Formation of Nitric Oxide in a Multi-Staged Air LPG Flame

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Introduction

Increasing awareness over the environmental pollution, coupled with a need to implement more stringent pollution control legislation, has accelerated a developmental installation of NOx reduction and control system in combustion devices. One of effective ways in controlling the NO emission is the air staged combustion technique that has been installed in many fossil fuel-fired combustion systems. Air staged-burner is normally fired sub-stoichiometrically so that it is operating with less than a theoretical amount of combustion air, while the remaining air is supplied farther downstream via staged air nozzles. This type of firing leads to a reduction of peak flame temperature, which then results in lowering thermal NO formation[1].

In order to predict NO formation correctly in a multi-staged air burner flame, it is necessary to understand thermal as well as chemical characteristics in the flow field. Furnace wall condition must be also relevant to determining the temperature distribution in furnace.

In this study, the objective of this study is to develop a numerical simulation which is capable of predicting the characteristics of NO formation in pilot scale combustor (0.2MW) adopting the air-staged burner flame. The numerical prediction is done by means of establishing the mathematical models for turbulence, turbulent combustion, radiation and turbulent nitric oxide chemistry. The radiative transfer equation is calculated using the discrete ordinates method (DOM) with weighted-sum-of-gray-gases model (WSGGM) for the non-gray gas effects by CO_2 and H_2O. Thermal NO and prompt NO chemical reaction rates are statistically averaged using the β probability density function[2]-[5]. Experimental measurements are also made when the liquefied petroleum gas (LPG) is used. The numerical results are then validated in comparison with the experimental data. This work is consequently considered to be a combined approach of modeling and experimenting the NO formation in multi-staged air LPG flame.

Experiments

Experiments have been performed to provide a comparative data for temperature distribution and species concentrations in the flow field of multi-staged air LPG flame. A schematic of three air-staged LPG burner of 0.2 MW is shown in Figure 1. The fuel nozzle is of hollow cone type with jet angle of 30^o. Its flow rate is monitored using a calibrated orifice flowmeter. The staged combustion air is supplied through a calibrated air flowmeter to the primary, secondary and tertiary air nozzles which are concentrically positioned. One swirler with vane angle 60^o is coaxially installed in the primary nozzle and another one with vane angle 30^o in the tertiary nozzle for flame stabilization. Figure 2 shows a schematic of experimental combustor. In order to measure the temperature and species concentrations in combustor, inspection holes (ϕ 25.4 mm) are made every 10 cm along the axial direction of the furnace wall.

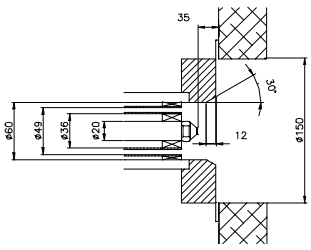

Figure 1. Dimensional configuration of the multi-staged air burner.

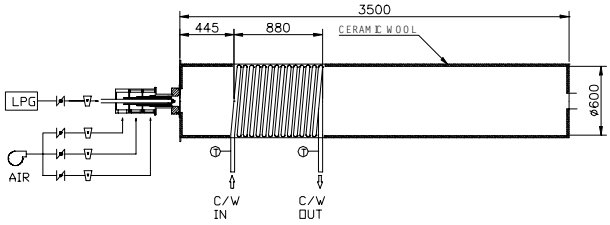

Figure 2. Schematic diagram of experimental equipment.

Table.1 Experimental conditions

Fuel mass flowrate	15.2 kg/hr
Fuel jet angle	30^o
Total air mass flowrate	260 kg/hr
Primary, secondary, tertiary air flow rates	20 %, 45 % , 35 %
Primary air stage vane angle	60^o
Secondary air stage vane angle	0^o
Tertiary air stage vane angle	30^o

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Mathmatical model

To analyze pollutive gas formation as well as gas phase combustion in this type of combustion chamber, a two-dimensional mathematical model is introduced here. It consists of the overall mass continuity, momentum equation for axial, radial and tangential directions, energy equation, turbulence model and chemical species conservation equation.

The equations can be written in the following generalized form for each variable:

$$\frac{\partial(\rho U\Phi)}{\partial x}+\frac{1}{r}\frac{\partial(r\rho V\Phi)}{\partial r}=\frac{\partial}{\partial x}\left(\Gamma_\varphi\frac{\partial\Phi}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\varphi\frac{\partial\Phi}{\partial r}\right)+S_\varphi \tag{1}$$

Turbulence effects are modeled using the widely employed standard k-ε model in which the effective turbulent viscosity and the wall function is used in near wall region, where the viscous effect is dominant [6].

The numerical calculation of multi-staged air LPG flame is here carried out using the propane gas (C_3H_8), since LPG used in this experiment is composed of 95 % of propane and 5% of other gas. The reaction model for oxidation of propane is assumed as a two-step mechanism as follows;

$$C_3H_8+7/2O_2\rightarrow 3CO+4H_2O \tag{R-1}$$

$$CO\ +1/2O_2\rightarrow CO_2 \tag{R-2}$$

The source or sink terms due to combustion, S_φ, in the species conservation equations are modeled using the eddy dissipation model [7].

In order to take account of the non-gray gas effects by CO_2 and H_2O, DOM is combined with weighted sum of gray gases model (WSGGM) such that the RTE can be written for k-th gray gas as follows;

$$\mu_l\left(\frac{\partial I_k^l}{\partial x}\right)+\frac{\xi^l}{r}\frac{\partial\left(rI_k^l\right)}{\partial r}-\frac{1}{r}\frac{\partial\left(\eta^l I_k^l\right)}{\partial\psi}=-\kappa_k I_k^l+\kappa_k w_k I_b \tag{2}$$

where κ_k, I_k, and w_k are the absorption coefficient, directional intensity and weighting factor for k-th gray gas respectively.

The reaction rate of thermal NO formation originally proposed by Zeldovich can be written as

$$\frac{d[\mathrm{NO}]_t}{dt}=\frac{2[O]\left(k_{1f}k_{2f}[O_2][N_2]-k_{1b}k_{2b}[NO]^2\right)}{k_{2f}[O_2]+k_{1b}[NO]} \tag{3}$$

where $[X_i]$ is mole fraction of species i

The source or sink of thermal NO formation (S_{t-NO}) is then expressed by

$$S_{t-NO}=W_{NO}\frac{d[NO]_t}{dt} \tag{4}$$

For the case of hydrocarbon combustion, Fenimore (1979) suggested a following reaction mechanism of prompt NO formation [8]

$$CH + N_2 \leftrightarrow HCN + N \quad \text{(R-3)}$$

$$C + N_2 \leftrightarrow CN + N \quad \text{(R-4)}$$

Based on these, De Soete (1975) proposed a following chemical reaction rate for prompt NO formation [9]

$$\frac{d[\mathrm{NO}]_p}{dt} = C\frac{W^{1+b}}{\rho^{1+b}}[\mathrm{O_2}]^b[\mathrm{N_2}][\mathrm{C_xH_y}]\exp\left(-\frac{E_a}{RT}\right) \quad (5)$$

$$S_{p-NO} = W_{NO}\frac{d[NO]_p}{dt} \quad (6)$$

where $C = 6.4\times10^6\,\mathrm{s}^{-1}$, $E_a = 3.038\times10^8\,\mathrm{J/kmol}$ and b=0.5.

The above equations (5) and (6) are based on data obtained from laboratory laminar premixed flames or shock tube studies where the conditions for molecular diffusion are well defined. In order to account for the turbulent effects, a statistical method is chosen in this study so that a probability density function (pdf) is used for estimating the average value of the NO reaction rate.

Results and discussions

The measured radial temperature distribution are plotted for four axial locations of 0.1, 0.5, 1.0, and 2.6m and compared with two numerical results in Figure 3. One is calculated without considering the effects of radiation while the other takes account of the non-gray radiation effects of CO_2 and H_2O. In the figure the results with radiation are seen to yield higher temperature distribution than those with radiation, since there is a radiative heat loss through exit for the case with radiation. In overall the numerical results considering the effects of radiation represent a much better agreement with the experimental results. But a discrepancy is observed for the radial temperature distribution at x=0.5m where the cooling pipe is placed around the furnace wall.

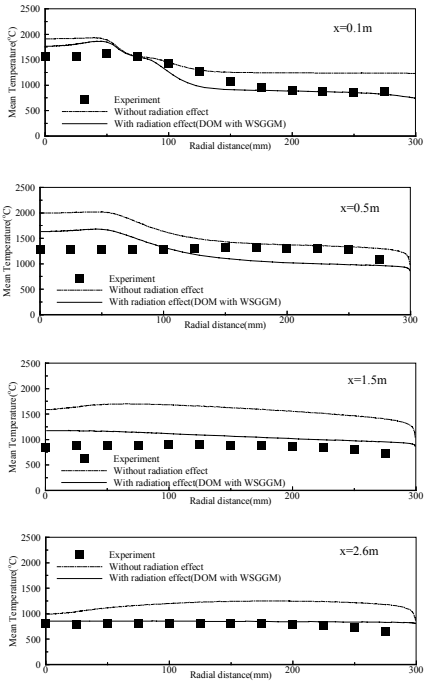

Figure 3. Radial temperature distribution

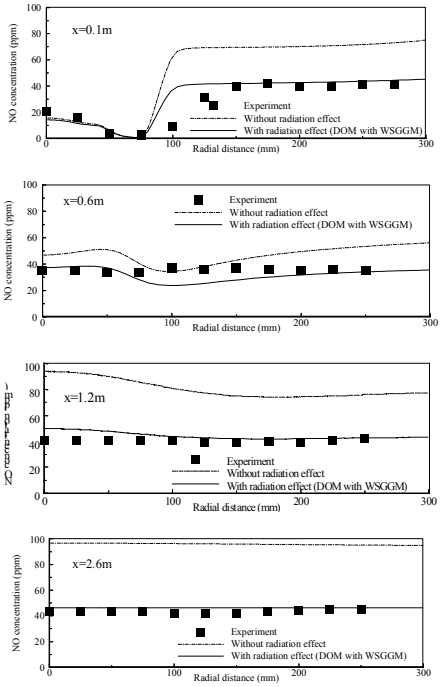

Figure 4. Radial NO distribution.

This results from the fact that in this experiment the cooling pipe is placed inside the furnace, while in the calculation the wall is considered smooth. Nevertheless, the overall results obtained by considering radiation are satisfactory compared with the experimental ones. Based on these, it can be inferred that the inclusion of appropriate radiation model is very important in modeling the gas-fired combustion.

Numerical distribution of NO is plotted in Figure 4 and compared with measurements. As noted in the figure, when the radiation effect is disregarded in the modeling, the predicted thermal NO over-predicts the measurements since the temperature is higher. For the case with radiation, there is a small difference between the numerical and experimental results at x=0.2 and 0.6 m, while the difference is much smaller farther downstream at x=1.2 and 2.6 m. Therefore, the thermal and prompt NO prediction models used in this study, which are based on the oxygen, temperature fields and empirical constants, are enough to be used for numerical modeling of NO formation with the discrete ordinates method for radiation and weighted sum of gray gases model in the multi-staged air LPG flame.

In Figure 5 a spatial distribution of the thermal and prompt NO formation is depicted. It is noted that the source of prompt NO is much higher than that of thermal NO at the flame front. This results from the fact that the prompt NO is created from CH radical, which is formed as an intermediate at flame front only so that the prompt NO is primarily generated at flame front [8]. Consequently, the NO concentration at x=0.1 m in Figure 4 is considered to mainly originate from prompt NO generated. On the other hand, the thermal NO is broadly produced while most of them are located at a high temperature region exceeding 1000 ^{o}C based on the Zeldovich reaction mechanism since thermal NO requires very high activation energy.

In Figure 6 the isolines of NO concentration are illustrated with/without radiation effects. In both cases the peak NO concentration lies downstream of the peak temperature zone since NO is accumulated downstream due to diffusive and convective gas flow. It is also observed that much less NO is produced for the case with radiation.

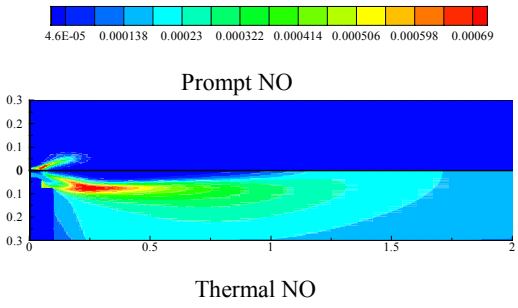

Figure 5. Thermal NO and Prompt NO distribution (kg/m^3/sec).

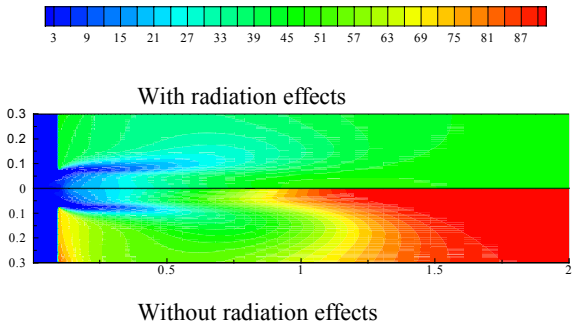

Figure 6. NO distribution with/without radiation effects(ppm).

Conclusion

In this study the combustion characteristics of an axisymmetric multi-staged air flame was examined to predict the nitric oxide formation with the decoupled kinetic model. A simplified non-gray radiation model, i.e., the weighted sum of gray gases model for CO_2 and H_2O was combined with the discrete ordinates method (DOM) to solve the radiative transfer equation together with the other mass, momentum, energy and species conservation equations. For its validation, a 0.2 MW pilot multi-staged air burner has been designed and constructed.

A better agreement of numerical gas temperature with measurements was obtained only when the radiation was taken into consideration. Consequently, the inclusion of radiation was prerequisite for modeling gas-fired combustion. This was also true of the prediction of the NO formation, since it strongly depended on temperature.

A prediction of species concentrations such as CO, CO_2 and O_2 in the field, as a whole, yielded a good agreement with the

measurements, except the upstream region of combustor near the burner inlet.

References

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