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PUBLISHER

Institute of Fluid Science (IFS), Tohoku University

VERSION

AM (Accepted Manuscript)

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Miyamoto, Hiromu, Shota Akaotsu, Yohsuke Matsushita, Hideyuki Aoki, and Weeratunge Malalasekera. 2019. “Prediction of Polycyclic Aromatic Hydrocarbons Formation Using Flamelet Approach with Additional Transport Equations”. figshare. https://hdl.handle.net/2134/10282886.v1.

Prediction of Polycyclic Aromatic Hydrocarbons Formation using Flamelet Approach with Additional Transport Equations

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ABSTRACT

It is known that the formation of minor species such as polycyclic aromatic hydrocarbons (PAHs) cannot be well captured by the standard flamelet/progress-variable (FPV) model. In this study, the extended method in which additional transport equations for PAHs were solved (FPV-TE model) was verified in the numerical simulations of a laminar counter-flow diffusion flame. The numerical results obtained from FPV-TE model were in better agreement with the solutions of the detailed chemistry than that in the standard FPV model in terms of the mass fractions of PAHs.

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) are widely recognized as the precursors of soot, which has adverse effects on health and environment. Reducing the emission of PAHs is one of the major goals in designing new combustion equipment, and numerical predictions of its emissions have played important roles. Generally, the computational cost in the simulation of PAHs formation is very high because high-molecular weight species such as PAHs are generated through thousands of chemical reactions. Especially in industrial applications with complex geometries and/or turbulent flows, the reasonable combustion model is needed to perform the simulation with realistic computational cost.

To reduce the computational cost without losing accuracy, the flamelet approach, such as the flamelet/progress-variable (FPV) model [1] has been used recently. The mixture fraction (*Z*) and the progress variable (*C*), which represents the progress of chemical reactions, are used to determine thermochemical quantities from a look-up table called flamelet library. In the FPV model, the calculation of fluid flow can be separated from that of chemical reactions by assuming much faster chemical reactions. On the other hand, the formation of minor species such as PAHs is not well captured because of relatively large time-scale of its reaction. To overcome this problem, M. Ihme and H. Pitsch [4] developed a new method in which additional equations was solved for the prediction of NO, and the proposed model gave a good agreement with experimental measurements in a turbulent partial-premixed flame.

In this study, the PAHs formation in a laminar counter-flow diffusion flame was predicted using the FPV model. Also, the additional equations of the mass fraction of PAHs were solved, and the accuracy of the numerical results was investigated in comparison with the solution based on the detailed chemistry.

2. Method

2.1 Construction of the flamelet library

One-dimensional calculations of a counter-flow diffusion flame were performed using the FlameMaster code [2]. For the detailed chemical mechanism, KAUST PAH Mechanism 2 [3], which comprises 202 species and 1351 reactions, was used. As stated before, thermochemical quantities obtained from the pre-calculations were tabulated by *Z* and *C*, which is defined as a combination of major species. In this study, *C* was defined as the sum of mass fractions of CO_2, CO, H_2, and H_2O.

2.2 PAHs modeling

Two approaches were investigated in this work. In the standard FPV model, the mass fractions of PAHs were directly retrieved from the flamelet library. In the other method, the mass fractions of PAHs (Y_k) were calculated by the additional transport equations as the post-process using a convergent solution in the standard FPV model. To identify the two types of the FPV models, this method is called as "FPV-TE model" in the later section. The transport equations of PAHs are as follows:

$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla \cdot (\rho \mathbf{u} Y_k) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k, \qquad (1)$$

where D_k, $\mathbf{u}$, ρ and $\dot{\omega}_k$ are diffusion coefficient, velocity vector, density and net production rates of chemical species, *k*, respectively. Note that the flow field was not assumed to be affected by the PAHs in FPV-TE model. As the chemical species calculated in the post-process, benzene and 11 PAHs species from C10 to C24 were selected. Using the concept of M. Ihme and H. Pitsch [4], net production rates were estimated by forward and backward reaction rates of PAHs ($\dot{\omega}_k^+$ and $\dot{\omega}_k^-$) such as the following equation:

$$\dot{\omega}_k = \dot{\omega}_k^+ + Y_k \left(\frac{\dot{\omega}_k^-}{Y_k^{flm}} \right), \qquad (2)$$

where Y_k^{flm} are the mass fractions of PAHs species *k* taken from the flamelet library.

2.3 Governing equations and numerical setup

Governing equations in this study were a continuity equation, momentum equations and transport equations for *Z* and *C*, and they were discretized by the finite volume method. The target flame is the counter-flow

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diffusion flame of ethylene [5]. Fig. 1 illustrates the schematic of the computational domain, which is the two-dimensional plane along the vertical center line between the nozzles. The number of grids is 2000. The boundary conditions are specified in Table 1.

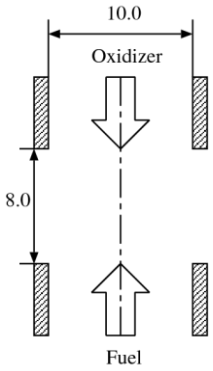


Fig. 1 The schematic of computational domain.

Table 1 Details of boundary conditions.

Fuel side ($Z = 1$)	Temperature	[K]	298
	Inflow velocity	[m/s]	0.2
	Mass fraction of C_2H_4	[-]	1.00
Oxidizer side ($Z = 0$)	Temperature	[K]	298
	Inflow velocity	[m/s]	0.2
	Mass fraction of O_2	[-]	0.233
	Mass fraction of N_2	[-]	0.767

3. Results and Discussion

Axial profiles of the temperature and the mass fractions of major chemical species are shown in Fig. 2. Overall, the numerical results obtained from the FPV model are in relatively good agreement with the solution of the detailed chemistry. Thus, it was confirmed that the FPV model was able to represent the temperature and the production of major chemical species predicted by the detailed chemistry. Fig. 3 shows the axial profiles of the mass fractions of PAHs. Although the FPV model describes the overall behaviors of the mass fractions of $C_{10}H_8$, $C_{16}H_{10}$, and $C_{22}H_{12}$ roughly, the model underestimates the absolute value; this discrepancy becomes larger in the mass fraction of $C_{24}H_{12}$. This is because $C_{24}H_{12}$ is formed in a relatively slow reaction, which is not consistent with the assumption of the flamelet approach. In the FPV-TE model, the absolute values and the peak positions are well captured, and it can be concluded that the accuracy for PAHs formations is improved by solving the additional transport equations.

4. Concluding Remarks

In this work, PAHs formations in the counter-flow diffusion flame was simulated using two-types of flamelet/progress-variable (FPV) model: the FPV model and the FPV-TE model. In the FPV-TE model, the mass fractions of PAHs were estimated by solving additional transport equations while those were directly retrieved from flamelet library in the FPV model. Although the numerical results of the FPV model were in reasonable agreement with the solutions of the detailed chemistry for the mass fractions of major species, the model underestimated those of PAHs due to its different characteristic time scale from the other major species. This discrepancy was reduced by solving additional transport equations, and the FPV-TE model yielded more accurate results than those obtained from the standard FPV model in terms of the mass fractions of PAHs.

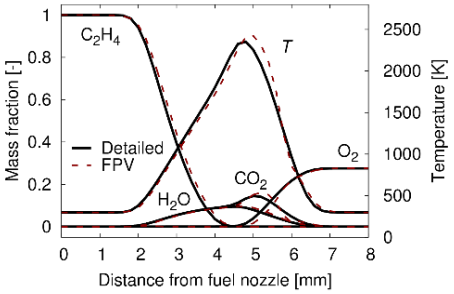


Fig. 2 Axial profile of the temperature and the mass fractions of major chemical species between nozzles.

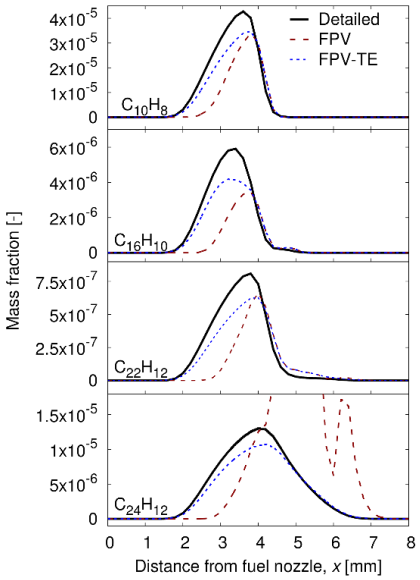


Fig. 3 Axial profile of the mass fractions of PAHs between nozzles.

Acknowledgments

This work was supported by Leading Young Researcher Overseas Visit Program in Tohoku University, JSPS KAKENHI [grant number JP18K03964] and JSPS Grant-in-Aid for Research Fellows [grant number JP18J11135].

References

[1] C.D. PIERCE, P. MOIN, *J. Fluid Mech.* 504 (2004) 73–97.

[2] H. Pitsch, FlameMaster v3.3.10: A C++ Computer Program for 0D Combustion and 1D Laminar Flame Calculations, (1998).

[3] Y. Wang, A. Raj, S.H. Chung, *Combust. Flame.* 160

(2013) 1667–1676.
[4] M. Ihme, H. Pitsch, *Phys. Fluids.* 20 (2008).
[5] Y. Wang, A. Raj, S.H. Chung, *Combust. Flame.* 162
(2015) 586–596.