The CJ detonation speedsD_{CJ} with various mole fractions are presented in Fig.1. D_{CJ} is independent on the blend ratio in case A. In case B and C, D_{CJ} steeply increases when the blend ratio of H_2 become over 60%. Fig.2 indicates the induction length L_{OH} with various mole fractions. L_{OH} rapidly decreases when 20% of C_3H_8or H_2 is added to CH_4 in Case A and B in Fig.2. Especially in Case A, when the ratio of methane changes from 100% to 80%,L_{OH} decreases to 25%. Since the induction length is proportional to a detonation cell size, it is possible to reduce the scale of PDEs by changing blend ratio. The blend ratio of C_3H_8-H_2 gives little influence to L_{OH} in Case C.

To figure out ZND mechanisms from the views of chemical reactions, steady

computations are carried out with ZND [6]. GRI-Mech 3.0 [8] is adopted as a reaction mechanism. The mole fractions of each chemical component behind the shockwave are examined in Case A. According to the results, the important chemical substances are chosen. The profiles of selected components are plotted in Fig. 3 (100% CH_4 case), Fig. 4 (80% CH_4 and 20% C_3H_8 case), and Fig. 5 (100% C_3H_8 case). Although the blend ratio of CH_4 increases as much as 80% from Fig.3 to Fig.4, there is no remarkable change between these two graphs. This tendency is also observed in L_{OH}. It is implied that the following two paths have a great impact on L_{OH} in the ZND structure. The first path is the reaction from H_2 to OH. When OH radical becomes the maximum, the mole fraction of H_2 decreases rapidly. Therefore it is obvious that most OH radical is directly generated from H_2. The second path is the decomposition reaction of HCO. We observe that only the profile of HCO changes its shape from Fig. 3 to Fig. 4 and suggest that HCO plays an important role of the rising L_{OH} as a trigger. HCO is generated from the substances including CH_3, CH_2O, C_2H_4, and C_2H_6 in decomposition reactions. These components comparatively exist a lot as seen in Figs. 3-5.

Figure 6 indicates the static pressure histories at the thrust wall in Case A. The initial high pressure by the driver gas decreases rapidly, and the plateau pressure is sustained until about $3.0t/t_{CJ}$. The influence of the mixture ratio on the thrust wall pressure is weak in Fig. 6, and the same tendencies are obtained in Case B-C. Figure 7 shows numerical and theoretical impulse I_{cyc}. Theoretical plots are derived from Endo *et al.* [9]. In Case A and B, I_{cyc} increases by 76% and 704% respectively when mole fraction of CH_4 rises from 20% to 80%. The numerical results are in good agreements with the theoretical analysis, and the differences between numerical and theoreticalI_{cyc} in Case A-C are 1.7%, 1.3%, and 1.0% at maximum. Figures 8 and 9 display the dependence of I_{sp} and I_{spf} on the mole fraction of mixed fuel, respectively. In Fig. 8, the blend ratio of mixed fuel has little effect onI_{sp}. By contrast, the ratio of mixed fuel has great influence on I_{spf} in Fig. 9. When mole fraction of H_2 rises from 20% to 80% in Case B and C, I_{spf} also increases by 29% and 16%, respectively.

Conclusion

A numerical study on the mixed fuel PDEs has been performed with the detailed 42-reaction and 163-step mechanism. We used CH_4-C_3H_8, CH_4-H_2,and C_3H_8-H_2 as mixed fuels. With changing blend ratios of these mixed fuels, we examined the characteristic features of detonations and performances of PDEs. As for the case of CH_4-C_3H_8 and CH_4-H_2, it was confirmed that the reduction of L_{OH} by adding C_3H_8 and H_2 to CH_4 enables us to reduce the scale of PDEs. It was suggested that the steep elongation of L_{OH} in one dimensional simulation is influenced by two chemical paths. The first is H_2 path: OH is directly generated from H_2.

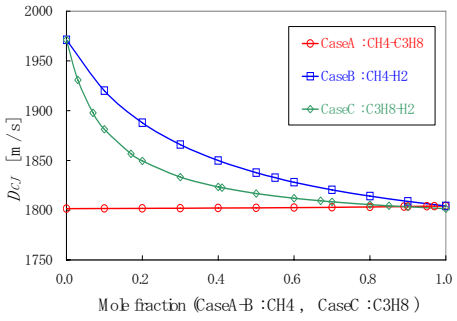

Figure 1: Chapman-Jouguet speed D_{CJ}.

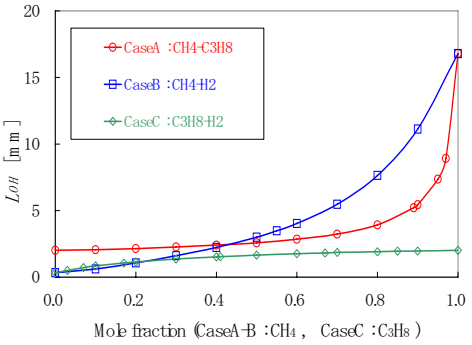

Figure 2: Induction length L_{OH}.

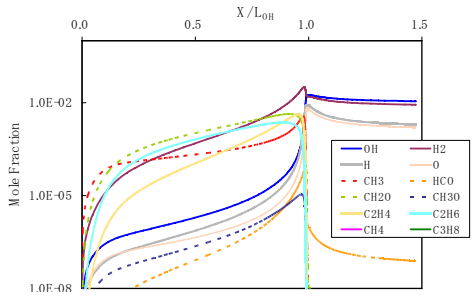

Figure 3: Selected mole fraction profiles in 100% CH_4 case.

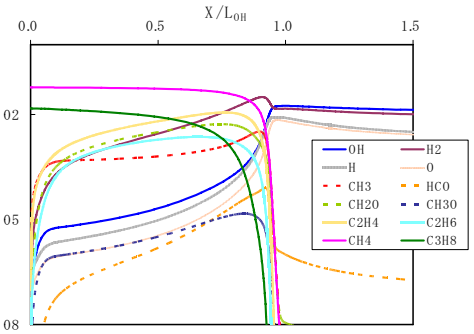

Figure 4: Selected mole fraction profiles in 80%CH_4 - 20% C_3H_8 case.

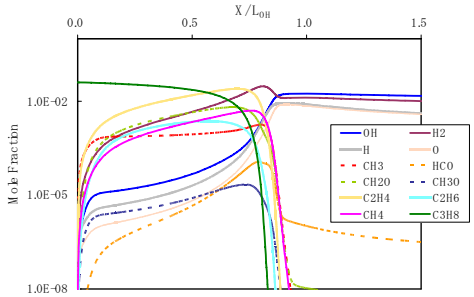

Figure 5: Selected mole fraction profiles in 100% C_3H_8 case.

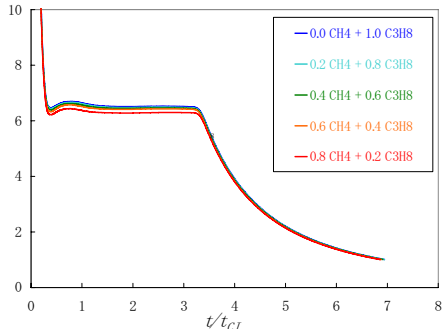

Figure 6: Pressure History at the thrust wall in Case A.

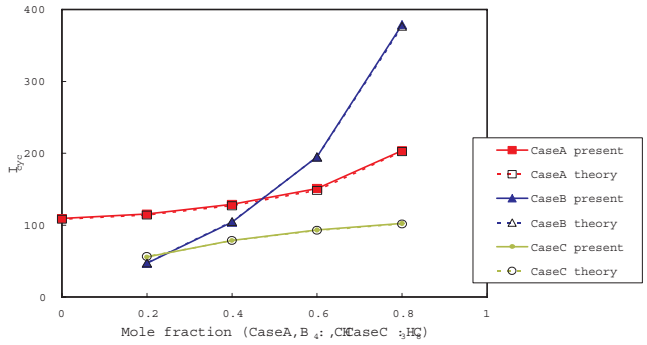

Figure 7: Dependence of I_{cyc} on mole fraction.

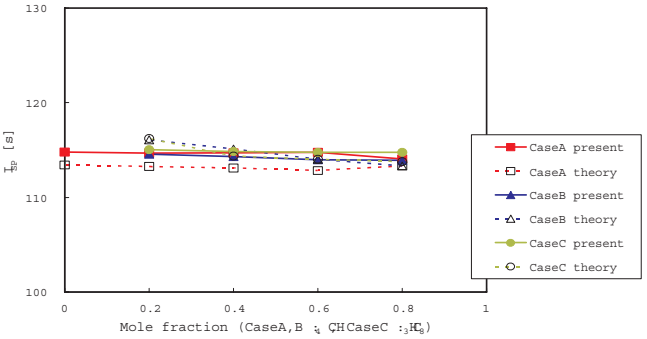

Figure 8: Dependence of I_{sp} on mole fraction.

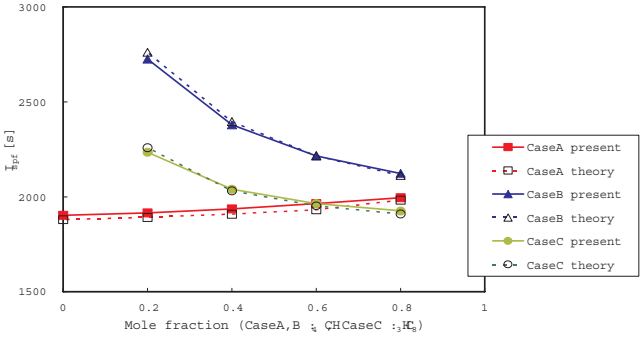

Figure 9: Dependence of I_{spf} on mole fraction.

The second is HCO path: OH is generated from HCO by decomposition reactions. Although the mole fraction of CH_4 increased from 0% to 80% inCH_4-C_3H_8 case, drastic variations of chemical compositions were not observed. When the mole

fraction of CH_4 in CH_4-C_3H_8 and CH_4-H_2 mixtures becomes large, I_{cyc} increases by 76% and 704%, respectively. In a similar way, when the mole fraction of H_2 in CH_4-$H_2$and C_3H_8-H_2 mixtures increase from 20% to 80%, I_{spf} increases by 29% and 16%, respectively.

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References

1. Kailasanath, K. (2000): "Review of Propulsion Applications of Detonation Waves," *AIAA J.*, Vol.38, No.9, pp. 1698-1708.
2. Roy, G. D., Frolovb, S. M., Borisovb, A. A., Netzerc, D. W. (2004): "Pulse detonation propulsion: challenges, current status of, and future perspective," *Progress in Energy and Combustion Science*, 30, pp. 545-672.
3. Yoshida, A., Okuda, Y., Yatsufusa, T., Endo, T., Taki, S., Aoki, S., Umeda, Y. (2005): "Detonation properties of mixed-fuel-and-air gas mixtures," *Proceeding of 20th ICDERS*.
4. Inaba, K., Kato, J., Yamamoto, M. (2006): "Numerical simulation of mixed fuel detonations," *AIAA paper* 2006-4309.
5. Westbrook, C.K., and Pitz, W.J. (1984): "A Comprehens Kinetic Mechanism for Oxidation and Pyrolysis and Propene," Comb. Sci. Tech 37,117.
6. Tanaka, K., AISTJAN http://www.aist.go.jp/RIODB/ChemTherm/gas.html
7. J. E. Shepherd, ZND http://www.galcit.caltech.edu/EDL/public/32bitChemkinPC/znd/
8. GRI Mech, http://www.me.berkeley.edu/gri_mech/
9. Endo, T., Kasahara, J., Matsuo, A., Inaba, K., Sato, S, Fujiwara, T. (2004): "Pressure History at the Thrust Wall of a Simplified Pulse Detonation Engine", *AIAA J.*, 42, pp. 1921-1930.