# 직접연소식 초임계 $CO_2$ 순산소 연소조건내 메탄 대항류 화염의 질소산화물 발생특성에 관한 수치해석적 연구

정기성*·박현수*·Nam Danh Nguyen*·이복직*·유춘상*†

# A numerical study of the NOx emission characteristics of methane counterflow flame under direct-fired supercritical oxyfuel combustion condition

Ki Sung Jung*, Hyun Su Bak*, Nam Danh Nguyen*, Bok Jik Lee**, Chun Sang Yoo*†

The direct fired supercritical carbon dioxide ($sCO_2$) power cycle using $CO_2$ as a working fluid is recently highlighted not only because it has a high thermal efficiency with small machinery footprints but also because it can ideally capture $CO_2$ up to 99 %. Since $N_2$ can infiltrate the combustor of the cycle mainly because natural gas has impurity in its chemical composition, this paper investigates the effects of $N_2$ amount in the fuel stream on the NOx emissions characteristics at supercritical conditions of the $sCO_2$ power cycle.

In this study, 1-D numerical simulations of nonpremixed counterflow methane flame are performed using OPPDIF code [1] with real gas effects [2]. San Diego mechanism [3] with NOx sub mechanism [4] is adopted because its validation range covers the relatively high pressure condition. All simulations are conducted with the boundary condition that inlet temperature of fuel and oxidizer side are fixed to 300 and 100 K, respectively. The mole fraction of $O_2$ at the oxidizer side and that of $CH_4$ at the fuel side range from 0.15 to 0.30 and from 0.9 to 1.0, respectively. We defined the global strain rate, $a$, as $a = (|U_F| + |U_O|)/H$, where $U$ is the axial velocity, and $H$ is the distance between two inlets. The subscripts F and O represent the fuel and oxidizer inlets, respectively.

The flame structures for counterflow nonpremixed $CH_4/O_2/CO_2$ flames at 300 atm for various global strain rates are shown in Fig. 1a, while Fig. 1b indicates the overall flame structures for various pressure with $a$=100 s$^{-1}$.

As shown in Fig. 1a, both the maximum flame temperature and reaction zone thickness decrease with the increase of $a$ due to the shortened residence time. As $a$ further increase to the upper-limit extinction strain rate, an extinction occurs due to the insufficient residence time for the mixture to sustain the flame structure (not shown here). In addition, the flame temperature increases with the increase of pressure up to 20 atm, but the maximum flame temperature does not change much as pressure further increases.
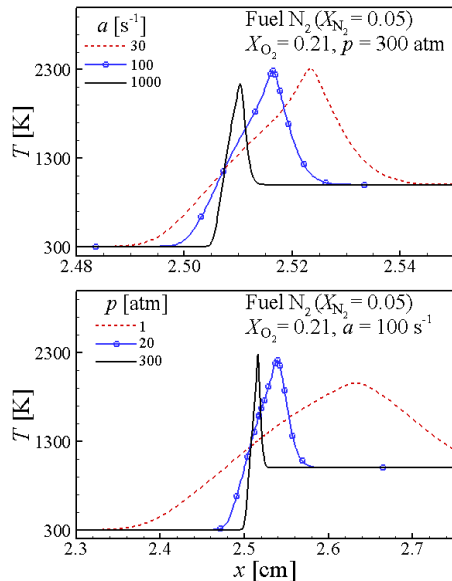


Figure 1. The temperature profiles of counterflow nonpremixed $CH_4/O_2/CO_2$ flames for (a) various strain rates at 300 atm and (b) various pressures at with $a$ = 100 s$^{-1}$.

The flame temperature effect on the NOx emission at the direct-fired $sCO_2$ relevant

* 울산과학기술원 기계공학과
** 서울대학교 기계항공공학부
† 연락저자, csyoo@unist.ac.kr

condition (i.e. $p$ = 300 atm and $a$ = 100 s$^{-1}$) is investigated. To remove the dilution effect and properly compare the amount of NO$_X$ formation, the emission index of NO$_X$, EINO$_X$ [g−NO$_x$/kg−CH$_4$], is defined as [5],

$$\text{EINO}_x = \frac{\int_0^H (\dot{\omega}_{NO} W_{NO} + \dot{\omega}_{NO_2} W_{NO_2})\, dx}{-\int_0^H \dot{\omega}_{CH_4} W_{CH_4}\, dx} \times 1000$$

where $x$ is the axial distance in 1−D counterflow configuration, $\dot{\omega}_k$ the production or consumption rate of species $k$ at each grid point of the domain, and $W_k$ the molecular weight of species $k$.

The mole fractions of N$_2$ in the fuel inlet are ranged from 0.0 to 0.1 and that of O$_2$ in the oxidizer inlet are also varied from 0.15 to 0.30. The maximum flame temperature, $T_f$, difference between undiluted CH$_4$ fuel jet and diluted CH$_4$ with $X_{N_2}$ of 0.1 is negligible (i.e., < 20 K). Therefore, $T_f$ in Fig. 2 is mainly varied as O$_2$ dilution level changes. It can be found that the production of NO$_X$ is more sensitive to the oxidant dilution level rather than the amount of N$_2$ in the fuel inlet. In addition, the EINO$_X$ generally very low when $T_f$ equals to or lower than 2300 K. On the other hand, as $T_f$ increases to be higher than 2500 K, an even small amount of N$_2$ ingress can no longer to be negligible. Considering that the maximum flame temperature of the previous sCO$_2$ combustor reaches up to 2750 K, the formation of NOx should be taken into account for the practical sCO$_2$ combustor design.

The relative NO$_X$ formation/consumption characteristics, the effect of pressure on the relative contribution of each NO$_X$ formation, and the effect of fuel concentration at the fuel inlet or overall NO$_X$ concentration levels will be further studied in a future study.
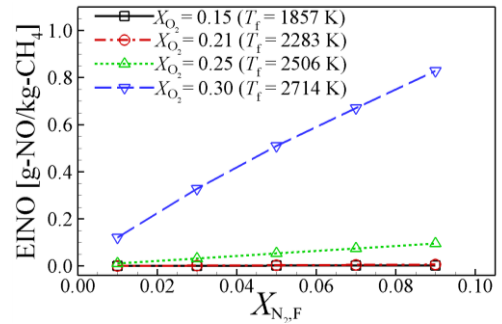


Figure 2. The flame temperature effect on the NO$_X$ emissions ($p$ = 300 atm, $a$ = 100s$^{-1}$)

## Acknowledgements

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