

Numerical investigation of the prediction performance of the chemical kinetics for the MILD combustion

Yu Jeong Kim and Chang Bo Oh
Department of Safety Engineering, Pukyong National University
Busan, Republic of Korea

1 Introduction

The Moderate or Intense Low oxygen Dilution (MILD) combustion is a promising combustion technique which can reduce the pollutants emission and enhance the thermal efficiency of combustion system. In this technology, combustion products are recirculated and mixed into air-stream, thereby it reduces the concentration of O₂ and temperature of combustion chamber [1]. This combustion mode shows a high thermal efficiency and effectiveness in CO₂ reduction. And it has advantage of low NO_x emission since internal temperature of combustion chamber becomes low and uniform. Currently, many studies focuses on the fundamental MILD combustion characteristics are in progress for simple geometries [2-4]. A CFD study of the MILD combustion requires an optimal chemical kinetic mechanism to simulate the MILD combustion efficiently and accurately. Some chemical kinetics have been validated for the MILD combustion of a certain fuel [5-6]. However, more specific information of chemical kinetics for various fuels is still required.

The objective of this study is to investigate the prediction performance of the various chemical kinetic mechanisms which are suitable for the numerical simulation of the methane MILD combustion in a confined jet.

2 Modeling approach

Numerical simulations were performed for methane turbulent MILD jet combustion with the commercial code Fluent 13.0 [7]. A modified standard κ - ϵ turbulence model with $C_{1\epsilon}=1.6$ was adopted in the simulation. The discrete ordinates (DO) radiation model and the weighted sum of gray gases model (WSGGM) were incorporated to treat the radiation heat transfer.

In this study, the prediction performance of five different chemical kinetics was investigated by comparing the flame structure and pollutants emission predicted by each chemical mechanism. The five chemical kinetics considered are:

- (1) 3-step global reaction mechanism of Westbrook and Dryer (3Step) [9],
- (2) modified 4-step global reaction mechanism of Westbrook and Dryer (WD4) [5],
- (3) skeletal mechanism consists of 16 species and 41 reactions (Skeletal) [10],
- (4) shorten full mechanism of GRI-v1.2 consists of 21 species and 84 reactions (DRM-19) [11],
- (5) GRI-v2.11 full mechanism consists of 49 species 279 reactions (GRI-2.11) [12].

For all reaction parameters of these chemical kinetics, please refer to the references. To consider NO_x emission in MILD combustion, the formation routes of thermal, prompt and N₂O intermediate NO were considered in the simulations.

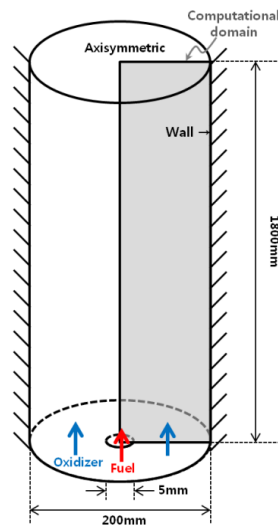


Figure 1. Axisymmetric confined coflow jet geometry for MILD combustion.

Table 1. Velocity (m/s) of the air-stream with the variation of dilution rate.

T_{air}	Dilution rate(Ω)			
	0.0	0.3	0.5	0.7
1100K	0.375	0.530	0.740	1.221

Table 2. Composition of the main species in the air-stream with the variation of dilution rate.

Species	Dilution rate(Ω)			
	0.0	0.3	0.5	0.7
O_2	0.210	0.147	0.105	0.063
N_2	0.790	0.766	0.750	0.734
CO	0.000	0.003	0.005	0.007
CO_2	0.000	0.027	0.045	0.063
H_2O	0.000	0.057	0.095	0.133

Figure 1 shows the geometry of the wall-confined coflow jet combustor with a diameter of 200 mm and height of 1.8 m. The geometry was axisymmetric and a structured non-uniform two-dimensional (2D) grid system was made for the computations. Total number of grids was about 50,400. The inner diameter of fuel nozzle was 5 mm and the thickness of fuel nozzle was neglected for simplicity. Air was supplied at the radially outside of the fuel nozzle. Pure methane was used as a fuel, and the fuel velocity was fixed to 12 m/s, which corresponds to a Reynolds number of approximately 3,400.

The global equivalence ratio (Φ) defined by the amounts of fuel and oxygen in the air-stream was fixed to 0.7. The inlet velocities of air-stream for each condition were provided in Table 1. In this study, only four species of CO_2 , CO, H_2O and N_2 were considered as main ones in combustion product. The concentrations of the four species were obtained by the simulation with an UPSR code [8]. In the UPSR simulation, the combustion products of perfectly mixed methane-air mixture were calculated at $\Phi=1.0$. Table 2 shows the composition of the main species mole fraction in air-stream with the variation of dilution rate (Ω). The dilution rate was defined as:

$$\Omega = \frac{\text{volume of product gases}}{\text{volume of total gases in air steam}} \quad (1)$$

The temperatures of fuel and air-stream were fixed to 300 K and 1100 K, respectively. The wall temperature was fixed to 900 K, which was determined by considering the previous experimental studies for MILD combustor [13]. An outflow boundary condition was given at the outlet of jet flow field, and no-slip condition was given at the wall.

3 Results and Discussions

Figure 2 shows 2D temperature distributions simulated by five different chemical kinetics for $\Omega=0.3$ and $\Omega=0.5$. In the figure, the black border represents the temperature band ranging from 1,250 K to 1,300 K, and it was introduced to distinguish the high temperature region of flame. For $\Omega \leq 0.3$, the temperature distributions predicted by different chemical kinetics were almost identical. However, for $\Omega \geq 0.5$, the flames obtained with DRM-19 and GRI-2.11 was found to be lifted off while the flames simulated with two global and skeletal mechanisms were established near the fuel nozzle. These overall flame features influenced the distributions of species concentration and pollutants emission

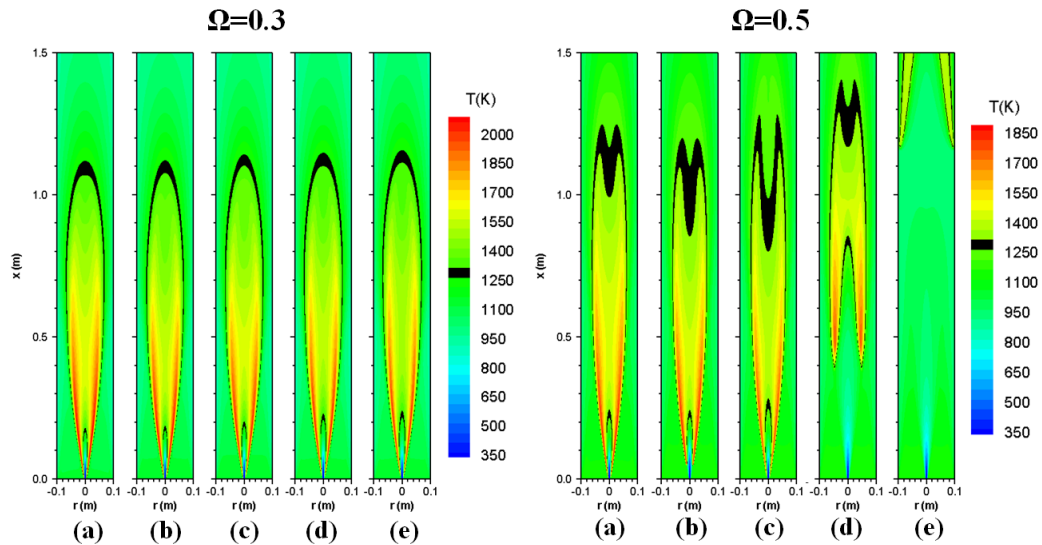


Figure 2. 2D temperature distributions of CH₄ jet when the chemical kinetics were varied for $\Omega=0.3$ and $\Omega=0.5$. (a)3step; (b)WD4; (c)Skeletal; (d)DRM-19; (e)GRI-2.11.

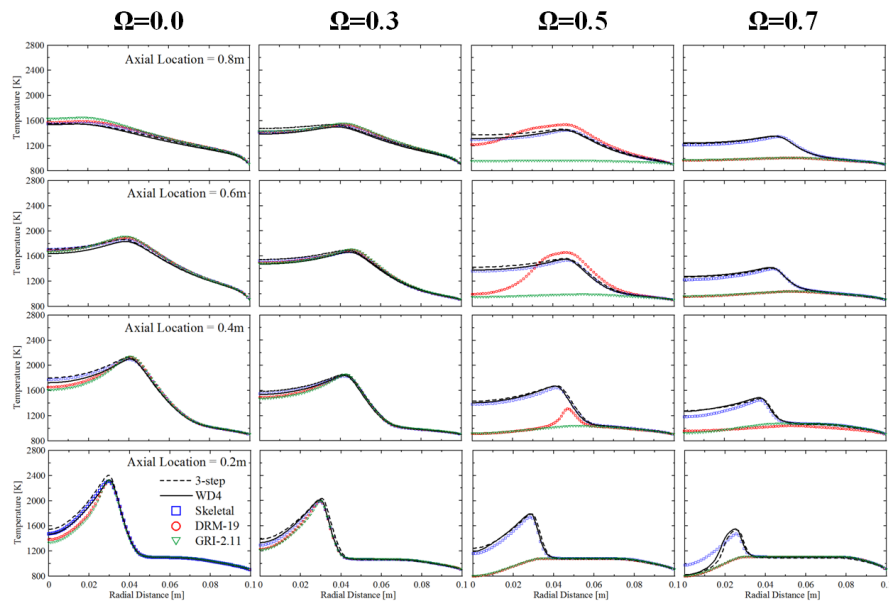


Figure 3. 1D temperature distributions when the chemical kinetics were varied for 3-step, WD4, Skeletal, DRM-19 and GRI-2.11 at various axial locations.

directly, and the relevance of those features is discussed at the following figures.

Figure 3 shows cross-sectional temperature distributions at selected axial locations for given conditions. For $\Omega=0.0$, the flame temperature was high compared to the other dilution rates, and the flame temperature decreased and became uniform with increasing the dilution rate. For $\Omega \leq 0.3$, where flames were not lifted off, the temperature profiles simulated by five chemical kinetics agreed relatively well each other. However, the simulated temperature profiles were not in good agreement because the prediction performance of flame lift-off by each chemical kinetics was different.

Figure 4 shows cross-sectional CO distributions at selected axial locations for given conditions.

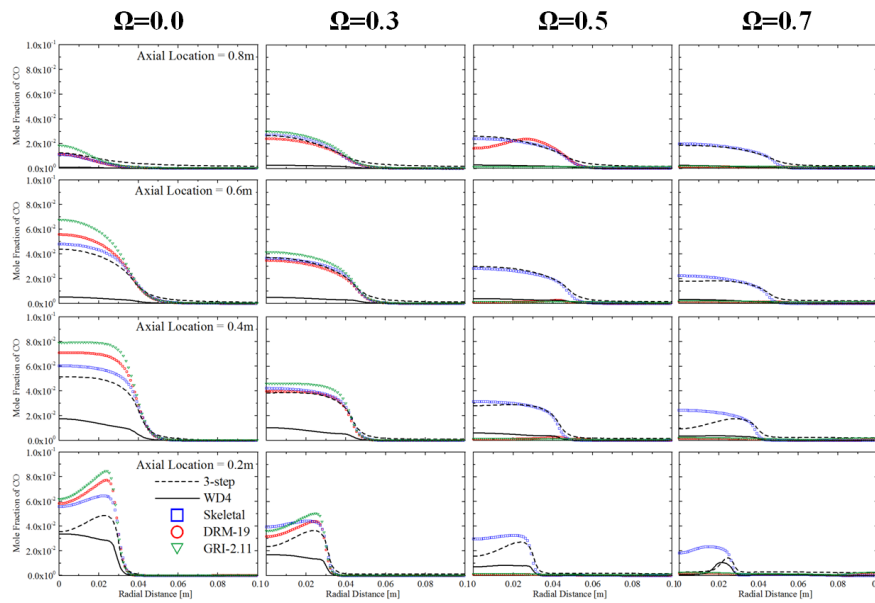


Figure 4. 1D distributions of CO mole fraction when the chemical kinetics were varied for 3-step, WD4, Skeletal, DRM-19 and GRI-2.11 at various axial locations.

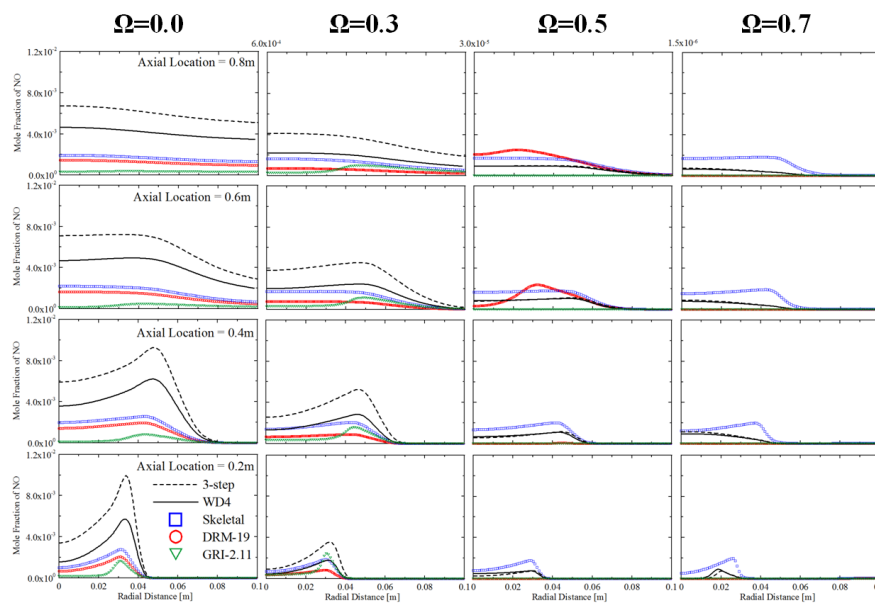


Figure 5. 1D distributions of NO mole fraction when the chemical kinetics were varied for 3-step, WD4, Skeletal, DRM-19 and GRI-2.11 at various axial locations.

It can be seen that CO concentration decreased with the dilution rate. A large difference in the CO distributions predicted by the five chemical kinetics was identified at upstream than at downstream for each dilution rate. The distribution of CO predicted by DRM-19 was much similar to that of GRI-2.11 for the conditions where the flame was not lifted off. The maximum CO concentration predicted by the chemical kinetics was, from highest to lowest, as $\text{GRI-2.11} > \text{DRM-19} > \text{Skeletal} > \text{3-step} > \text{WD4}$. It was already known that WD4 was good for the simulation of flame temperature and species concentration of CH_4/H_2 MILD combustion [5]. However, it was found that the prediction performance of the global reaction mechanisms for CO was not so good compared to others at

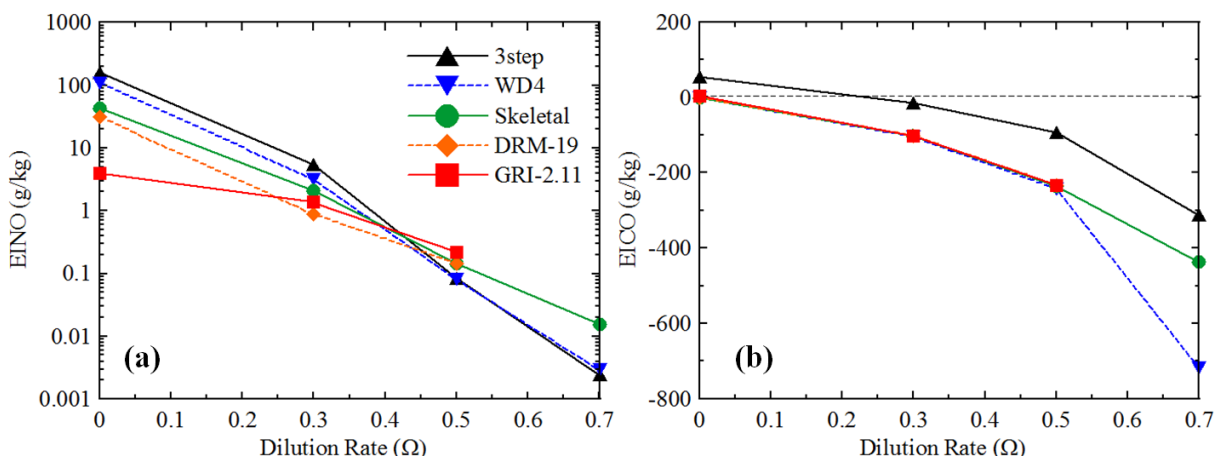


Figure 6. Variation of emission index for (a)NO, (b)CO with variation of the dilution rate.

upstream.

Figure 5 shows the distributions of NO mole fraction predicted by five chemical kinetics at selected axial locations. The maximum scales for NO mole fraction in the vertical line were different for given dilution rates. Predicted NO concentrations decreased with increasing the dilution rate regardless of chemical kinetics. The difference in the prediction performance by each chemical kinetics was large compared to that for other species. Four chemical kinetics predicted the NO concentration higher than GRI-2.11. At $\Omega = 0.0$, the predicted NO mole fraction by each chemical kinetics was, from highest to lowest, as 3step > WD4 > Skeletal > DRM-19 > GRI-2.11. Prediction performance for the NO distributions by DRM-19 and GRI-2.11 were not discriminate at this stage. Additional validation is required for NO prediction by DRM-19 and GRI-2.11 by comparing with experiment for NO concentration. As mentioned before, the flame structure including the NO distribution for $\Omega \geq 0.5$ was affected by the flame stabilization characteristics. Although not shown here, the prediction performance of radicals, such as H, O and OH, by the DRM-19 was almost similar to that of GRI-2.11 while the Skeletal over-predicted the radical concentrations compared to the DRM-19 and GRI-2.11. Consequently, it can be seen that DRM-19 was very similar to GRI-2.11 in predicting the flame temperature and species concentrations except for NO.

Figure 6 shows the emission indices for NO and CO with the variation of the dilution rate. As the dilution rate increased, both the EINO and EICO decreased. However, the degree of decrease in EINO was significant. For $\Omega \leq 0.3$ where the flames were stabilized near the fuel nozzle, the magnitude of EINO by each chemical kinetics was, from largest to smallest as 3step > WD4 > Skeletal > DRM-19 > GRI-2.11. Moreover, it can be seen that the degree of decrease in the EINO predicted by the GRI-2.11 decreased gradually compared with the other chemical kinetics. For $\Omega \geq 0.5$, overall flames was not captured in the simulation domain for some chemical kinetics, the discussion of EINO was meaningless. In terms of EICO, the EICOs by all chemical kinetics decreased with increasing the dilution rate. For $\Omega \leq 0.5$, the values of EICO were very similar to each other except for 3step even though the local CO distributions were somewhat different. Here, it should be noted that the EICO have negative value for higher dilution rates. This means that some part of CO supplied to the air-stream as a combustion product can be destroyed in the MILD combustion field. Moreover, this negative EICO implies that the MILD combustion might be very effect in destroying CO. Thus, it seems that an additionally study including experiment of the validation for this CO destruction in MILD combustion is required in near future.

4 Conclusions

The prediction performance of the five different chemical kinetics for the methane MILD jet combustion was investigated numerically.

The predicted temperature distribution appeared similar for all chemical kinetics for $\Omega \leq 0.5$. For $\Omega \geq 0.5$, temperature distribution was depended on the lift-off characteristics, and the reasonable prediction of the flame stabilization location was important for the high dilution rates.

The predictions of CO distribution by each chemical kinetics were not agreed well at upstream compared to at downstream. WD4 was the worst for the prediction of CO distribution at upstream. NO distribution was predicted differently by each chemical kinetics. The EINO with all the chemical kinetics decreased rapidly with increasing the dilution rate. The magnitude of EINO by each chemical kinetics was, from largest to smallest, as 3step > WD4 > Skeletal > DRM-19 > GRI-2.11.

The EICOs with different chemical kinetics also decreased with the dilution rate, and were very similar to each other except for 3step. Interestingly, the EICO had a negative value for large dilution rates. The negative EICO means that the CO supplied in the air-stream was destroyed in the MILD combustion. Thus, an additional study of CO destruction in MILD combustion is required to discussed the phenomena in more detail.

Acknowledgments

This work was supported by Joint International Research Program in Energy Efficiency and Resources R&D Business (20102030200051) under the Ministry of Knowledge Economy in Korea .

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