Construction of Compact Reaction Models for Methane and Natural Gas using Genetic Algorithms

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1 Introduction

The size of a reaction model has a great impact on the computation cost of Computational Fluid Dynamics (CFD) for combustion. To reduce the computational costs, methods of generating reduced reaction models have been developed, e.g., Direct Relation Graph (DRG) [1]. In reduction methods like DRG, unimportant species were removed from a detailed reaction model, and rate parameters of a detailed reaction model were maintained. Due to the process of the reduction concept, there is a trade-off relation between reducing the size of a model from a detailed model and prediction accuracy. In addition, it is known that reaction models have irremovable key species, which limits the numbers of species and reactions that can be reduced [2]. In other words, too small a set of species and reactions with inherited rate parameters makes it impossible to reproduce combustion properties within practically acceptable errors.

To overcome this issue, we proposed a new way to build a compact reaction model using abbreviated reaction pathways (ARP) and a genetic algorithm (GA). ARP is a simplified reaction pathway using a few virtual species and reactions. Virtual species lamped and replaced key species in a detailed reaction model. Virtual reactions were reactions that contain virtual species. Reduction methods provide the numbers of species and reactions after the reduction process, while the proposed method first decided on the numbers of species and reactions of a compact model. The rate parameters of virtual reactions were optimized and determined by GA so that the compact model can reproduce combustion properties determined by users, e.g., ignition delay time (IDT) and laminar flame speeds (LFS). GA was used to optimize the rate parameters of a reaction model to improve the prediction accuracy [3], because of its robustness.

In this study, we apply ARP and GA for generating compact models of methane at first. Rate parameters of virtual reactions in the compact methane model were optimized so that the compact model predicted both IDT and LFS of single fuel component. After that, we apply this method for generating a compact model of natural gas and confirm the validity of the proposed method for a practical fuel.

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2 Method of generating compact models

There are four steps in the method of generating a compact model using ARP and GA. (1) Deciding the reaction configuration, (2) Defining the optimization problem, (3) Optimization, (4) Evaluation. At first, we decide on the reaction configuration of compact models. A conceptual diagram of ARP is shown in Figure 1.

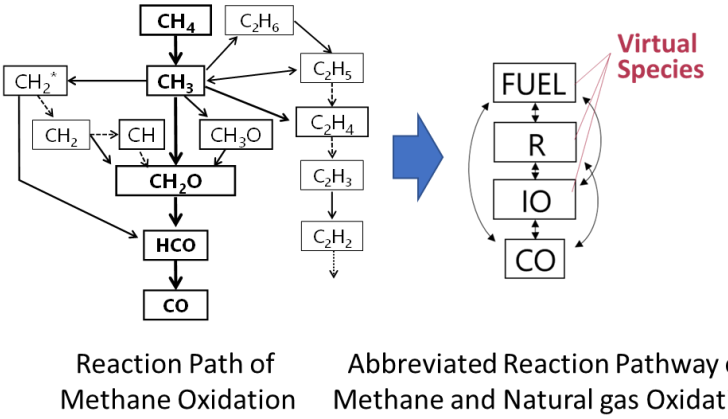

Figure 1: Conceptual diagram of reaction path of CH_4 oxidation and abbreviated reaction pathways of CH_4 and natural gas.

Because the primary component of natural gas is methane, we applied the same reaction configuration for methane to natural gas. For both fuels, we abbreviated the oxidation pathways from fuel to CO using two intermediates as FUEL→R→IO→CO, where FUEL, R, and IO were virtual species. FUEL, R, and IO respectively represented fuel, fuel radical, and aldehyde. The thermodynamic and transport properties of R and IO were the same as those of CH_3 and CH_2O in Aramco 3.0 [4], respectively. The transport property of FUEL was taken from that of CH_4 in Aramco 3.0. In methane case the thermodynamic property of FUEL was taken from that of CH_4 in Aramco 3.0, whereas in natural gas case that of FUEL was calculated using FITDAT with Aramco 3.0, where the natural gas composition was set to CH_4: 96.91 vol%, C_2H_6: 2.33 vol%, C_3H_8: 0.54 vol%, *n*-C_4H_{10}: 0.10 vol%, and *i*-C_4H_{10}: 0.12 vol% [5]. And then, a compact model was composed of virtual reactions and detailed H_2-O_2/CO reactions. The vertical reactions were chosen with each virtual species + X, namely, FUEL + X, R + X, and IO + X, where X was H_2-O_2 radicals (H, O, OH, and HO_2).Reactions of H_2-O_2/CO subsets were used from Aramco 3.0 as it was. The total size of the compact reaction model was 14 species and 55 reactions.

As the second step, the objective function f to be minimized by GA was defined as follows:

$$f = w_{IDT} f_{IDT} + w_{LFS} f_{LFS}, \tag{1}$$

$$f_i = \sqrt{\frac{1}{N_i} \sum_{j=1}^{N_i} \left(\log_{10} \frac{i_{c,j}}{i_{d,j}} \right)^2} \tag{2}$$

Where N_i was the number of the test conditions for combustion property i, w_i was the weighting factor for i, $i_{c,j}$ was the combustion property computed with a compact reaction model at the jth test condition, and $i_{d,j}$ was a combustion property computed with Aramco 3.0 at the jth test condition.

Combustion properties of both IDT and LFS were evaluated by linear combination with weighting factors which were set to w_{IDT} = 1 and w_{LFS} =5. IDT at atmospheric pressure and equivalence ratios of 0.5, 1.0, and 2.0 over a high-temperature range were evaluated (N_{IDT} = 9 at ϕ = 0.5, 1.0, 2.0, T_0 = 1250, 1538, 2000 K, P_0 = 1 atm). LFS at atmospheric pressure and normal temperature over an equivalence ratio range of 0.7 to 1.45 were evaluated (N_{LFS} = 9 at ϕ = 0.7, 0.8, 0.9, 1.0, 1.05, 1.15, 1.25, 1.35, 1.45, T_0 = 300 K, P_0 = 1 atm). Computations of IDT and LFS were conducted using Cantera 2.5 [6]. We can strictly control the error of user-defined combustion characteristics in each condition.

To apply GA to reaction model systems, one compact model was regarded as an individual which had 84 designed variables (28 virtual reactions × 3 Arrhenius parameters per reaction) to be optimized. Initial values of design variables were randomly given by Gaussian distribution with a mean of 0 and a standard deviation of 10. Conversion of design variables ν to each Arrhenius parameter was made as follows: 10^{ν} for a pre-exponential factor, 0.01ν for a temperature exponent, and $1000|\nu|$ for activation energy in cm^3-mol-cal-s units. Population size, elite fraction, and mutation ratio were 640, 0.2, and 0.15, respectively. A GA function in the global optimization toolbox of MATLAB R2022a (MathWorks Inc.)[7] was used for the implementation of the optimization. The error ratio was defined as the percentage of $(i_{c,j} - i_{d,j}) / i_{d,j}$.

3 Results and Discussions

3.1 Methane Case

In the case of the compact model of methane, the optimization was terminated at the 400th generation when the objective function of the best individual reached 0.10 (f_{IDT} = 0.05 and f_{LFS} = 0.05). We regarded the best individual of 400th as the optimized compact model of methane.

Figure 2 shows the prediction results of LFS computed with the optimized compact model of methane and Aramco 3.0 at the test conditions of the objective function. The maximum error ratio in those conditions was 4.1% at ϕ = 1.45. The minimum error ratio in those conditions was 0.3% at ϕ = 1.25. The optimized compact model of methane well replicated the LFS predicted by Aramco 3.0.

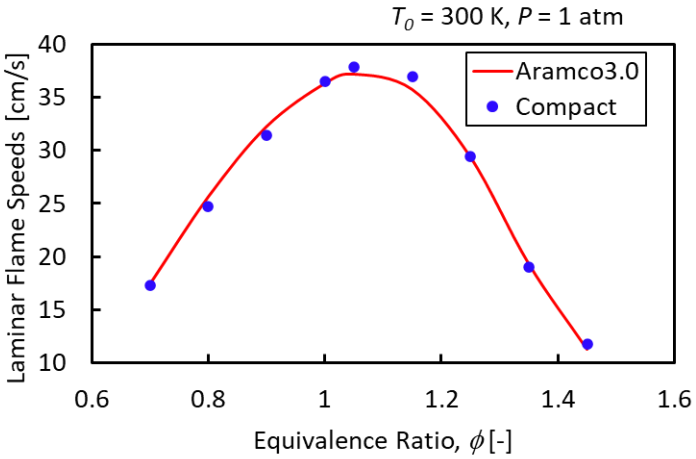

Figure 2: Comparison of laminar flame speeds using the optimized model of CH_4 and Aramco 3.0. (P_0 = 1 atm, T_0 = 300 K, ϕ = 0.7, 0.8, 0.9, 1.0, 1.05, 1.15, 1.25, 1.35, and 1.45)

Figure 3 shows IDT computed with the optimized compact model of methane and Aramco 3.0 at the test conditions of the objective function. The maximum error ratio in those conditions was −22.3% at ϕ = 2.0, T_0 = 2000 K. The minimum error ratio in those conditions was 0.2% at ϕ = 1.0, T_0 = 1250 K. The optimized compact model of methane well reproduced IDT predicted with Aramco 3.0. The

optimized compact model of methane generated by the present method reproduced both LFS and IDT with high accuracy.

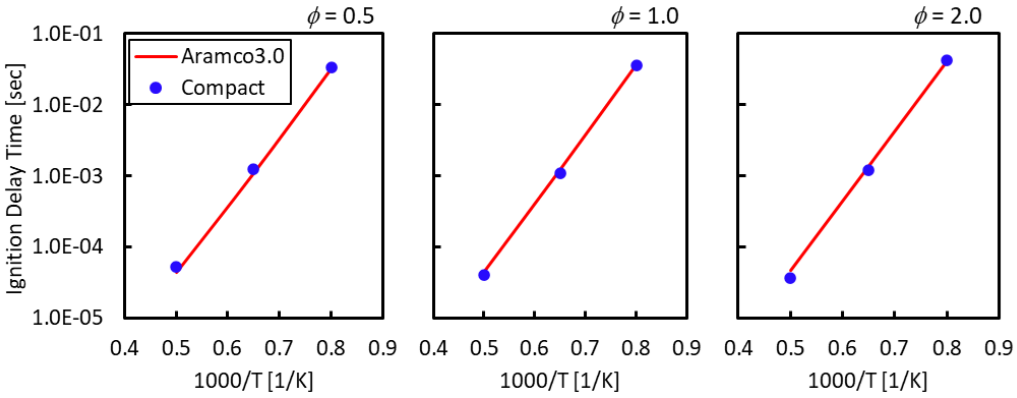

Figure 3: Comparison of ignition delay times (P_0 = 1 atm, T_0 = 1250, 1538, 2000 K, ϕ = 0.5, 1.0, 2.0) using the compact model of CH_4 and Aramco 3.0.

3.2 Natural Gas Case

In the natural gas case, the optimization was terminated at the 450th generation when the objective function of the best individual reached 0.16 (f_{IDT} = 0.09 and f_{LFS} = 0.07). We regarded the best individual of the 450th generation as the optimized compact model of natural gas.

Figure 4 shows LFS computed with the optimized compact model of natural gas and Aramco 3.0 at the test conditions of the objective function. The maximum error ratio in those conditions was 7.2% at ϕ = 1.45. The minimum error ratio in those conditions was −0.2% at ϕ = 0.7. The optimized compact model of natural gas well reproduced LFS predicted with Aramco 3.0. Note that LFS of natural gas are very similar to those of methane.

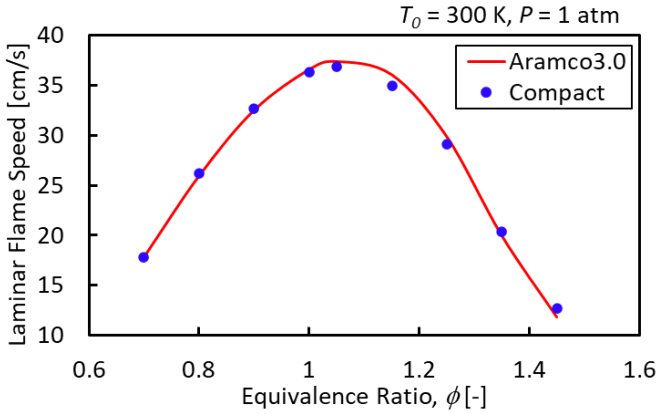

Figure 4: Comparison of the prediction results for laminar flame speeds (P_0 = 1 atm, T_0 = 300 K, ϕ = 0.7, 0.8, 0.9, 1.0, 1.05, 1.15, 1.25, 1.35, 1.45) using the compact model of natural gas and Aramco 3.0.

Figure 5 shows IDT computed with the optimized compact model of natural gas and Aramco 3.0 at the test conditions of the objective function. The maximum error ratio in those conditions was 25.1% at ϕ = 0.5, T_0 = 2000 K. The minimum error ratio in those conditions was −0.3% at ϕ = 0.5, T_0 = 1250 K. The optimized compact model of natural gas well reproduced IDT predicted with Aramco 3.0. The figure also plots IDT computed with the optimized compact model of methane and Aramco 3.0 at the

test conditions of the objective function for methane. Because of the high reactivity components of C2 – C4 hydrocarbons in natural gas, IDT of natural gas are two to three times shorter than that of methane. The present method generated the optimized compact model of natural gas without including C2 – C4 hydrocarbons and their reaction pathway, namely, keeping the number of species as 14 in the model.

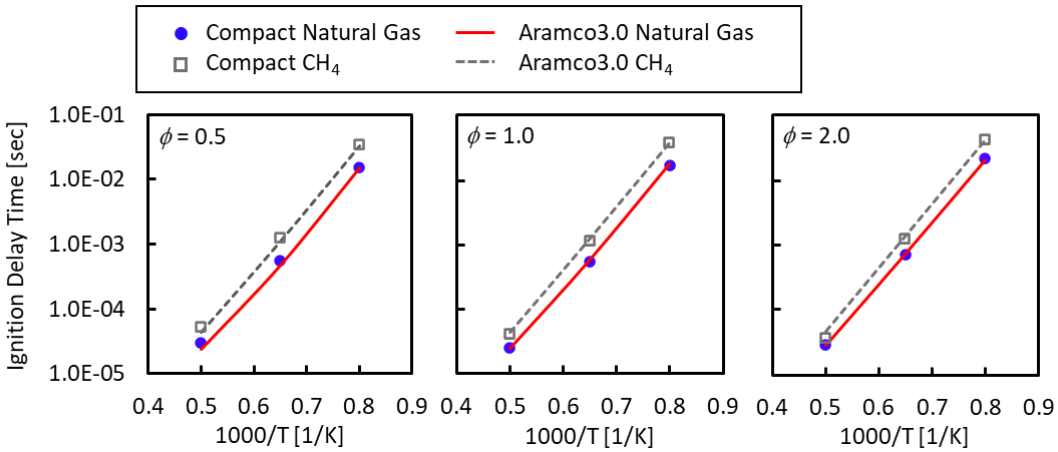

Figure 5: Comparison of the prediction results for ignition delay times (P_0 = 1 atm, T_0 = 1250, 1538, 2000 K, ϕ = 0.5, 1.0, 2.0) using the compact model of natural gas and Aramco 3.0. Results in the methane case shown in Figure 4 are also plotted as a reference.

4 Conclusions

The new method of generating a compact reaction model using abbreviated reaction pathways (ARP) and a genetic algorithm (GA) was proposed and applied to methane and natural gas. The present method generated a compact model of methane with 14 species and 55 reactions. The generated models well reproduced both laminar flame speeds and ignition delay times predicted with Aramco 3.0.

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