Reduced Chemical Reaction Model of Methane/Oxygen Mixture

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1 Introduction

Methane fuel has many advantages; such as good availability, low cost, and clean burning for gas turbine or rocket engines. Therefore, there are many experimental or numerical researches to use methane fuel commercially. However, the stagnation pressure in the chamber is much higher than the atmospheric pressure. So that, it is difficult to do experiments in order to understand the combustion process in detail. On the other hand, when the methane combustion is numerically simulated, it is important to select the reliable chemical reaction model in order to obtain the good results. The GRI-Mech[1], which is widely used for the numerical simulations for the methane combustion, is reported that the results such as ignition delay time agree well with the experimental data under atmospheric pressure state, however, it cannot predict them under high pressure state[2]. Recent computers are improving rapidly. To understand methane combustion in detail, the combustion process can be predicted not only by ignition delay times and laminar flame velocity but also by CFD simulations to be understood in detail. However, the detailed chemical reaction models are commonly not available for CFD simulations including compressible effect because they have many species and elemental reactions. So reduced chemical reaction models are required for CFD simulations especially for the combustion under high pressure environment. But even detailed chemical reaction models are not available for high pressure states so it is necessary to estimate the reliability of detail and reduced chemical reaction models or to construct a new model.

The present paper shows the comparison between the numerical results and the experimental data. Then, new reduced reaction models are constructed by using the reliable detailed chemical reaction model.

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2 Comparison of Experimental Data and Numerical Results

k3l1[3] is selected as a detailed chemical reaction model and Petersen & Hanson model[4] is selected as a reduced chemical reaction model. k3l1 includes 68 species and 325 elementary reactions. Petersen & Hanson model, which is reduced from RAMEC[2], includes 24 species and 35 elementary reactions. Ignition delay times and laminar flame velocities are calculated by CHEMKIN4.1.1. to compare with the experimental data.

The numerical results of ignition delay time at various temperatures are compared with the experimental data by Petersen et al.[5]. The condition of methane/air mixture is as follows, the equivalence ratio = 3 and the pressure = 115 atm. Figure 1 shows the ignition delay times. This figure shows that the numerical results of k3l1 and Petersen & Hanson model agree well with the experimental data by Petersen et al.

The numerical results of laminar flame velocities at various equivalence ratios are compared with the data measured by Vagelopoulos et al.[6,7] and Rozenchan et al.[8]. The condition of methane/air mixture is the pressure of 1 bar, and the temperature of 298 K. Figure 2 shows the experimental data and numerical results. It presents that the calculations with k3l1 agree well with the experimental data, however, those with Petersen & Hanson model do not agree with the experimental data. Petersen & Hanson model can predict accurate ignition delay times. However, it cannot calculate accurate laminar flame velocities. This is because Petersen & Hanson model is only reduced with respect to the ignition delay times therefore this model cannot simulate accurate laminar flame velocities. The present results indicate that more reliable model is necessary to be constructed for calculating the combustion process in detail.

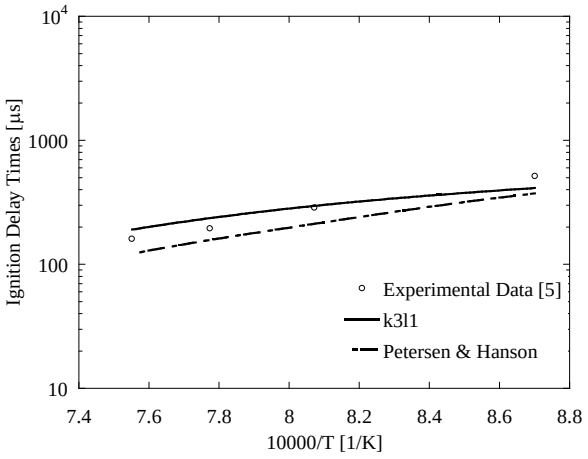

Figure 1. Comparison of experimental data and numerical results of ignition delay time for $0.2CH_4+0.133O_2+0.67N_2$ at 115 atm

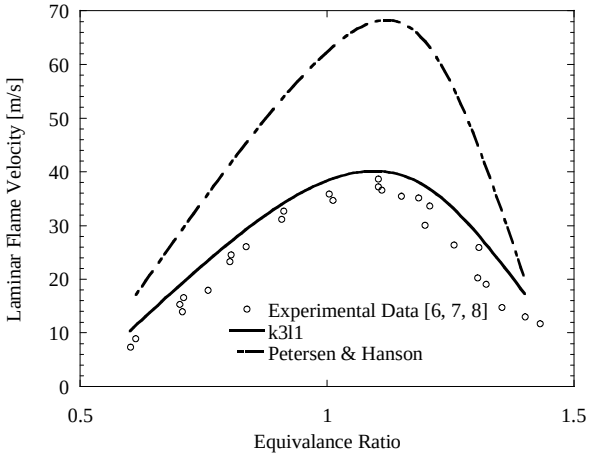

Figure 2. Comparison of experimental data and numerical results of 1D laminar flame velocity for methane-air at 1 bar, 298 K

3 Constructing Reduced Chemical Reaction Model

In order to construct a reduced chemical reaction model, the Direct Relation Graph method [8] is applied. From Figs. 1 and 2, k3l1 is chosen as the reliable chemical reaction model and it is used as a base for new reduction models. Two sets of chemical reaction models are constructed by adjusting threshold values such as 0.1 and 0.3. Table 1 shows the obtained reduced chemical reaction models. They are named as DRG01 and DRG03, respectively. DRG01 has 35 species and 134 elementary reactions and DRG03 has 27 species and 120 elementary reactions. As in section 2, the comparisons

are conducted with not only the experimental ignition delay times but also the experimental laminar flame velocities. So the laminar flame velocities and ignition delay times are calculated using DRG01 and DRG03. The numerical results are compared with the ignition delay times by Petersen et al. [5] and the laminar flame velocities by Vagelopoulos et al. [6, 7] and Rozenchan et al. [8]

Figure 3 shows the comparison of ignition delay times between the experimental data and numerical results. DRG01 agrees well with the experimental data but DRG03 does not agree well with them. Note that the numerical results by DRG01 and k3l1 are almost same. Figure 4 shows the comparison of laminar flame velocities between the experimental data and the numerical results. Both DRG01 and DRG03 agree with the experimental data, however, the equivalence ratios for maximum flame velocity calculated by both models differ from the experimental data and numerical results by original k3l1.

From the above discussions, DRG01 would simulate accurate combustion phenomena rather than DRG03, however, the numerical results of laminar flame velocities by DRG01 differ from these by k3l1 at equivalence ratios > 1. This is because some elementary reactions related with C_2-hydrocarbon are reduced from k3l1 by DRG method. In addition, DRG01 still has so many species and elementary reactions that this model is difficult to be used for CFD simulations. So we found that it is hard to construct reduced chemical reaction models only with DRG method. Therefore, DRG01 has to be reduced more by other reduction method, or the original model, k3l1, has to be reduced by other reduction methods.

Table 2. The reduced chemical reaction model with DRG method

Model	Threshold Value	Species	Elementary reaction
k3l1 (original)	-	68	325
DRG01	0.1	35	134
DRG03	0.3	27	120

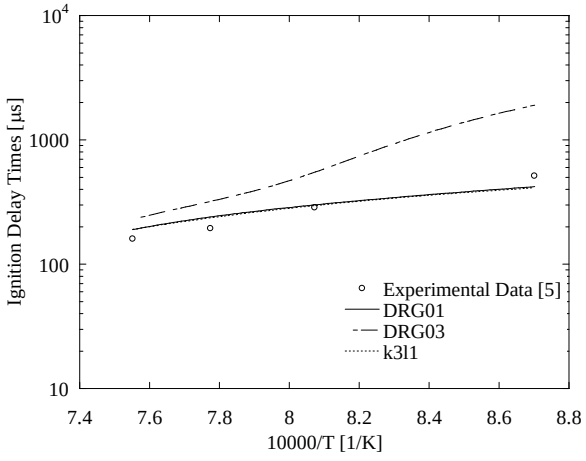

Figure 3. Comparison of experimental data and numerical results of ignition delay time for $0.2CH_4+0.13O_2+0.67N_2$ at 115 atm

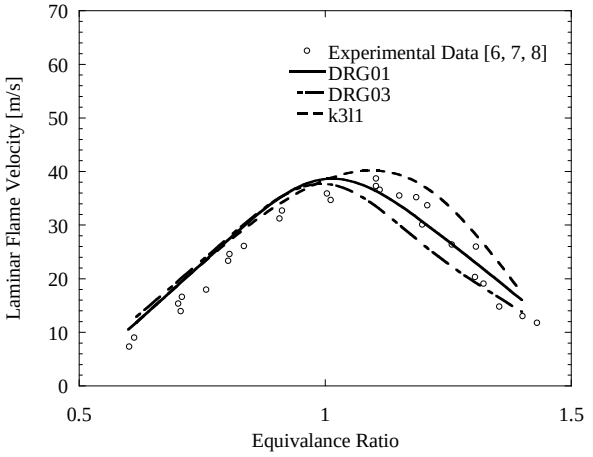

Figure 4. Comparison of experimental data and numerical results of 1D laminar flame velocity for methane-air at 1 bar, 298 K

4 Conclusion

The numerical results with k3l1 or Petersen & Hanson model are compared with experimental data to be checked if they agree well with experimental data or not. Because of this, k3l1 agrees well with

experimental data but Petersen & Hanson model agrees well with the experimental data of ignition delay time but not of laminar flame velocity. So it is necessary to construct a new reduced chemical reaction model. DRG01 and DRG03, reduced from k3l1, are constructed as reduction models for methane combustion. It is found that DRG01 agree well with experimental data of ignition delay times and laminar flame velocities at equivalence ratios under 1. The results of laminar flame velocities with DRG01 are different from the results with k3l1 at higher equivalence ratios than 1. This is because some elementary reactions related with C_2-hydrocarbon are dropped from k3l1 by DRG method. DRG01 still has too many species and elementary reactions to apply for CFD simulations and differs from the results by k3l1. So DRG01 has to be reduced more or that k3l1 has to be reduced by other methods.

Acknoledgement

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