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Improvement of the prediction accuracy of NO emissions in counter-flow diffusion flames on using NO mass fraction as a progress variable

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Abstract

Computational fluid dynamics has been widely used to predict the production of nitrogen oxide (NO). Flamelet approach is commonly used as a modelling technique to perform turbulent combustion simulations. As the prediction of NO emissions with the flamelet approach is not reliable, when predicting the NO emission, the NO emissions are calculated with the conservation equation of NO mass fraction, and the NO production rate is predicted with the flamelet approach. In this study, we used the mixture fraction and NO mass fraction to predict the NO production rate in the conservation equation of the NO mass fraction, comparing the numerical results calculated with proposed method with those with the conventional methods and detailed chemistry model. Numerical simulations of counter-flow diffusion flames where NO was not supplied, that was supplied with fuel, and that was supplied with oxidizer indicated that the distribution of NO mole fraction calculated with the proposed method was in better agreement with that of the detailed chemistry model than that of the conventional methods.

Introduction

Nitrogen oxide (NO) produced by combustion systems is causes of acid rain and photochemical smog, and triggers health issues. Predicting the production and flow of the NO is necessary to decrease the NO emission in combustion systems. Computational fluid dynamics has been widely used to predict the production of NO. Flamelet approach (e.g., SLFM [1], FPV [2], FGM [3], and FPI [4]) is commonly used as a modelling technique to perform turbulent combustion simulations. As the prediction of NO emissions with the flamelet approach is not reliable, when predicting the NO emission, the NO emissions are calculated with the conservation equation of NO mass fraction, and the NO production rate is predicted with the flamelet approach [5-7]. In those studies, the prediction accuracy was discussed in comparison with the experimental results. However, the turbulent flames simulated in those studies were too complicated to investigate the prediction accuracy of the production of NO. For example, the difficulty is the effect of the diffusion of NO produced upstream on the downstream reaction. In this study, to simplify the problem, laminar counter-flow diffusion flames where NO was not supplied and that was supplied with the fuel or oxidizer were simulated to consider the downstream reaction zone, and the results calculated with the FPV model combined with the conservation equation of the NO mass fraction and a detailed chemistry model were compared to investigate the accuracy of the production of NO In general, the NO production rate is usually calculated by the controlling variable of mixture fraction and the progress variable of major products in conventional FPV and FGM model. Interestingly, studies that used the NO mass fraction as the progress variable have been rarely observed. Therefore, the results calculated with a method that the NO mass fraction was applied as a progress variable to lookup the database were compared with those calculated with the conventional methods.

Flamelet/progress variable (FPV) model

In FPV model [2], a database is necessary to be prepared before the combustion simulation. In this study, the database was generated by FlameMaster [8] with GRI-Mech 3.0 [9]. As the boundary conditions of chemical species, the composition of fuel was assumed CH_4/N_2 with a volume ratio of 23/77, and that of oxidizer was O_2/N_2 with a volume ratio of 23/77. The temperatures at both the sides were 300 K. Lewis number was assumed to be unity. Radiation heat transfer was neglected. The calculations were carried out for the cases with various scalar dissipation rates, and the results were remapped by the mixture fraction and progress variable (PV) to produce the database (143×101). The PV dose not rise monotonically for the scaler dissipation rate as shown in Fig. 1. In this study, the monotonically increased data was collected when producing the database. Note that a linear combination of CO, CO_2, H_2, and H_2O mass fraction or NO mass fraction was applied as conventional progress variables ($PV_{Conv.}$), and proposed progress variable (PV_{NO}), respectively.

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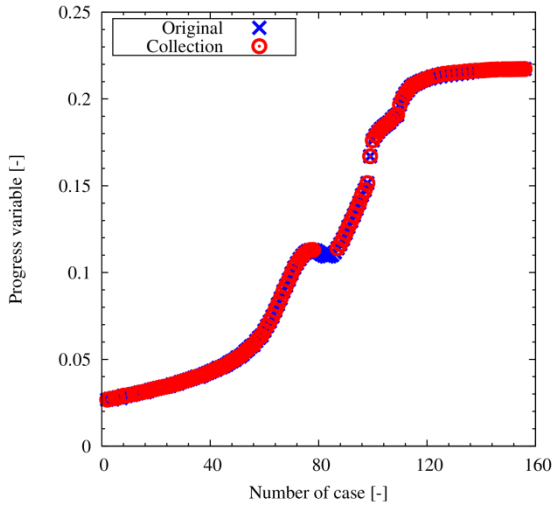


Figure 1. A relationship between the progress variable and the scalar dissipation rate.

Numerical simulation of combustion

A laminar counter-flow diffusion flame [10] was simulated as shown in Fig. 2 . The oxidizer and fuel flowed from the top and bottom of the computational region with a velocity of 0.255 m/s, respectively. As the analytical object was assumed to be two-dimensional, the slip condition was applied for the boundary conditions in the depth direction. Unstructured grids with collocated arrangement were employed, and the computational domains were divided into 3000 hexahedrons. The FPV model and a detailed chemistry model were used as the combustion model.

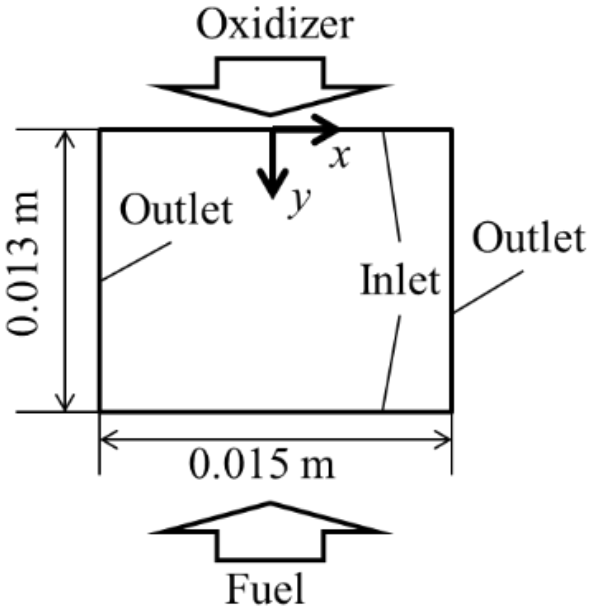


Figure 2. Analytical object for the simulation.

The continuity, momentum, mixture fraction, PV, and NO mass fraction conservation equations were discretized based on the finite volume method when using FPV model combined with the conservation equation of NO mass fraction. In the case of detailed chemistry model, the continuity, momentum, enthalpy and each species conservation equation were discretized. The second-order central differencing scheme was used for the discretization of the diffusive terms of all the equations and the convective term of the momentum, and the total variation diminishing scheme (limiter function of Min-Mod) was used for the discretization of the convective terms of the other scalars. The second-order Adams-Bashforth method was used to advance time for the momentum equation, and the pressure–velocity coupling scheme was SMAC. The implicit Euler method was used to advance time for the other scalar equations. The simulation was conducted using the constant time step (10^{-5} s) from 0 s (initial condition) to 0.2 s.

In the case of using FPV model, combustion temperature, major species, the production rate of PV_{Const}, flow properties, and thermophysical properties except for the diffusion coefficient in the conservation equation of the mixture fraction, PV, and each species mass fraction were looked up from the database by using the mixture fraction and $PV_{Const.}$. The diffusion coefficient was given by thermal diffusivity for the assumption that Lewis number is unity. NO mass fraction was calculated with the conservation equation of the NO mass fraction. The production rate of the NO mass fraction in the conservation equation was looked up from the database of PV_{Conv}. (referred to as the conventional method [5]), looked up from the database of PV_{NO} (referred to as the proposed method), or formulated with Eq. (1) (referred to as the Ihme and Pitsch's method [11]),

$$\dot{\omega}_{NO}=\dot{\omega}_{NO_Positive}(Z,C)-\frac{\dot{\omega}_{NO_Negative}(Z,C)}{Y_{NO}(Z,C)}\times Y_{NO,coservation} \quad (1)$$

where C is $PV_{conv.}$, Y_{NO} is the NO mass fraction, Z is the mixture fraction, $\dot{\omega}_{NO}$ is the production of NO. In the present study, Table 1 shows the boundary conditions for the conservation equation of NO mass fraction to consider the downstream reaction zone where NO diffused. Note that the database obtained for case 1 was used in each case because the same database is used for whole combustion region in turbulence combustion simulation. On the other hand, when using the detailed chemistry model, conservation equations of 53 species and enthalpy were calculated, and the production rates of each species were obtained with VODE [12] to predict the temperature and mass fraction of all chemicals. The reaction mechanism, flow properties and thermophysical properties, and the boundary condition of temperature in the calculation with the detailed chemistry model were same as those in calculation with FPV model. The boundary conditions of mass fraction of each species were set up for the case 1–3.

Table 1. the boundary conditions of NO mass fraction

	Fuel side	Oxidizer side
case 1	$Y_{NO} = 0$	$Y_{NO} = 0$
case 2	$Y_{NO} = 0.00024027$	$Y_{NO} = 0$
case 3	$Y_{NO} = 0$	$Y_{NO} = 0.0002106$

Results and discussion

The calculated temperatures and mole fraction of major species on the *y*-axis are shown in Fig. 3 with the experimental data [10]. With respect to both the distribution of temperature and mole fraction of major species, the results of the FPV and detailed chemistry model are in good agreement with those of the detailed chemistry and the experimental data. This indicates that the results of the FPV and detailed chemistry method are reasonable, and the FPV model can predict the reasonable reaction field with lower computational cost than the detailed chemistry model.

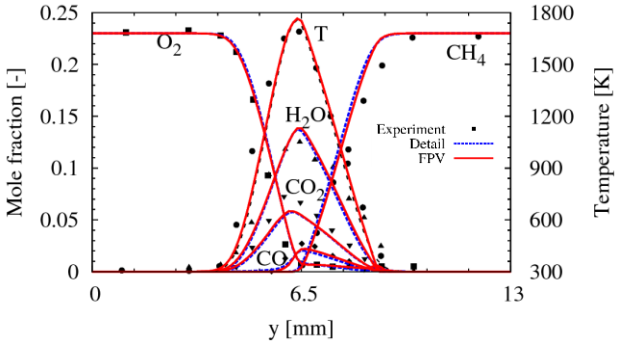


Figure 3. Temperature and major species profiles computed with the FPV or detailed chemistry model and the results of compared with the experimental data [10]

Fig. 4 shows the calculated NO mole fraction distribution on the *y*-axis in the case 1 whose condition is the same as experiment [10]. The results of proposed and Ihme and Pitsch's method are almost the same as the results of the detailed chemistry method. However, the conventional method underestimated the NO mole fraction in comparison with the detailed chemistry model. To take the difference between the conventional method and Ihme and Pitsch's method into account, the reason of underestimating is that the amount of NO reduction is overestimated in the case of the conventional method because of lacking information of the NO in the computational cell.

The NO mole fraction distribution calculated with each method in the case 2 was shown in Fig. 5. Although the results of proposed method is in better agreement with those of the detailed chemistry model than those of the conventional methods, the results of proposed method could not predict the minimal value appeared around y = 6.5. This is because the amount of NO reduction should be underestimated due to using the database made in the case 1. The conventional method overestimated the NO mole fraction in comparison with the detailed chemistry model. This could be explained by the fact that the conventional method neglects the amount of NO in the computational cell when predicting the production rate of NO. On the contrary, Ihme and Pitsch's method underestimated the NO mole fraction in

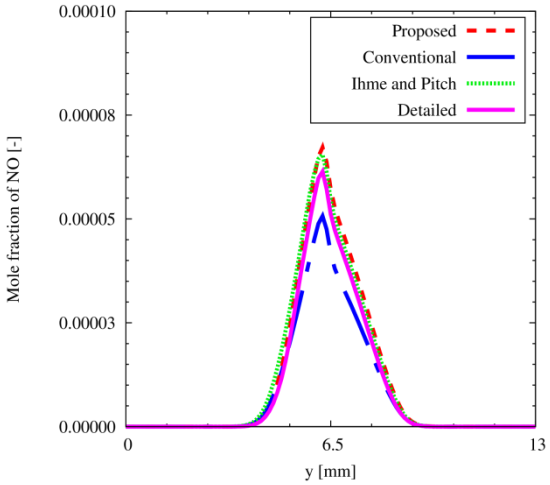


Figure 4. NO mole faction distribution calculated with the proposed, conventional, Ihme and Pitsch's method, and the detailed chemistry model on y axis in the case 1.

comparison with the detailed chemistry model. This suggests that the amount of NO reduction calculated with Ihme and Pitsch's method might be overestimated in the case that the NO mass fraction in the computational cell is higher than that looked up from the database.

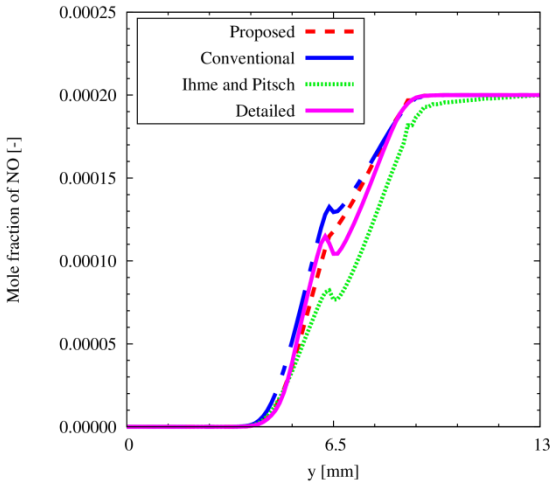


Figure 5. NO mole faction distribution calculated with the proposed, conventional, Ihme and Pitsch's method, and the detailed chemistry model on y axis in the case 2.

Fig. 6 shows NO and NO_X mole faction distributions calculated with the detailed chemistry model and NO mole fraction distribution calculated with the proposed, conventional, and Ihme and

Pitsch's methods in the case 3. Note that NO_X mole fraction is a linear combination of NO and NO_2 mole fraction. It is indicated that the results of proposed method are in better agreement with those of the detailed chemistry model than the conventional methods similar to Fig. 5. The minimal value which appeared in the results of the detailed chemistry model around y = 6 mm was not estimated when using proposed, conventional, Ihme and Pitsch's method. In the case of the NO_X mole fraction distribution, the minimal value did not appear. This indicates that the reaction between NO and NO_2 leads to produce the minimal value of the NO mole fraction distribution. Thus, the FPV method combined with the conservation equation of NO mass fraction might not estimate the reaction rate between NO and NO_2 accurately, so far. This should be explained by the large difference of reaction rate between NO and NO_2.

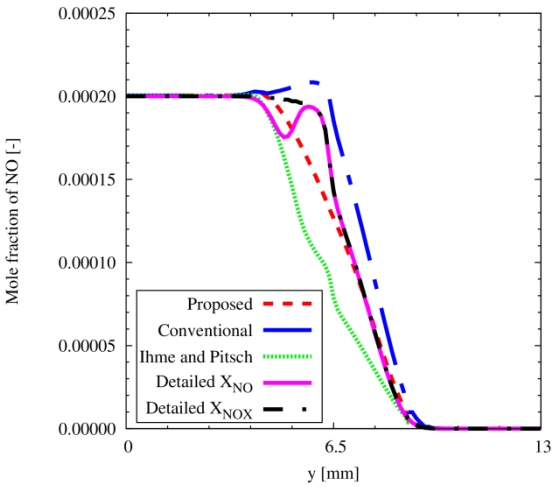


Figure 6. Comparison between the computed profiles of NO mole faction distribution with the proposed, conventional, and Ihme and Pitsch's method, and mole faction distribution of NO and NO_X calculated with the detailed chemistry model in the case 3.

Conclusions

In this study, the counter-flow diffusion flames were simulated with the FPV model combined with the conservation equation of NO mass fraction or the detailed chemistry model. We proposed a new method that used the NO production rate looked from the database with the NO mass fraction as a progress variable, and the results of proposed and conventional methods were compared to ensure the prediction accuracy of the NO mole fraction. The results showed that the proposed and conventional method estimated NO mole fraction in good agreement with the detailed chemistry model in the case that the boundary conditions of CFD and the database for FPV model are the same. On the other hand, the results of the proposed method were in better agreement with those of the detailed chemistry model than those of the conventional method when the boundary condition of CFD and database are different with respect to the NO like a combustion zone where downstream reaction occurs.

Acknowledgments

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