

DME 연료의 대향류 비예혼합 화염에서 냉염의 화염구조 및 에지 거동에 관한 수치해석적 연구

김재중*, 김승현**, 박정**, 유춘상*†

Numerical Study on the Flame Structures and Edge Dynamics of DME Nonpremixed Counterflow Cool Flame

Jae Jung Kim*, Seung Hyun Kim**, Jeong Park**, Chun Sang Yoo*†

Low-temperature flames, also referred to as "cool flames", were first observed in the early 19th century in fuel-air premixtures exposed to heated metal surfaces. Cool flames are distinguished by their extremely faint luminosity in contrast to conventional flames, commonly known as "hot flames". One of their unique characteristics is the substantial production of aldehydes while emitting very low amount of carbon dioxide. This phenomenon suggests a profound connection between the existence of cool flames and the negative temperature coefficient (NTC) region.

Over an extended period, premixed cool flames have been extensively investigated using a variety of hydrocarbon fuels. These investigations revealed the presence of diverse flame structures, not limited to solely low-temperature chemistry reactions. Instead, they are accompanied by intermediate- or high- temperature chemistry reaction zones, distinguishing them from the straightforward cool flames primarily sustained by low-temperature chemistry alone. This spectrum of flames has been classified under various labels, such as warm flame, double flame, three stage flame, and so forth, following systematic criteria [1].

Remarkably, in the 2010s, researchers achieved a groundbreaking discovery by experimentally detecting cool and warm flames in non-premixed conditions, thereby opening up new avenues for exploration.

In this context, the current study focuses on non-premixed counterflow cool flames employing dimethyl ether (DME) as the fuel,

thereby contributing to the evolving body of knowledge in this domain. DME is widely employed as a fuel in numerical studies of cool flames due to its small molecular size.

Numerical calculations are performed in both one- and two- dimensions. For fundamental and repetitive parameter studies, OPPDIF[2], a Fortran code for simulating diffusion flames between two opposing nozzles in a one-dimensional domain is used. To calculate the entire domain of a counterflow flame using an axisymmetric two-dimensional approach, laminarSMOKE [3-4], an open-source CFD solver for laminar reacting flows with detailed kinetic mechanisms based on OpenFOAM [5] and OpenSMOKE++ [6], is employed.

Several detailed kinetic mechanisms for the oxidation of DME are used in the current study. First, the most widely used kinetic model developed by Zhao [7] is selected when the addition of ozone in the oxidizer stream is not considered. Additionally, another DME oxidation kinetic model developed by Wang [8] is used, which is directly validated for use with the ozone sub-mechanism developed by Hao [9].

The numerical domain is generated based on the detail structure of the counterflow burner used in the experimental study in progress. A schematic of the domain is provided in Fig. 1. The domain consists of two opposing main nozzles with a diameter of 25 mm and two opposing annular coaxial curtain nozzles with a 35 mm outer diameter. Curtain nozzles play a role in stabilizing the counterflow flame by preventing external disturbances using an inert gas flow. The nozzle separation distance is fixed at 15 mm. A uniform 50 μm mesh is employed within the region of the outer edge of the nozzle components (43 mm in diameter),

* 울산과학기술원(UNIST) 기계공학과

** 부경대학교 기계공학과

† 연락처, csyoo@unist.ac.kr

TEL : (054)217-2322 FAX : (052)-217-2309

while the remaining area is covered with a stretched mesh to reduce computational costs.

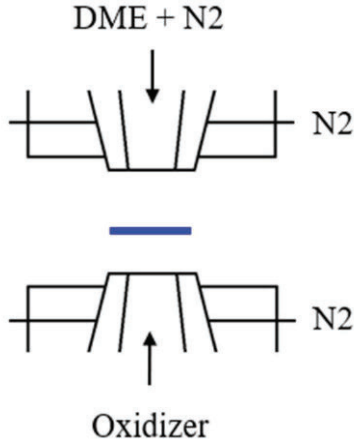


Figure 1 Schematic of the domain.

In the counterflow flames, the global strain rate is defined by Seshadri and Williams [10].

$$a_g = \frac{2U_0}{L} \left[1 + \frac{U_F}{U_0} \left(\frac{\rho_F}{\rho_0} \right)^{\frac{1}{2}} \right] \quad (1)$$

To adjust the position of stagnation point at the center, the momenta of both streams are equated, resulting in the determination of exit velocities through the following equations.

$$\rho_F U_F^2 = \rho_O U_O^2 \quad (2)$$

$$a_g = \frac{4U_0}{L} \quad (3)$$

To minimize the shear-layer effect, the velocities of the curtain flows are set equal to the velocity of each main nozzle.

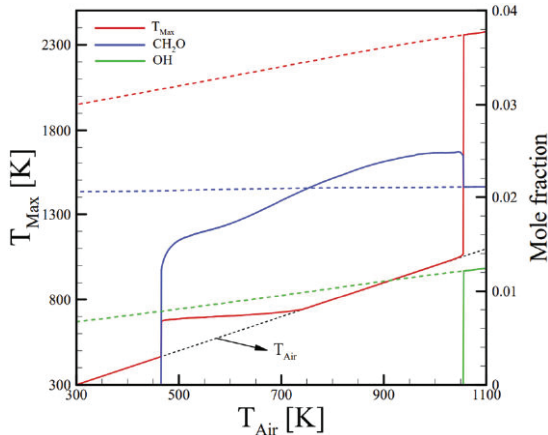


Figure 2 Extinction of cool flame and transition from cool flame to hot flame.

Figure 2 illustrates the results obtained by gradually changing the temperature of the oxidizer stream in one-dimensional calculations. Mole fraction of fuel is held constant at 0.5, and air is employed as the oxidizer. To maintain a constant global strain rate of 60 s^{-1} while the density of oxidizer side changes, the velocity of the fuel stream is continuously adjusted.

The curve starts from the initial point of the cool flame at an air temperature of 600 K, with a flame temperature of 703 K. The significantly high formaldehyde and extremely low OH mole fractions support the classification of this flame as a cool flame. When the air temperature decreases, the cool flame is extinguished at an air temperature of 465 K. On the other hands, when the air heated to 1056 K, the flame undergoes a sudden transition into a hot flame with a flame temperature of around 2300 K. This transition results in sharp changes in the mole fractions of radicals. Additionally, the dashed lines in Fig. 2 represent the path of the hot flame obtained by decreasing the air temperature again. In contrast to the cool flame, the hot flame persists until the air reaches room temperature.

A remarkable region is observed in Fig. 2, between 750–1050 K. Despite the fact that the maximum temperature does not exceed the air temperature, the presence of formaldehyde indicates the occurrence of reactions similar to those observed in common cool flames. To investigate these phenomena, two-dimensional steady simulations are performed for two representative cases with air temperatures of 600 K and 800 K.

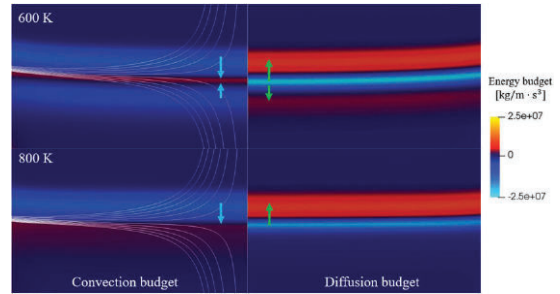


Figure 3 Convection and diffusion energy budget in two cases of air temperature.

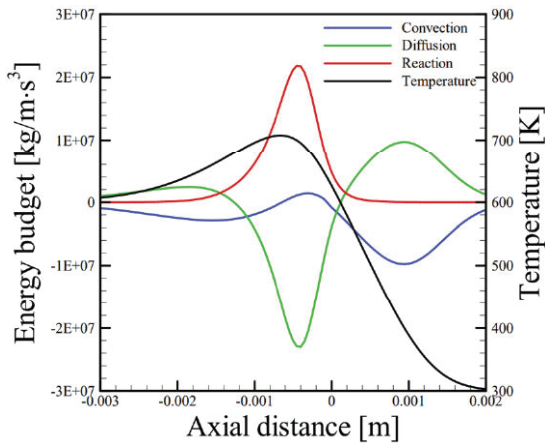


Figure 4 Structure of energy transport in case of 600 K air along the centerline.

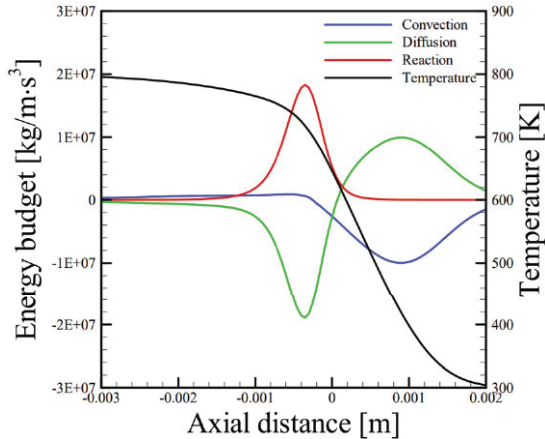


Figure 5 Structure of energy transport in case of 800 K air along the centerline.

Fig. 3 displays the results of an energy budget analysis, a method used to analyze the production and transportation of thermal energy by decomposing convection, diffusion, and reaction terms of the energy equation. The blue arrow and green arrow represent the directions of thermal energy transport via convection and diffusion, respectively. The white lines on the left side indicate the streamlines of the flow. In the case of 600 K, it can be observed that thermal energy is diffused on both sides from the center, while the fluid flow causes the energy to gather in the center by convection. Meanwhile, in the case of 800 K, thermal energy is exchanged only on the fuel side, where the stream is not

preheated. Figures 4 and 5 depict the budgets and the temperature along the centerline, showing clear difference between both cases. It can be observed that the reaction budgets, also referred to as heat release rates, exhibit similar structures in both cases. On the other hands, the convection budgets and diffusion budgets on the oxidizer side become notably monotonous at 800 K. This can be attributed to the temperature distribution. In the case of 600 K, the temperature curve has a peak near the center, thereby allowing the thermal energy diffusion to naturally occur in both directions. However, there is no peak in the case of 800 K. Diffusion has no choice but to occur in only a single direction. Furthermore, in the absence of a reaction, convection must be balanced with diffusion, thereby affecting the behavior of convection as well.

후 기

This research used the computational resources of UNIST Supercomputing Center.

참고 문헌

- [1] Y. Ju, Understanding cool flames and warm flames, *Proc. Combust. Inst.* 38 (2021) 83–119.
- [2] Lutz, A. E, Kee, R. J, Grcar, J. F, Rupley, F, *OPPDIF: A Fortran program for computing opposed-flow diffusion flames*. (1997)
- [3] A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, Numerical modeling of laminar flames with detailed kinetics based on the operator-splitting method, *Energy Fuels* 27 (2013) 7730–7753
- [4] A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, A computational tool for the detailed kinetic modeling of laminar flames: application to C₂H₄/CH₄ coflow flames, *Combust. Flame* 160(2013) 870–886.
- [5] H.G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, *Comput. Phys.* 12(1998) 620–631.
- [6] A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms, *Comput. Phys. Commun.* 192

(2015) 237-264

[7] Z. Zhao, M. Chaos, A. Kazakov, F.L. Dryer, Thermal decomposition reaction and a comprehensive kinetic model of dimethyl ether, *Int. J. Chem. Kinet.* 40(2008) 1-18.

[8] Z. Wang, X. Zhang, L. Xing, L. Zhang, F. Herrmann, K. Moshhammer, F. Qi, K. Kohse-Höinghaus, Experimental and kinetic modeling study of the low-and intermediate-temperature oxidation of dimethyl ether, *Combust. Flame*, 162(2015) 1113-1125.

[9] Z. Hao, Y. Xueliang, J. Yiguang, Kinetic studies of ozone assisted low temperature oxidation of dimethyl ether in a flow reactor using molecular-beam mass spectrometry. *Combust. Flame*, 173(2016) 187-194.

[10] K. Seshadri, F.A. Williams, Laminar flow between parallel plates with injection of a reactant at high Reynolds number, *Int. J. Heat Mass Transf.* 21(1978) 251-253.