A numerical study of the NO\textsubscript{x} emission characteristics of methane counterflow flame under direct–fired supercritical oxyfuel combustion condition

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The direct fired supercritical carbon dioxide (sCO\textsubscript{2}) power cycle using CO\textsubscript{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\textsubscript{2} up to 99%. Since N\textsubscript{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\textsubscript{2} amount in the fuel stream on the NO\textsubscript{x} emissions characteristics at supercritical conditions of the sCO\textsubscript{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 NO\subscript{X} 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\textsubscript{2} at the oxidizer side and that of CH\textsubscript{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, \( \alpha \), as \( \alpha = \frac{\left| U_F \right| + \left| U_O \right|}{H} \), 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\textsubscript{4}/O\textsubscript{2}/CO\textsubscript{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 \( \alpha = 100 \text{ s}^{-1} \).

As shown in Fig. 1a, both the maximum flame temperature and reaction zone thickness decrease with the increase of \( \alpha \) due to the shortened residence time. As \( \alpha \) 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\textsubscript{4}/O\textsubscript{2}/CO\textsubscript{2} flames for (a) various strain rates at 300 atm and (b) various pressures at with \( \alpha = 100 \text{ s}^{-1} \).
The flame temperature effect on the NOX emission at the direct-fired sCO2 relevant condition (i.e. $p = 300$ atm and $\alpha = 100$ s$^{-1}$) is investigated. To remove the dilution effect and properly compare the amount of NOX formation, the emission index of NOX, $\text{EINO}_X$ [g-NOX/kg-CH4], is defined as [5],

$$\text{EINO}_X = \frac{\int_{0}^{\lambda} (\omega_{NO} W_{NO} + \omega_{NO2} W_{NO2}) \, dx}{\int_{0}^{\lambda} \omega_{CH4} W_{CH4} \, dx} \times 1000$$

where $x$ is the axial distance in 1-D counterflow configuration, $\omega_k$ 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 N2 in the fuel inlet are ranged from 0.0 to 0.1 and that of O2 in the oxidizer inlet are also varied from 0.15 to 0.30. The maximum flame temperature, $T_f$, difference between undiluted CH4 fuel jet and diluted CH4 with $X_{N2}$ of 0.1 is negligible (i.e., < 20 K). Therefore, $T_f$ in Fig. 2 is mainly varied as O2 dilution level changes. It can be found that the production of NOX is more sensitive to the oxidant dilution level rather than the amount of N2 in the fuel inlet. In addition, the EINOX 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 N2 ingress can no longer to be negligible. Considering that the maximum flame temperature of the previous sCO2 combustor reaches up to 2750 K, the formation of NOX should be taken into account for the practical sCO2 combustor design.

The relative NOX formation/consumption characteristics, the effect of pressure on the relative contribution of each NOX formation, and the effect of fuel concentration at the fuel inlet or overall NOX concentration levels will be further studied in a future study.

Figure 2. The flame temperature effect on the NOX emissions ($p = 300$ atm, $\alpha = 100$ s$^{-1}$)

Acknowledgements

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (NRF-2018R1A2A2A05018801) and Korea Electric Power Corporation (Grant number: R19X001-25).

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