Numerical investigation on the combustion characteristics of
turbulent premixed ammonia/air flames stabilized by a swirl burner

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Abstract
The present study is dedicated to understand the combustion characteristics of turbulent premixed swirl flames for ammonia (NH₃)/air mixture in gas turbine combustors by a numerical investigation. Although, NH₃ has been identified recently as a sustainable fuel because of the carbon-free nature, some physical and chemical characteristics of NH₃, such as very low laminar burning velocity, production of large amount of fuel NO during the combustion, hampered the utilization of the NH₃ as a commercial fuel. Hence, the large eddy simulation (LES) numerical technique was used to produce a detailed and multi-scale information about the reacting flow field and the chemical species distributions of turbulent premixed NH₃/air flames by three dimensional calculations. The study realized that a swirl burner successfully stabilizes the NH₃/air premixed flames without any additives. In addition, the study found that even though there is an enormous NO emission than that of the ordinary hydrocarbon fuel at the stoichiometric condition, in the rich flame condition, NO emission is significantly decreased, whereas unburnt NH₃ increases with respect to the equivalence ratio. Accordingly, there is an impressive operating condition for NH₃/air mixtures, which gives a minimal NO and unburnt NH₃ emissions even for turbulent swirl flames. The present study found that, at the initial mixture temperature of 500 K, the equivalence ratio of 1.225 gives the minimal NO and NH₃ emissions, and this is the best operating point for the selective catalytic reduction (SCR) process in the downstream of the burner.

Key words: Swirling flow, Ammonia, Turbulent premixed flames, Flame stabilization, NO/NH₃ emission reduction, LES

1. Introduction
In order to minimize the detrimental effects of fossil fuels on the earth, recently, ammonia (NH₃) has been identified as a sustainable fuel for various sectors because of its carbon-free nature like hydrogen. Similar to hydrogen, NH₃ is also a synthetic product that can be obtained either from fossil fuels, biomass, or other renewable sources. However, NH₃ has some advantages than hydrogen, such as less expensive cost per unit of stored energy, higher volumetric energy density, easier production, handling and distribution with the existing infrastructure facilities, and better commercial viability (Zamfirescu and Dincer, 2008). Moreover, NH₃ has a narrow flammability range, and hence, it is generally considered as non-flammable when transported. Therefore, NH₃ transportation is much safer than the hydrogen transportation. However, low burning velocity of NH₃, as low as 7 cm sec⁻¹ at the stoichiometric condition (Hayakawa et al., 2015a), should lead to the least flame stabilities. In addition, NH₃ contains the nitrogen itself, and consequently it may lead to higher production of fuel NOx. Therefore, the flame stabilization and emission reduction have become the major challenges in the NH₃ fueled gas turbine development.

On the other hand, one of the most promising gas turbine combustion techniques to respect the strict legislative limits on the combustion pollution emission is the adaptation of lean premixed flames for hydrocarbon fuels. However, lean turbulent premixed flames, which also show the lower burning velocities, lead to a flame instability, and a classical way...
of stabilizing the lean premixed flames consists in generating a large inner recirculation, where the low velocity zone
permits flame anchoring, by means of a swirling flow. Moreover, the recirculation of the hot burnt gases in the proximity
of the fresh mixture leads to a continuous supply of radicals and ignition of the reactive flow system. Nevertheless, as to
the best of the author’s knowledge, there is no any comprehensive numerical study on turbulent NH$_3$/air flames stabilized
by a swirl burner. Meanwhile, recent fundamental flame characteristics of NH$_3$/air laminar flames have been
clarified. The study of Hayakawa et al. (2015b) on the NO formation/reduction mechanisms of NH$_3$/air premixed flames
at various equivalence ratios and pressures revealed that the mole fraction of NO significantly decreases with an increase
in equivalence ratio of the rich flame side at the atmospheric pressure and the mixture temperature of 298 K, based on
the one-dimensional laminar flame analysis. This is caused by of excess NH$_i$ ($i=2$, $1$, $0$) radicals in the rich NH$_3$/air
mixtures. In addition, the laminar burning velocity and Markstein length at elevated pressures have been experimentally
clarified by Hayakawa et al. (2015a), and Brackmann et al. (2016) have investigated the structure of premixed NH$_3$/air
flames at the atmospheric pressure using the laser diagnostics and kinetic modeling.

Thus, the present study is dedicated to understand the combustion characteristics of the turbulent premixed swirl
flames for NH$_3$/air mixture. Accordingly, a relatively simple test case was chosen as an affordable test to evaluate the
feasibilities of more complex gas turbine combustors. However, gas turbine combustor modeling comprises a wide range
of computational and modeling challenges because of the involvement of the interactions of many complex physical
processes such as the turbulent-chemical interaction, and thereby, in the present study, large eddy simulation (LES) with
a finite rate chemistry is performed in three-dimensional computational domain in order to discuss a detailed resolution
of the reacting flow fields and flame structures in terms of the equivalence ratio.

2. Mathematical modeling
2.1 Governing equations and the sub-grid scale model

In computational fluid dynamics (CFD), large eddy simulation (LES) with the finite rate chemistry is one of the most
promising techniques to produce detailed and multi-scale information about reacting flow and scalar fields. In the present
study, the reacting flow simulation was conducted using the open-source code, OpenFOAM (http://www.openfoam.org).
The simulations were conducted using the scalar supercomputers, which consist of CPUs of Intel XeonE5-4650v2 2.40
GHz and memory of 8 TB, at the Institute of Fluid Science, Tohoku University, Japan. The LES in OpenFOAM with a
two-step chemistry has been successfully used to predict the low swirl stratified premixed methane/air flames (Nogenmyr
et al., 2009).

Spatially filtered Navier-Stokes equations (Poinset and Veynante, 2005) are used in the LES of the present study as
shown in Eqs. (1) – (4).

Continuity equation:
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i)}{\partial x_i} = 0
\]  

Momentum equation:
\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial}{\partial x_j} \left[ \bar{\rho} (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) \right] + \frac{\partial \bar{f}_{ij}}{\partial x_i} + \frac{\partial \bar{p}}{\partial x_j} 
\]  

Species mass balance equation:
\[
\frac{\partial \bar{Y}_k}{\partial t} + \frac{\partial (\bar{Y}_k \bar{u}_i)}{\partial x_i} = -\frac{\partial}{\partial x_i} \left[ \bar{Y}_k \bar{u}_i \bar{u}_j \right] + \frac{\partial}{\partial x_i} \left( \bar{Y}_k \bar{u}_j \right) + \bar{\omega}_k \quad \text{for } k = 1, \ldots, N
\]  

Sensible enthalpy equation:
\[
\frac{\partial \bar{h}_s}{\partial t} + \frac{\partial (\bar{h}_s \bar{u}_i)}{\partial x_i} = -\frac{\partial}{\partial x_i} \left[ \bar{h}_s \bar{u}_i \bar{u}_j \right] + \frac{\partial}{\partial x_i} \left( \bar{h}_s \bar{u}_j \right) - \frac{\partial}{\partial x_i} \left( \bar{h}_s \bar{u}_j \right) + \frac{\bar{D}_p}{\bar{D}t} + \bar{\omega}_T 
\]  

Here
\[
\frac{\bar{D}_p}{\bar{D}t} = \frac{\bar{D}_p}{\bar{D}t} + \bar{u}_i \frac{\partial \bar{p}}{\partial x_i}
\]

where $t$ is time; $u_i (i = 1, 2, 3)$ are the velocity components in the Cartesian coordinates $x_i (i = 1, 2, 3)$ directions,
respectively. The quantities with over-bars, $\bar{f}$ denote the spatially filtered values from the instantaneous quantities, $f$
whereas the quantities with over-tildes denote density weighted spatial filtering, $\bar{f} = \bar{\rho} \bar{f} / \bar{\rho}$. In addition, here, $\rho$
is the density, $p$ the pressure, $\tau_{ij}$ the viscous tensor, $Y_k$ the mass fraction of the species $k$, $h_s$ the sensible enthalpy of the
mixture, \( h_{s,k} \) the sensible enthalpy of species \( k \), \( \dot{\omega}_k \) the reaction rate of species \( k \), \( \dot{\omega}_T \) the total heat release rate, \( \lambda \) the heat conductivity of the mixture, and \( V_{k,i} \) the \( i \) component of the diffusion velocity of species \( k \).

Moreover, filtered laminar diffusion fluxes for species and enthalpy in the Eqs. (3) and (4) are modeled through a simple gradient assumption such as:

\[
V_{k,i} = -\rho D_k \frac{\partial \tilde{Y}_k}{\partial x_i} \quad \text{and} \quad \frac{\partial \tilde{T}}{\partial x_i} = \frac{\lambda}{\rho} \frac{\partial T}{\partial x_i}
\]

Here, \( D_k \) is the diffusivity of the species \( k \). In addition, the first terms of the right hand side of Eqs. (2), (3) and (4) are required to model because, in the LES approach, scales smaller than the grid size are not resolved, and accordingly, accounted through the subgrid scale tensor, \( T_{ij} \), as given by:

\[
T_{ij} = u_i \bar{u}_j - \bar{u}_i \bar{u}_j
\]

Most subgrid scale models are based on an eddy-viscosity assumption to model the subgrid scale tensor:

\[
T_{ij} = -\frac{1}{3} T_{kk} \delta_{ij} - 2 \nu_t \tilde{S}_{ij}
\]

where \( \delta_{ij} \) is the Kronecker delta function and the rate of strain tensor, \( \tilde{S}_{ij} \), is given by:

\[
\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]

Moreover, unresolved fluxes of species and enthalpy are described as a gradient assumption:

\[
\bar{u}_i \tilde{Y}_k - \bar{u}_i \bar{Y}_k = -\frac{\nu_t}{S_{ck}} \frac{\partial \tilde{Y}_k}{\partial x_i}
\]

\[
\bar{u}_i \tilde{h}_s - \bar{u}_i \bar{h}_s = -\frac{\nu_t}{P_{rt}} \frac{\partial \tilde{h}_s}{\partial x_i}
\]

where \( S_{ck} \) and \( P_{rt} \) are subgrid scale Schmidt number and subgrid scale Prandtl number, respectively.

In addition to the governing Eqs. (1) – (4), a modeled transport equation for the turbulent kinetic energy, \( k \), as shown in Eq. (15), (Kim and Mennon, 2010) is solved and the value of \( k \) is used for the turbulent combustion modeling.

\[
\frac{\partial \tilde{k}}{\partial t} + \frac{\partial \tilde{p} \tilde{u}_i \tilde{k}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\nu_t}{\sigma_k} \frac{\partial \tilde{k}}{\partial x_i} \right) + 2 \nu_t \tilde{S}_{ij} \tilde{S}_{ij} - \frac{2}{3} \tilde{p} \frac{\partial \bar{u}_i}{\partial x_i} - \frac{C_e \tilde{k}^{1/2}}{l}
\]

where constants of \( \sigma_k \) and \( C_e \) are 1 and 1.048, respectively.

In the present study, the conservation equations were solved by the existing OpenFOAM codes, whereas newly developed codes were added the main program for the solving of the subgrid scale viscosity.
2.2 Numerical models and conditions

A second order finite volume scheme is used for the discretization of spatial terms in the transport equations of momentum, mass fraction and sensible energy, whereas a second order implicit scheme is employed for the time integration. The turbulent-chemistry interaction is accounted with a partially stirred reactor model (Golovichev et al., 2000). The Miller’s chemical kinetics for the oxidation of NH$_3$ in flames (Miller et al., 1983) which included 23-species and 98-elementry steps, was selected for the finite chemistry calculation. Even though the laminar burning velocity estimations by Miller’s chemical kinetics has a slightly over prediction than the experimental measurements (Hayakawa et al., 2015a) the mechanism was selected in the present study because it consists of a lower number of chemical species. However, still the chemical kinetics became a barrier to adopt the finite rate chemistry LES model, because of the higher computational cost, and accordingly, an in-situ adaptive tabulation algorithm library (Contino et al., 2011) was used to calculate the composition changes through the chemical reaction, and thereby reduce the computational burden.

The unstructured three dimensional computational domain consists of the cylindrical combustion chamber, which was installed in vertically, and an annulus swirl was installed at the center of the bottom of the combustion chamber. The computational grid was consisted of the 4.2 million cells, and a cell volume was approximately 0.25 mm$^3$.The inner and outer diameters, $D_i$ and $D_o$, of the swirler were 14 mm and 24 mm, respectively. The chamber had inner diameter of 72 mm (=3$D_o$), and a height of 150 mm. The circular outflow channel, which was placed at the top of the cylinder, had a diameter of 36 mm (=1.5$D_o$) and length of 10 mm. The swirler flow inlet was located 1 mm upstream from the bottom of the chamber. The origin of the coordinates was set at the center of the swirl burner exit, and the axial, radial, and tangential coordinates are indicated by $z$, $r$, and $\theta$ respectively. The mean velocity at the outlet of the swirl burner was 39.1 m/s, and the swirl angle, $\alpha$ was approximately 40 degree. Accordingly, the swirl number, $S$ was calculated by the Eq. (16) (Lefevle and Ballal, 2010) and, the swirl number was 0.675.

$$S = \frac{2}{3} \left[ 1 - \left( \frac{D_i}{D_o} \right)^3 \right] \tan \alpha$$ (16)

Based on the typical initial fuel/air mixture temperature of commercial gas turbines, all calculations are carried out at the initial temperature of 500 K and for the equivalence ratios, $\phi$ of 1, 1.25 and 1.4. A relative turbulence intensity of 30% was set for the inlet flow in order to retain a higher turbulent intensity in the flow field, whereas LES characteristic length scale in the flow field is approximately 0.63 mm, which corresponds to a cubic root of a computational cell. The walls of the furnace are non-slip and adiabatic, and the outlet is specified by the continuity boundary condition. The operating pressure is 0.1 MPa. The initial CFD time-step was selected as $1 \times 10^{-6}$ s with a corresponding Courant number of approximately 0.4, whereas the initial chemical time-step was selected as $1 \times 10^{-7}$ s. The resolution of computational grid is comparable with the study of Hernandez-Perez et al. (2014) on large eddy simulation of lean hydrogen-methane turbulent premixed flames in the methane-dominated regime.

In addition, one-dimensional unstretched planer flame simulations were carried out using the CHEMKIN-PRO (2010). The inlet temperature was set to 500 K and the Miller’s chemical kinetics for the oxidation of NH$_3$ in flames (Miller et al., 1983) was employed.

3. Results and discussion

3.1 Instantaneous reacting flow field

Figures 1 (a), (b), and (c) show the instantaneous streamlines and velocity distribution in a vertical plane, turbulence intensity, $u'$, and iso-surfaces of the second invariant of the velocity gradient tensor, $Q$, as shown in Eq. (17) (Hinze, 1959), at $3 \times 10^{-7}$ (selected as a median value), shaded with the mass fraction of NH$_3$, $Y_{NH_3}$, respectively.

$$Q = -\frac{1}{2} \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i}$$ (17)

The flow field consists of inner and outer recirculation zones as shown in Fig. 1(a). In the swirl flow, inner recirculation zone (IRZ) strongly associated with the vortex breakdown bubble owing to low pressure of backside in the swirling flow, whereas an outer recirculating zone (ORZ), or a toroidal recirculating region generated by the rapid expansion of the annular swirler into the combustor (Chiterev et al., 2014). The recirculation zones bring the free radicals
and hot burnt gases to the upstream of the combustion chamber and leads to the mixing of burnt and unburnt gases whereas maintaining a continuous chemical reaction. Moreover, as shown in Figs. 1 (a) and (b), the flow field in the near downstream of the burner is directed towards the furnace wall owing to the centrifugal force from the swirl motion and the sudden expansion of the annuals flow in to the combustion chamber. The turbulence intensity, $u'$, was calculated from the turbulent kinetic energy by the isotropic assumption. Figure 1 (b) clearly shows the small eddies along the main flow field in the near downstream of the combustion chamber, which enhance the turbulent mixing of burnt and unburnt gases. In addition, the dissipation of the turbulent intensity is moderately high because of the sudden expansion of the geometry at the swirler outlet. Hence, even though the turbulent intensity at the outlet of the swirl burner is approximated to 11 m/s, the turbulent intensity of the central flow region of the combustion chamber is about 2 m/s. However, mean flow velocity in the central flow region of the chamber is about 10 m/s, and hence, the relative turbulence intensity is still conserved at about 20%. Moreover, vortices in the flow field are visualized in Fig. 1(c) by using the iso-surfaces of second invariant of the velocity gradient tensor, $Q$, at $3 \times 10^7$. The iso-surfaces are shaded according to the mass fraction of the NH$_3$, $Y_{NH3}$. Figure 1 (c) clearly shows the rotational flow structures in the near downstream of the swirl burner.

3.2 Flame structure at the stoichiometric condition

In the present study a swirler stabilized NH$_3$/air flame structure at the stoichiometric condition and initial mixture temperature of 500 K is discussed by means of temperature distribution, distribution of OH mole fraction, $X_{OH}$, and the heat release rate (HRR) distribution as shown in the Figs. 2 (a), (b), and (c), respectively. Hereafter, $X_k$ shows the mole fraction of species of $k$. Figures 2 (a), (b) and (c) clearly show that the swirling flow at the stoichiometric condition produce a V flame topology, and the reaction zone starts rather close to the exit of the swirl burner and it inclines towards the furnace wall as shown in Fig. 2 (c). The flame height is about 100 mm. The flame region temperature has an almost uniform distribution, and is about 2000 K. Even though at the flame front, OH mole fraction has a slightly larger value, the flame region has a uniform OH distribution as shown in Fig. 2 (b), and consequently, the OH mole fraction distribution verifies that flame has been completely filled in the combustion chamber and the longer flame length than ordinary
hydrocarbon flames (Obserleithner et al., 2015, and Stohr et al., 2014) should be related with the lower laminar burning velocity of the NH$_3$/air mixture (Hayakawa et al., 2015a).

Fig. 2 Flame structure at the stoichiometric condition: (a) temperature distribution; (b) distribution of OH mole fraction, $X_{\text{OH}}$; (c) heat release rate (HRR) distribution.

Fig. 3 Emission characteristics under the stoichiometric condition: (a) distribution of NO mole fraction; (b) distribution of NH$_3$ mole fraction; (c) distribution of H$_2$ mole fraction.
3.3 Emission characteristics under the stoichiometric condition

The NH3/air combustion emission characteristics under the stoichiometric condition and initial mixture temperature of 500 K are shown in the Figs. 3 (a), (b), and (c) in terms of mole fraction distribution of NO, NH3 and H2, respectively. The almost uniform NO distribution is resulted in the flame region, as shown in Fig. 3 (a), and the greater amount of NO generation should be associated with the fuel NO production. Moreover, this NO generation behavior is qualitatively agreed with the 1-dimentional study of the NH3/air mixture at the stoichiometric condition and initial temperature of 298 K by Hayakawa et al. (2010b). Then, in order to find the space and time averaged values of the emissions, the space averaged values for all emissions at the exit of the combustion chamber were plotted against the time until the system reached to the steady state. Subsequently, the space and time averaged NO emission at the furnace exit was calculated, and is about \(8266 \times 10^{-6}\) and the value is much higher than that of ordinary hydrocarbon flames, which produce the thermal NO significantly at above the flame temperature of 1800 K (Flagan and Seinfeld, 1988). However, NH3 has almost completely burnt in this initial mixture conditions and space and time averaged NH3 at furnace exit is about \(0.001 \times 10^{-6}\). Since the flame has a V topology, unburnt NH3 has accumulated at the corners of the cylindrical combustion chamber. In addition to the NO and unburnt NH3 emissions, in the present study, small amount of unburnt H2 emission was identified, and the space and time averaged value at the furnace exit is about \(991 \times 10^{-6}\). Possibly, NH3 cracking may cause the H2 generation. According to these emission characteristics, further studies on NH3 fueled low NO combustion systems are expected.

3.4 Emission characteristics under the rich flame condition

Enormous NO emission of the NH3 flame under the stoichiometric condition has urged a firm solution for the NO reduction if NH3 is needed to be use as a sustainable fuel. The one-dimensional study of Hayakawa et al. (2010b) shows that at the equivalence ratio of 1.1 (and initial mixture temperature of 298 K), there is a significant NO reduction, and this was caused by the excess NH (i=2, 1, 0) radicals in the rich flame condition as shown in Eq. (18) (Hayakawa et al., 2010b). In addition, Warnatz et al. (2006) has described that there is a possibility for NO reduction in exhaust gases of ordinary hydrocarbon fuels by externally adding of small amount of NH3, which produces the NH radicals and starts the reactions as shown in Eq. (18).

\[
\begin{align*}
\text{NH}_2 + \text{NO} & \leftrightarrow \text{N}_2\text{H} + \text{OH} \\
\text{NH} + \text{NO} & \leftrightarrow \text{N}_2\text{H} + \text{O} \\
\text{N} + \text{NO} & \leftrightarrow \text{N}_2 + \text{O} \\
\end{align*}
\]  

(18)

Thus, in the present study, a one-dimensional flame simulation for NH3/air mixture was carried out using the CHEMKIN-PRO (2010) at the initial temperature of 500 K and over the wide range of equivalence ratio in the lean and rich conditions. The study showed, as seen in the later part of this paper, that NO emission has maximum value around the equivalence ratio of 0.9, and then decreased with an increase in the equivalence ratio. In rich flame conditions, NO was almost zero, nevertheless unburnt NH3 emission was significantly increased after the equivalence ratio of 1.25. Eventually, the one-dimensional study found that at the equivalence ratio of 1.25 the NO and unburnt NH3 mole fractions are minimal, and both are having the value of less than \(300 \times 10^{-6}\).

Then, the three dimensional study was carried for NH3/air mixtures at the equivalence ratios of 1.25 and 1.4 with same other initial mixture conditions. Figures 4 (a), (b), and (c) show the emission characteristics at the equivalence ratio of 1.25 in terms of NO mole fraction, NH3 mole fraction, and H2 mole fraction, respectively. Similar to the one-dimensional study, NO emission has significantly reduced compare to the stoichiometric condition. In this case, the space and time averaged value of NO emission is about \(203 \times 10^{-6}\), and there is a quantitative agreement with a one-dimensional study. In addition, the space and time averaged unburnt NH3 emission at the furnace exit is about \(1426 \times 10^{-6}\), and it is slightly above the one-dimensional study. However, H2 generation is very significant at the rich flame condition and the space and time averaged of unburnt H2 emission is about \(67000 \times 10^{-6}\) by NH3 cracking. Another significant difference of the flames between the stoichiometric and equivalence ratio of 1.25 (and 1.4 also) conditions is the change of flame from V to M topology. Guiberti et al. (2015) demonstrated that when the tip of a swirl flame is quenched at the combustor side wall, V to M flame topology transition are triggered by flashback of the flame front.
Fig. 4 Emission characteristics at the equivalence ratio of 1.25: (a) distribution of NO mole fraction; (b) distribution of NH₃ mole fraction; (c) distribution of H₂ mole fraction.

Fig. 5 Space and time averaged NO, NH₃, and H₂ mole fraction variations at the furnace exit in terms of the equivalence ratio with one-dimensional calculations.
along this wall. Owing to the change of flame topology from V to M, there is no unburnt NH$_3$ accumulation at the corners of combustion chamber, and flame height is also significantly reduced.

Eventually, the summary of the space and time averaged NO, NH$_3$, and H$_2$ emissions, at the furnace exit, in terms of the equivalence ratio is shown in the Fig. 5 with the one-dimensional emission values, as shown by broken lines. Here, the mole fractions of one-dimensional flame simulations were calculated at the 40 mm downstream from the maximum heat release position of each flame. The three-dimensional calculations are almost quantitatively agreed with the one-dimensional calculations for NO and H$_2$ mole fractions. However, the unburnt NH$_3$ mole fractions in the rich flame conditions are higher than that of one-dimensional estimations, and moreover, the unburnt NH$_3$ emission is rapidly increased with an increase in the equivalence ratio. Figure 5 shows that the unburnt ammonia is 7 times larger at the equivalence ratio of 1.4 than that of 1.25. The NO and unburnt NH$_3$ emissions are minimal at the equivalence ratio of 1.25 by one-dimensional calculation, whereas at the equivalence ratio of 1.225 by three-dimensional calculation. This operating condition is more important for the selective catalytic NO reduction (SCR) at the downstream of the burner.

4. Concluding Remarks

Combustion characteristics of NH$_3}$/air swirl flames were numerically studied in details by using the large eddy simulation with a detailed chemistry. The following key findings were observed.

1. The stabilized NH$_3$/air flame was resulted using a swirl premixed reacting flow for the stoichiometric and rich flame conditions at the initial mixture temperature of 500 K and velocity of 39.1 m/s.
2. However, at the stoichiometric condition, almost uniformed NO distribution was resulted in the flame region, where NO concentration is much higher than the ordinary hydrocarbon flames.
3. Thus, NH$_3}$/air flames at rich conditions were studied, and, in this condition, it was found that NO emission was significantly decreased whereas unburnt NH$_3$ increases with respect to the equivalence ratio.
4. One and three dimensional calculations verified that there is a significant operating condition which gives minimal NO and unburnt NH$_3$ emissions for the NH$_3}$/air combustion.
5. According to the three dimensional calculation, at the equivalence ratio of 1.225, NO and NH$_3$ emissions are minimal and suitable for the selective catalytic reduction (SCR) at the downstream of the burner.

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