Research paper

Numerical approach to one-dimensional CH_4/O_2 detonation with the reduced chemical kinetic model DRG30

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Abstract

In order to understand the effect of the CH_4/O_2 chemical kinetic models for detonation phenomena, the numerical calculations use one detailed chemical kinetic model k3l1 and four reduced chemical kinetic models such as DRG30 model, DRG23 model, Petersen & Hanson model, and Soetrisno model. At first, the calculations of laminar flame velocity and one-dimensional ZND model are performed to compare with k3l1 model. Then, it is shown that DRG30 model is the most reliable reduced chemical kinetic model in four reduced kinetic models in these conditions. Next, the one-dimensional Euler simulations are performed with k3l1 model, DRG30 model, Petersen & Hanson model, and Soetrisno model. The results are discussed about detonation velocity history, and instantaneous pressure and temperature profiles. The detonations using k3l1, DRG30, and Petersen & Hanson models can propagate unstably, but Soetrisno model cannot reproduce a detonation. As a result, the similar features appear between the results with k3l1 model and DRG30 model.

Keywords : methane, detonation, CFD, chemical kinetic model

1. Introduction

Detonation is a shock-induced combustion wave propagating through a reactive mixture and has been studied from the safety engineering for long time. The detonation propagation limit is especially important to understand detonation phenomena and to prevent the detonation from propagating. The spinning detonation, which occurs near the limit states, is studied by experiments[1] and numerical simulations[2]. It is difficult to observe the detonation phenomena in detail by experiments because of its supersonic propagating velocity. Therefore, as for hydrogen fuel, three-dimensional detonation was simulated using a H_2/O_2 detailed reaction model by Tsuboi et al.[3], and the pressure dependence and the structures of spinning detonation were discussed in this work. However, as for hydrocarbon fuel, the oscillating behavior of detonation, which cannot be observed for hydrogen fuel, was reported[4] and six modes were classified depending on the stabilities of detonation velocity[5]. In this paper, the methane fuel

detonation is discussed because it's the simplest hydrocarbon and is important as a next generation fuel. The experiments of methane detonation near the limit were reported by our group[6]. Methane detonation also has oscillating behavior. Then, to understand the phenomena in detail, Computational Fluid Dynamics (CFD) simulation have to be performed.

The problems of numerical simulation of methane fuel with a detailed reaction model requires more computational time than the case of H_2/O_2 gas mixture, because the computational time increases with almost square of the chemical species. In order to reduce Computational time, one step model is used to calculate the detonation wave for hydrocarbon/oxygen gas mixture[7]. However, calculation with one step model cannot predict the detonation limit because the heat release rate is important around the detonation propagating limit. Therefore, a reliable reduction model is necessary to reduce computational time and to understand the detonation limit for hydrocarbon/oxygen gas mixture.

The objective of this work is to calculate CH_4/O_2 detonation to show the difference of chemical kinetic models. First of all, the calculations of laminar flame velocity and ZND model[8] with the proposed reduction model are discussed and compared with other reaction models. Finally, one-dimensional detonation simulations of CH_4/O_2 gas mixture are performed with three reduced kinetic models to show the effect of the reaction models on the detonation structure.

2. Numerical method and conditions

2.1 Chemical reaction models

The reduced chemical kinetic models DRG30 model and DRG23 model based on the detailed chemical reaction model k3l1 model[9] is constructed using Direct Relation Graph method[10] (DRG) to reduce computational time. This models are reduced to be fitted to the experimental laminar flame velocity at 1.01325×10^5 Pa[11], in order to study the methane fuel detonation under low-pressure environments. The other reduction models, Petersen & Hanson model[12] and Soetrisno model[13], are also chosen to be compared with DRG30 model and DRG23 model, because these reduced chemical kinetic models were constructed for the numerical simulations under high pressure states. The numbers of speceis and elementary reactions are shown in Table 1, respectively.

Table 1 Number of species and elementary reactions in chemical kinetic models.

Models	Species	Elementary reactions
k3l1	68	334
DRG30	30	150
DRG23	23	99
Petersen & Hanson	21	34
Soetrisno	12	19

2.2 One-dimensional numerical simulation using ZND model

The one-dimensional numerical simulation using ZND model is performed in order to estimate the difference of these models. The gas mixture is stoichiometric CH_4/O_2. Initial pressures are 1.01325×10^4 Pa and 1.01325×10^5 Pa, and initial temperature is 298 K. Chapman-Jouguet (CJ) values are calculated with AISTJAN[14]. The chemical kinetic models are k3l1 model, DRG30 model, DRG23 model, Petersen & Hanson model, and Soetrisno model as shown in Table 1.

2.3 Numerical simulation of one-dimensional CH_4/O_2 detonation

Four chemical kinetic models (k3l1 model, DRG30 model, Petersen & Hanson model, and Soetrisno model) in Table 1 are used for one-dimensional reactive flow simulation in order to study the difference of models in more detail than ZND model. The governing equations are the Euler equations with 68, 30, 21, and 12 chemical species, respectively. They are explicitly integrated using 3rd-order Total Variation Diminishing Runge-Kutta method[15]. The chemical reaction source term is integrated by the stiff solver Variable-Coefficient Ordinary Differential Equations solver[16] in order to avoid a stiff problem. Advection Upstream Splitting Method fllux Difference and flux Vector scheme[17] with2nd-order Monotone Upstream-centered Scheme for Conservation Laws[18] and minmod limiter is used for the numerical flux in the convective terms. The number of computational grid is 40,000 with the grid size of 5μm and ignition zone uses 1000 grids. The gas mixtures are stoichiometric CH_4/O_2. Initial pressure and temperature are 1.01325×10^4 Pa and 298.15 K. Ignition pressure and temperature are 8.106×10^5 Pa and 1800 K.

3. Results and discussion

3.1 Numerical results of the laminar flame velocities

The numerical results of the laminar flame velocities using the chemical kinetic models are in Figure 1. DRG30 model and DRG23 model are much more reliable reaction model than Petersen & Hanson model and Soetrisno model, because the results with Petersen & Hanson and Soetrisno models have twice value compared with the Rozenchan's experimental data in Figure 1.

3.2 One-dimensional numerical simulation with ZND model

The results with ZND model are shown in Figures 2 and 3. The temperature profiles for DRG30 model and k3l1 model show more similar feature than other reduced chemical kinetic models. Especially, the results with Petersen & Hanson model and Soetrisno model require larger ignition time to become a constant temperature, comparing with the results with k3l1 model. In addition, comparing the results for DRG30 model with DRG23 model, 23 chemical species at least are required for the reduced kinetic model, in order to fit the order of ignition time to become a constant temperature to that of k3l1

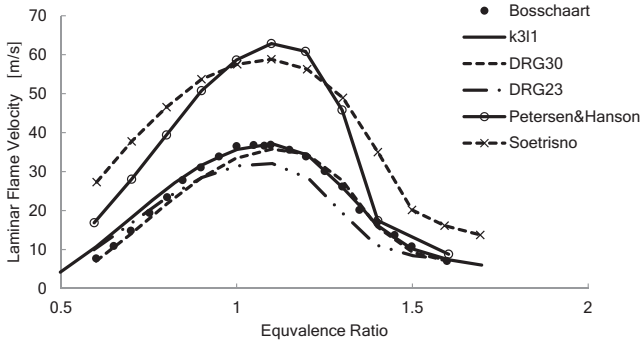
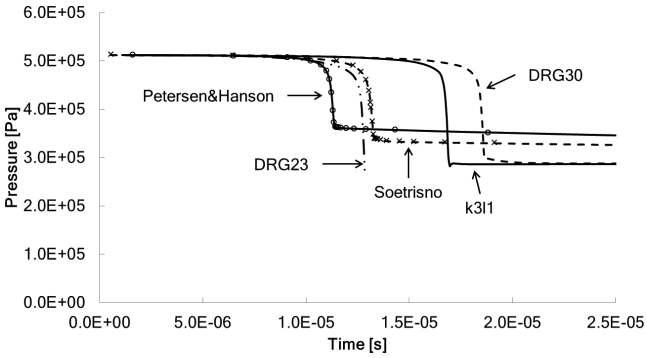


Figure 1 One-Dimensional laminar flame velocity of CH_4/O_2 for 1.01325x10^5 Pa.



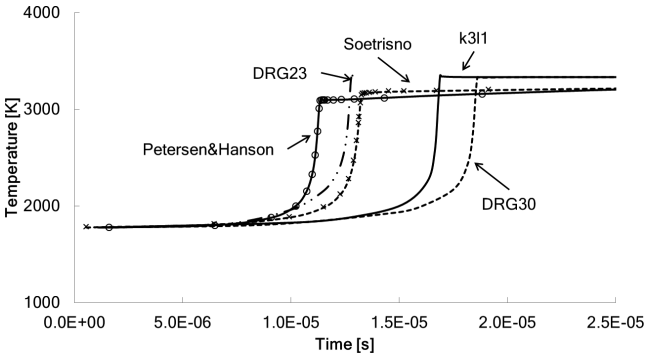
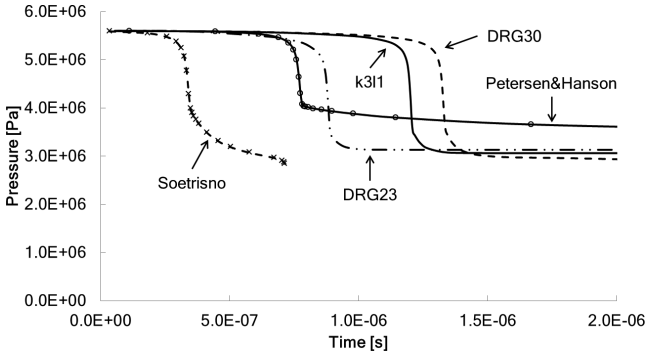


Figure 2 The pressure and temperature profiles for 1.01325x10^4 Pa.

model. DRG30 model is more reliable reduced chemical kinetic model than DRG23 model, Petersen & Hanson model, and Soetrisno model in these conditions. And from referring the experiences, the difference between k3l1 model and DRG30 model does not dominantly affect the results of CFD simulations. Therefore, we conclude DRG30 model can replace k3l1 model in these conditions.

3.3 Numerical simulation of one-dimensional CH_4/O_2 detonation

The comparison of computational time ratio for DRG30 is shown in Figure 4. The computational times depend on the number of species. The results of detonation velocities are shown in Figure 5. The velocities for k3l1 model, DRG 30 model, and Petersen & Hanson model are higher than CJ velocity, at first. After some strong peaks, however, the velocity becomes lower than CJ velocity. The strong peaks appear because the reaction and shock fronts closely interact. The one-dimensional detonation without a piston support is known that the detonation cannot self-sustain because of instability of fluids[19]. Therefore, the reaction



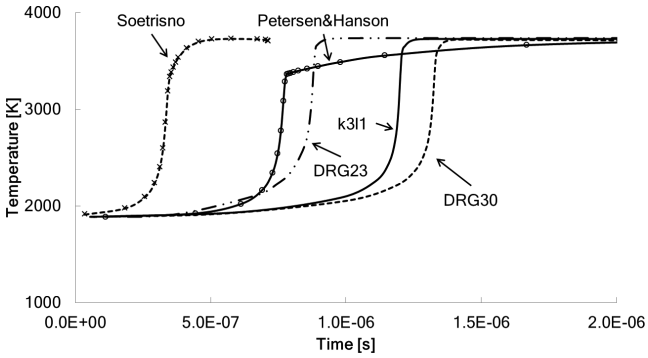


Figure 3 The pressure and temperature profiles for 1.01325x10^5 Pa.

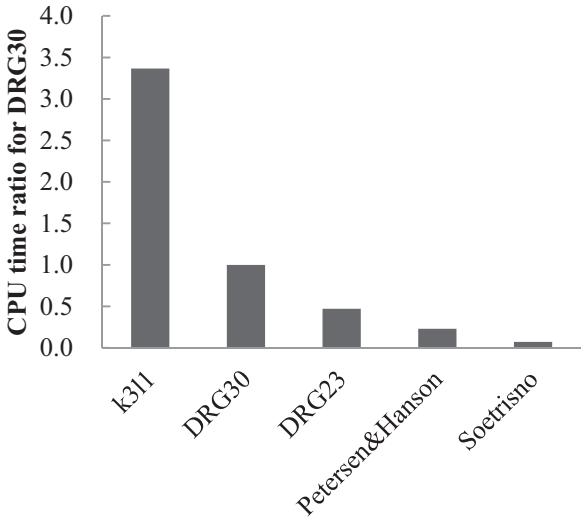


Figure 4 Comparison of computational times for DRG30.

and shock fronts are decoupled and its velocity becomes lower than CJ velocity. The results with Soetrisno model show the detonation wave can't propagate under this condition.

The results of instantaneous pressure and temperature with k3l1 model, DRG30 model, Petersen & Hanson model, and Soetrisno model are plotted in Figures 6-9. In Figures 6-8, the some pressure profiles have strong peaks near the wave front. The peak pressures appear just after the detonation velocities have the strong peaks. In Figures 6-8, the some temperature profiles have the peaks in the detonation front. They also appear just after the detonation velocities have the strong peaks. As shown in temperature profiles, it is clear that shock wave and combustion front are closely coupled during a detonation, but they are decoupled after the detonation disappeared.

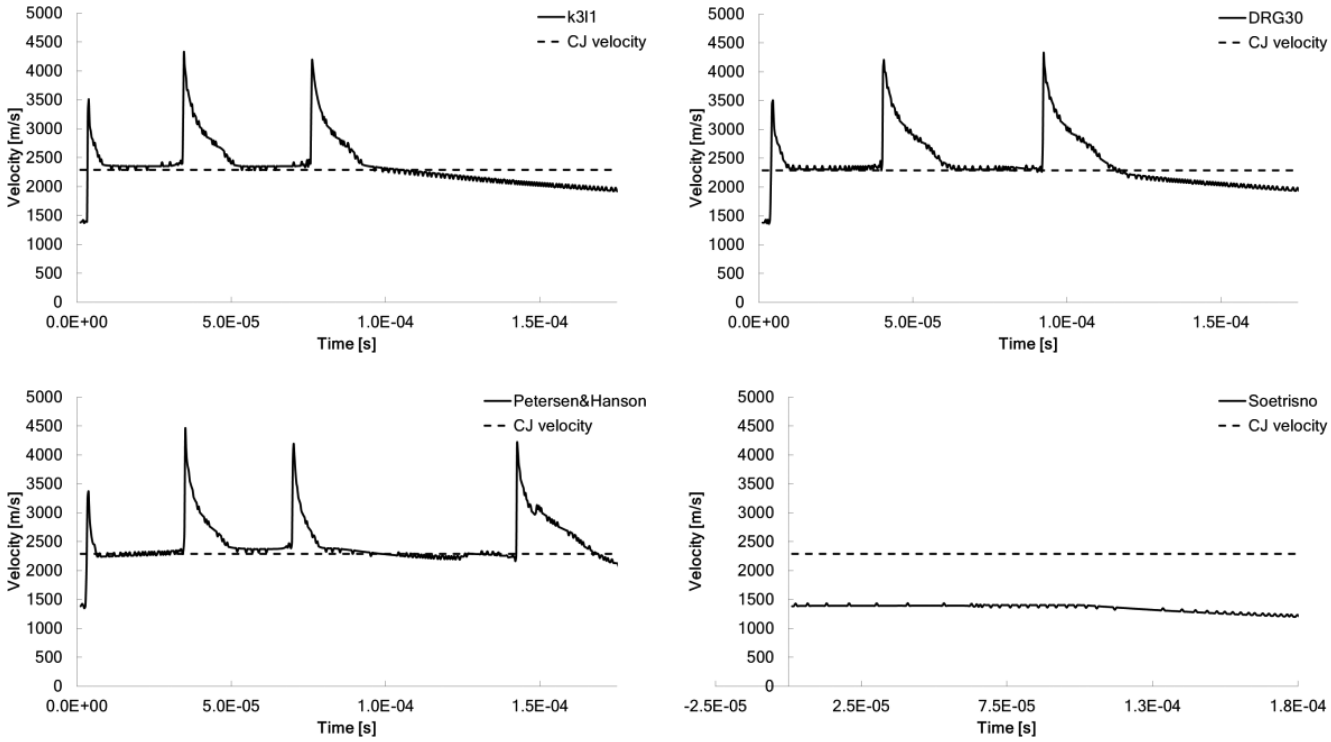


Figure 5 Comparison of detonation velocity between various chemical kinetic models. CJ velocity is 2290 m/s.

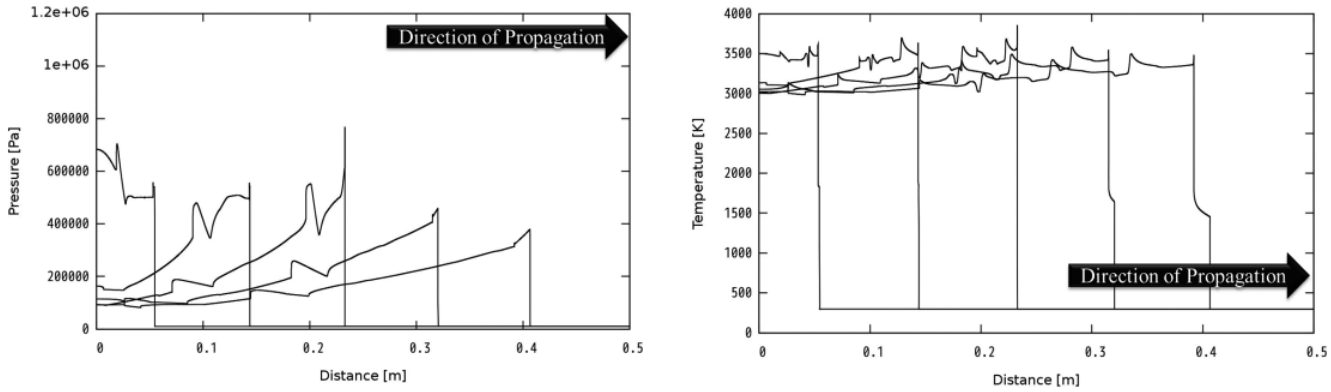


Figure 6 Instantaneous pressure and temperature profiles for k3l1 model at 1.83×10^{-5}, 5.20×10^{-5}, 8.62×10^{-5}, 1.24×10^{-4}, and 1.66×10^{-4}s.

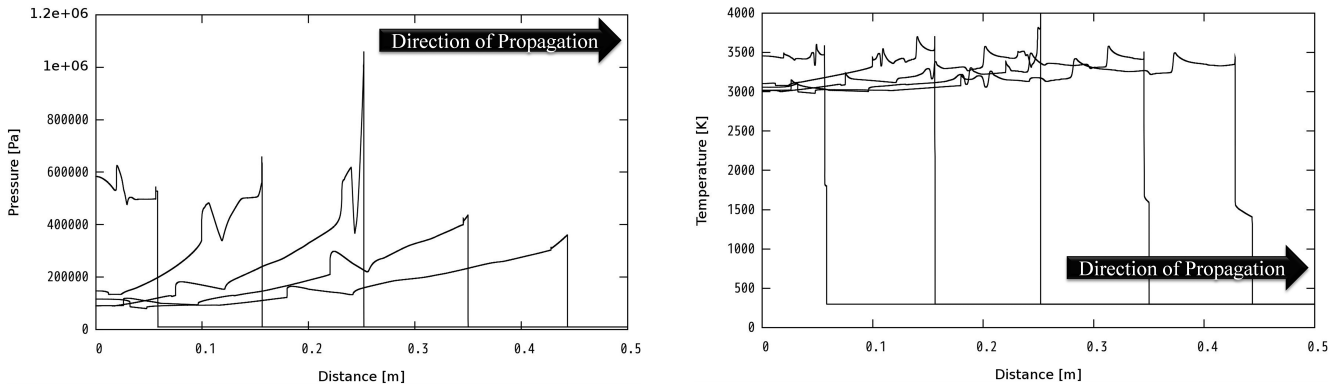


Figure 7 Instantaneous pressure and temperature profiles for DRG30 model at 2.02×10^{-5}, 5.68×10^{-5}, 9.56×10^{-5}, 1.35×10^{-4}, and 1.82×10^{-4}s.

As for Soetrisno model, the detonation does not appear in these conditions because there are no peaks in Figure 9.

Detonation is multi-dimensional phenomena and the two-dimensional simulations are requires to understand the effects of the chemical reaction models. Then, it's difficult to understand the effects of the chemical reaction models. However, the results with DRG30 model are almost similar with the results with k3l1 model. Then, the one-dimensional detonation in CH_4/O_2 gas mixture using the reliable reduction model DRG30 is successfully

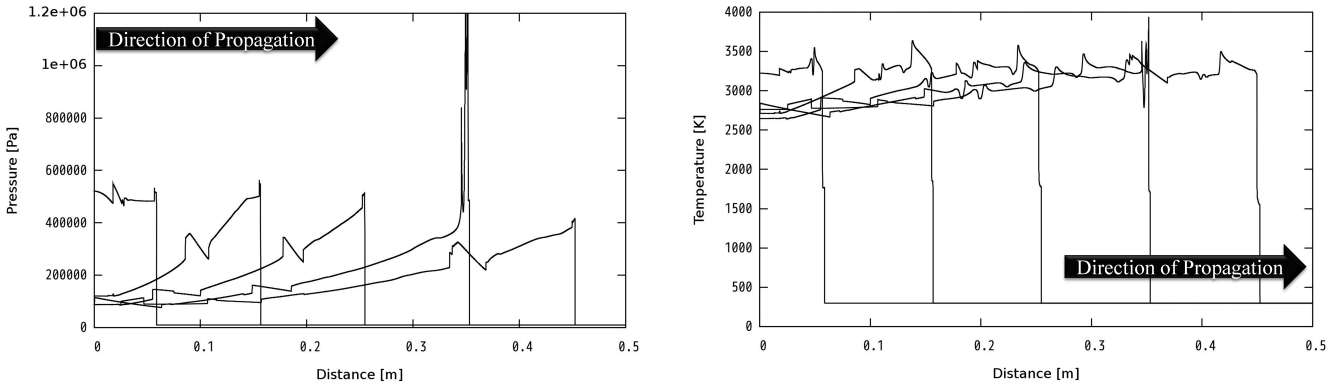


Figure 8 Instantaneous pressure and temperature profiles for Petersen & Hanson model at 2.09×10^{-5}, 5.89×10^{-5}, 9.82×10^{-5}, 1.42×10^{-4}, and 1.80×10^{-4}s.

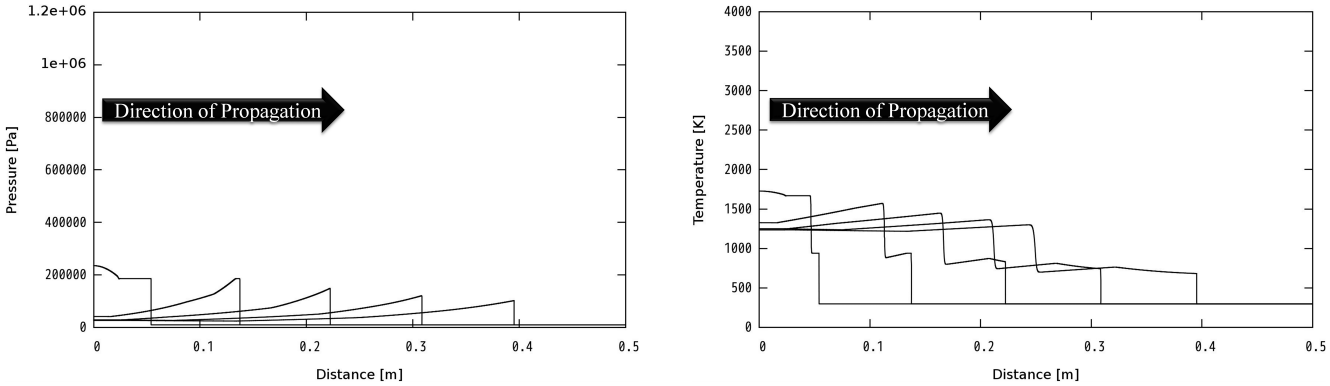


Figure 9 Instantaneous pressure and temperature profiles for Soetrisno model at 2.97×10^{-5}, 8.95×10^{-5}, 1.53×10^{-4}, 2.26×10^{-4}, and 3.06×10^{-4}s.

simulated.

4. Conclusions

The numerical simulation on CH_4/O_2 detonation with the chemical kinetic models, k3l1 model, DRG30 model, DRG23 model, Petersen & Hanson model, and Soetrisno model, are estimated in order to understand the effects of chemical kinetic models. The laminar flame velocity and ZND calculations with DRG30 model are more similar to those of k3l1 model. However, the results with Petersen & Hanson model and Soetrisno model don't agree well with those of k3l1 model. Therefore, DRG30 model is a reliable reaction model to simulate detonation in these conditions.

As for the one-dimensional simulation, the results with k 3l1 model, DRG30 model, and Petersen & Hanson model can propagate as a detonation wave. In the present simulation conditions, Soetrisno model cannot reproduce a detonation. As for results of instantaneous temperature and pressure profiles, there are similar features between k 3l1and DRG30 models. As a result, the simulations with DRG30 model can get more reliable results comparing with the results of other reduced chemical kinetic models, and can replace k3l1 model in these conditions.

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簡略化モデルDRG30を用いた 一次元メタン酸素デトネーションの数値解析に向けた研究

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メタン酸素の化学反応モデルが爆轟現象に与える影響を調査するために，詳細化学反応モデルのk3l1とDRG30, DRG23, Petersen & Hanson，Soetrisnoの４つの簡略化モデルを用いて計算を行った．まず初めに，層流火炎速度及びZNDモデルの計算を行い，詳細化学反応モデルk3l1で得られた結果との比較を行った．結果としてDRG30モデルは選択した４つのモデルの中では十分信頼性が高いことが分かった．次に一次元Euler方程式を解くことにより比較を行った．結果として，k3l1モデル，DRG30モデル，DRG23モデルはデトネーションとして伝播することが確認できたが，Soetrisnoモデルを持ちいた解析ではデトネーションとして伝播しなかった．比較の結果，DRG30モデルは詳細化学反応モデルk3l1とよく一致することが示され，メタン酸素爆轟計算においてDRG30モデルは十分利用可能であることが分かった．

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