

# Industrial Ammonia Burner and Modeling Capability Development

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## ABSTRACT:

Ammonia as a fuel for industrial heating and steam generation is being considered as an option to help reduce industrial greenhouse gas emissions, especially in regions without indigenous natural gas or pore space for CO<sub>2</sub> sequestration. Ammonia is attractive as a low-carbon fuel because of its energy density and resulting transportability compared to hydrogen and other alternatives; the presence of existing protocols, standards, and infrastructure for ammonia transportation; and to eliminate the need for additional facilities and energy consumption to convert ammonia from a carrier medium (ammonia/hydrocarbon) to fuel (hydrogen).

Due to its low laminar flame speed and propensity to form high concentrations of nitrogen oxides (NO<sub>x</sub>), ammonia presents challenges as a fuel when compared with gaseous hydrocarbon and hydrogen-based fuels. This paper describes the development to date of a commercial burner based on Zeeco's various burner concepts for use in industrial heating and steam generation applications. Additionally, it describes developments of modeling tools to allow the prediction of ammonia combustion performance in a burner for commercial applications.

The technical development work described here is part of a larger ammonia combustion program led by ExxonMobil, including basic research by the Massachusetts Institute of Technology (MIT) and Stanford University, aimed at furthering the understanding of ammonia combustion to allow the development of an ammonia burner for specific commercial applications.

Results from tests of Zeeco's modified GLSF FREE JET burner, which was selected from testing various burner models, have been presented here. Tests have been performed with different mixes of ammonia and hydrogen or natural gas at varying operating conditions, demonstrating progress on the development of an ammonia burner providing a stable flame with manageable NO<sub>x</sub>. Ammonia emissions test data are included in this paper from three commercial burner designs, along with supporting computational fluid dynamics (CFD) analysis and a discussion of how CFD can be used to predict combustion performance when firing ammonia. Using both combustion testing and CFD is essential for developing new technologies and predicting performance in commercial applications with reasonable certainty. Finally, this paper outlines the next steps in the commercial ammonia burner development program.

## 1.0 INTRODUCTION

Interest in combusting ammonia as a carbon-free fuel for energy systems is gaining traction, especially in geographical locations where indigenous natural gas (NG) and CO<sub>2</sub> sequestration are limited or

unavailable. Ammonia's high energy density, low Carbon Intensity and resulting transportability make it an attractive fuel compared to many alternatives including hydrogen. Additionally, though not in widespread use, industry already has existing protocols, standards, and infrastructure in place for ammonia handling and transport. Lastly, combusting ammonia directly eliminates the need for the facilities and additional energy consumption required to convert ammonia to hydrogen. Early adopters of ammonia firing can be seen at coal-fired power plants in Asia, where ammonia is being tested as a supplemental fuel. This configuration reduces CO<sub>2</sub> emissions but still relies on selective catalytic reduction (SCR) technology to reduce both thermal and fuel-bound NO<sub>x</sub> emissions.

In comparison with industrial fuel gases commonly used, ammonia properties are quite different and are shown in Table 1 below. It has low flame speed, lower flame temperature, narrow flammability limits, and slower chemical kinetics. These characteristics make ammonia a much more difficult fuel to combust. Also, as ammonia is decomposed at high temperatures, nitrogen reacts with free oxygen and hydroxyl radicals and other compounds, producing high amounts of oxides of nitrogen (NO, NO<sub>2</sub>, N<sub>2</sub>O). To enable the broad use of ammonia as a carbon-free fuel for industrial heating and electric power generation, these combustion challenges must be overcome.

*Table 1: Comparison of Ammonia and Common Fuel Gases*

| Fuel Gas | Higher Heating Value (MJ/m <sup>3</sup> ) | Density (kg/m <sup>3</sup> ) | Auto Ign.   Adiabatic Temps (°C) | Flame Speed (m/s) | SG @ 25°C & 1 atm | Flammability Limits (% vol) |
|----------|-------------------------------------------|------------------------------|----------------------------------|-------------------|-------------------|-----------------------------|
| Methane  | 38.7                                      | 0.716                        | 595   1950                       | 0.34              | 0.55              | 5.0 - 15.0                  |
| Propane  | 93.2                                      | 1.879                        | 470   1970                       | 0.4               | 1.52              | 2.1 - 9.5                   |
| Hydrogen | 141.8                                     | 0.099                        | 500   2370                       | 1.9               | 0.07              | 4.0 - 75.0                  |
| Ethylene | 51.9                                      | 1.178                        | 425   2130                       | 0.67              | 0.97              | 2.7 - 36.0                  |
| Ammonia  | 18.6                                      | 0.771                        | 651   1800                       | 0.07              | 0.59              | 15.0 - 28.0                 |

ExxonMobil and Zeeco have initiated a joint effort to develop a commercial ammonia burner that can be used in new and existing industrial heating equipment (process heating, steam generation, etc.). The development program is aimed at producing a burner that allows flexibility in fuel composition, gives stable performance across all operating conditions and aims to reduce GHG emissions. Emission targets for the project include NO<sub>x</sub> less than 200 ppm (ideally under 100 ppm), and ammonia slip less than 50 ppm (preferably under 10 ppm) at 3% O<sub>2</sub> dry. This paper describes the development efforts to date.

## 2.0 BURNER DEVELOPMENT, TESTING PLAN AND TEST FACILITIES

### 2.1 Development and Testing Plan

Three burner concepts were identified as starting points for the development of a commercial ammonia burner:

1. Zeeco's GB burner – a conventional raw gas burner with bluff body flame stabilization on a single, central fuel tip

2. Zeeco's GLSF FREE JET burner – an ultra-low NO<sub>x</sub> burner (ULNB) with staged fuel tips stabilized on a hot refractory tile and with flame from auxiliary fuel tips on the inside of the tile
3. Zeeco's GLSF DT burner – a ULNB with the same type of staged and auxiliary tips arranged around a refractory tile with an additional set of staged fuel tips around the periphery of the burner

Figure 1 shows the schematics for the three burner concepts.



Figure 1 - Burner Concepts in Initial Testing - (left to right) GB, FREE JET, DT

Initial testing and burner configuration optimization was conducted on natural draft, nominal 4 MMBtu/hr versions of these three burner types at Zeeco's Global Technology Center (GTC) near Tulsa, Oklahoma. Testing a burner size at the low end of the commercial scale allowed for a large number of tests to be quickly and economically conducted. The more intense fuel/air mixing enabled by higher combustion air pressure drop in forced draft burner designs can mask burner design deficiencies during initial concept development. Thus, natural draft testing was selected to better enable identification of burner configuration concepts for optimizing flame stabilization and NO<sub>x</sub> and NH<sub>3</sub> emissions.

For the initial burner testing phase, the GB burner blended ammonia with support fuel because there was only one gas stream fired. The ULNB designs (FREE JET and DT) used separate fuel streams for the auxiliary tips (tips in the center) and the main tips (tips around the burner tile), allowing use of 100% natural gas or hydrogen in the central auxiliary fuel tips while maximizing NH<sub>3</sub> content of the fuel in the main fuel tips. Natural gas and hydrogen were used as support fuel.

The results of this initial testing were then used to identify the most promising design concept, which was then further optimized to maximize the percentage of ammonia in the fuel blend that could be utilized while still producing a stable flame with reduced emissions. This most promising design will be used to produce a forced draft burner scaled up to the capacity range typically seen for most industrial heating applications.

Development of computational fluid dynamics (CFD) modeling techniques for ammonia combustion is an integral part of the commercial ammonia burner development. While hydrocarbon and hydrogen combustion are well understood with validated kinetics, ammonia combustion modeling is at its initial stage of development. The CFD work focused on improving the chemical kinetics and turbulence models

to better simulate ammonia combustion. The objective of the CFD work is to develop CFD tools to support burner design and predict burner performance in commercial applications.

## 2.2 Test Facilities

An existing vertical cylindrical (VC) single burner test furnace at Zeeco's GTC, appropriately sized for the 4 MMBtu/hr burner being tested, was selected for installation of facilities to accommodate burning of ammonia. The test furnace used had a radiant box height of about 14' and a tube circle diameter of 6', with a single burner being tested at the center of the furnace floor. Heater firebox temperature was controlled via water flow through tubes on one side of the VC, mimicking a commercial vertical cylindrical with multiple burners arranged in a circle inside a larger circle of process fluid tubes.

Fuel supply, vaporization, piping, and metering were all added or modified for handling ammonia. To ensure safe operation, a detailed safety review was completed to ensure adequate facilities were present, required operating procedures developed, and operating personnel trained to mitigate the risks associated with handling and operating with ammonia fuel. Operating procedures and training included consideration of personnel present in the facility at the time of testing, ambient conditions, wind speed and direction, etc.

Emissions measurement was another area that needed significant attention. Traditional  $\text{NO}_x$  measurement systems utilizing chemiluminescence can give misleading results due to potential interactions with  $\text{NH}_3$  slip present in the system. Also, it was important to measure  $\text{NH}_3$  slip and  $\text{N}_2\text{O}$  to achieve the program's burner development goals.  $\text{NO}_x$  emissions include  $\text{NO}$  and  $\text{NO}_2$ , but do not account for  $\text{N}_2\text{O}$ . In most combustion systems with blends of hydrocarbon and hydrogen fuels,  $\text{N}_2\text{O}$  emissions are very low, typically less than 5 ppm. However, with very high fuel-bound nitrogen in a high ammonia fuel blend, there is much greater potential for significant  $\text{N}_2\text{O}$  emissions.  $\text{N}_2\text{O}$  emissions have not historically been a concern, as they do not cause respiratory harm to people, unlike  $\text{NO}_x$ , which causes atmospheric ozone. Yet,  $\text{N}_2\text{O}$  is a powerful greenhouse gas, so it is of particular concern when using ammonia as a low-carbon fuel to abate  $\text{CO}_2$  emissions.

For emissions measurement, the following analyzers were installed on the test furnace. These included:

- A Fourier Transform Infrared Spectroscopy (FTIR) system to measure  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{O}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CO}$
- A Tunable Diode Laser (TDL) based system to measure  $\text{NO}$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{O}$
- Chemiluminescent and paramagnetic type analyzers for  $\text{NO}_x$ ,  $\text{NO}_2$ ,  $\text{O}_2$  dry, and  $\text{CO}$

The TDL system was installed in the stack (Figure 2), on two pairs of nozzle connections. The other two analyzer systems used independent heated sampling systems to bring the flue gas sample to the analyzers at the grade level.



*Figure 2 - TDL Analyzer on Test Furnace Stack*

There were a few challenges and observations from combusting high levels of ammonia, as listed below:

- High concentrations of moisture in the flue gas created challenges for the FTIR and the TDL systems (wavelength interference). An analyzer configuration to account for the expected range of flue gas water vapor concentration was required. At the writing of this paper, TDL configuration allowing validated measurements is still a work in progress, so all  $\text{NH}_3$  measurements quoted in this paper are from the FTIR analyzer.
- Ammonia is a “sticky” gas and can stay adhered to the sample line tubing wall for an extended period. This made it challenging to take test point measurements that did not carry ammonia slip from previous test points. A test was conducted where the analyzer initially read  $<1$  ppm  $\text{NH}_3$  before ammonia fuel was introduced; upon firing, ammonia measurement spiked to 2000–4000 ppm. The sample line was opened to the atmosphere, and it took 12 minutes for  $\text{NH}_3$  levels to drop below 10 ppm and 53 minutes to reach 2 ppm!
- Also, ammonia gets absorbed in the furnace insulation. On a separate test, the burner was shut down, and the furnace door was opened to the atmosphere. In the center of the furnace, the  $\text{NH}_3$  reading was zero, but read 9 - 17 ppm when measured 6” from the insulation. Also, there have been instances when the heater was started up on  $\text{H}_2$  (or natural gas), but  $\text{NH}_3$  was recorded because of ammonia trapped in the insulation even after overnight purging (opened in natural draft). Figure 3 shows a trend of  $\text{NH}_3$  measured by the FTIR analyzer vs. time after shutting off the burner when it was burning a high ammonia fuel (80+ vol%).
- There had been a few instances where ammonia condensed in fuel piping and dead-headed at the valve. The liquid didn’t burn well in the gas burner, and  $\text{NH}_3$  was recorded in the stack.

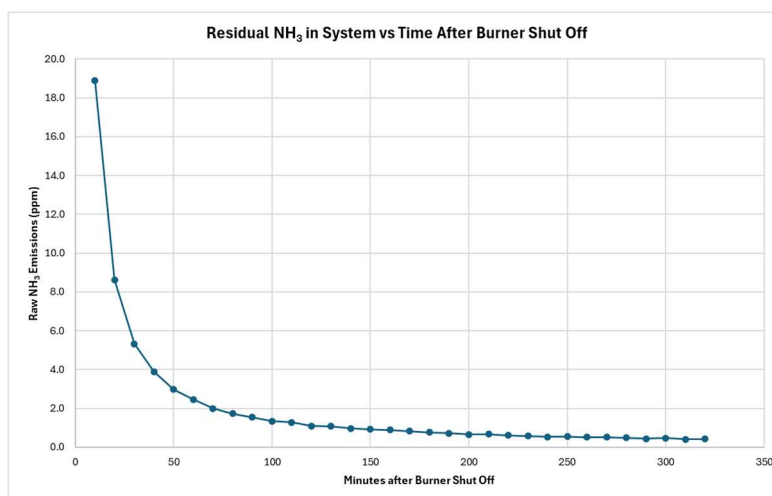


Figure 3: Residual NH<sub>3</sub> measured in stack vs. Time after shutting off burner

### 3.0 INITIAL BURNER TESTING RESULTS

For this initial development phase, burner testing was conducted across a range of excess O<sub>2</sub> levels at about 0.3" WC floor draft. Firebox temperature was maintained at 1600-1750F for most test points. Initially, none of the three burner concepts performed well, with each producing with high ammonia concentrations in the stack. Each underwent modifications to improve flame stability, reduce NO<sub>x</sub> and ammonia slip, and increase ammonia content in the fuel.

Table 2 shows a summary of test results for the three burner concepts after optimization. The conventional GB burner could combust up to 20% (\*) ammonia when mixed with natural gas and up to 60% when mixed with hydrogen. However, the NO<sub>x</sub> remained high. The GLSF FREE JET burner showed a marked improvement, producing a stable flame with 100% ammonia through the main tips, although ammonia slip became unacceptable with main fuel ammonia above 80%. It also delivered lower NO<sub>x</sub> emissions than the GB burner. The DT burner performed similarly to the FREE JET, offering no clear advantage. Based on these findings, it was decided to focus on the FREE JET design concept for further development.

(\*) All % compositions stated in this document are in volume percent, unless stated specifically otherwise

Table 2: Initial Test Results with Maximum Ammonia in Fuel

| Burner          | Main Fuel                               | Auxiliary Tip Fuel  | NH <sub>3</sub> /Total Fuel Flow | NH <sub>3</sub> /Total Heat Release | NO <sub>x</sub> <sup>1</sup> | NH <sub>3</sub> Slip | CO  | O <sub>2</sub> |
|-----------------|-----------------------------------------|---------------------|----------------------------------|-------------------------------------|------------------------------|----------------------|-----|----------------|
|                 | vol%                                    | vol%                | vol%                             | %                                   | ppm                          | ppm                  | ppm | vol%, dry      |
| Conventional GB | 20% NH <sub>3</sub> /80% NG             | N/A                 | 20%                              | 9%                                  | 1130                         | ---- <sup>2</sup>    | 0   |                |
|                 | 60% NH <sub>3</sub> /40% H <sub>2</sub> | N/A                 | 60%                              | 65%                                 | 2400                         | ----                 | 1   |                |
| GLSF FREE JET   | 85% NH <sub>3</sub> /15% NG             | 100% NG             | 77%                              | 57%                                 | 134                          | 41                   | 24  | 3.8            |
|                 | 90% NH <sub>3</sub> /10% NG             | 100% NG             | 82%                              | 63%                                 | 102                          | 79                   | 11  | 2.8            |
|                 | 85% NH <sub>3</sub> /15% H <sub>2</sub> | 100% H <sub>2</sub> | 67%                              | 73%                                 | 113                          | 26                   | 2   | 4.6            |
| GLSF DT         | 85% NH <sub>3</sub> /15% NG             | 100% NG             | 71%                              | 49%                                 | 260                          | 1                    | 1   | 2.9            |
|                 | 80% NH <sub>3</sub> /20% H <sub>2</sub> | 100% H <sub>2</sub> | 62%                              | 68%                                 | 151                          | 3                    | 0   | 3.7            |

<sup>1</sup> - Values corrected to 3% dry and 1700F

<sup>2</sup> - ---- indicates measurement for this parameter was not available during this test run

### 3.1 Initial Test Observations

A few key observations from the initial testing are summarized below:

- When increasing the  $\text{NH}_3$  content in the main fuel tips above 80 vol% on the GLSF FREE JET, the burner remained stable, but the flame length increased and resulted in significant  $\text{NH}_3$  slip (200 ppm to >1000 ppm) in the stack. The pictures in Figure 4 show stable flames with a variety of ammonia content in the main fuel tips up to 100% ammonia despite the very high slip at this condition. High ammonia slip may be seen with both natural gas and hydrogen support gas for test points with main fuel tip  $\text{NH}_3 > 80$  vol% in the data in Figure 5. Below 80% ammonia in the main fuel tips, most data points ranged between 0 – 5 ppm.
- In addition to reducing thermal  $\text{NO}_x$ , the ULNBs also reduced fuel-bound  $\text{NO}_x$  associated with the combustion of  $\text{NH}_3$  mixtures. The GB Conventional Burner produced  $\approx 2,400$  ppm  $\text{NO}_x$  emissions with 60%  $\text{NH}_3$  & 40% hydrogen. With the same fuel, the GLSF FREE JET burner produced 200 - 400 ppm  $\text{NO}_x$  emissions. It is surmised that the flue gas entrained into the flame by the FREE JET main fuel tips creates regions in which  $\text{NH}_2$  reduces the  $\text{NO}$  created in regions conducive to  $\text{NH}_3$  oxidation (high  $\text{O}_2$  and high temperature) to  $\text{N}_2$ .
- $\text{N}_2\text{O}$  emission correlated very strongly with  $\text{NH}_3$  slip. For test points where  $\text{NH}_3$  slip was < 5 ppm,  $\text{N}_2\text{O}$  was less than 10 ppm. Where  $\text{NH}_3$  slip was between 5 and 100 ppm,  $\text{N}_2\text{O}$  was between 10 and 50 ppm. For  $\text{NH}_3$  slip > 100 ppm,  $\text{N}_2\text{O}$  was 50-150 ppm. Thus, limiting  $\text{NH}_3$  slip results in preventing  $\text{N}_2\text{O}$  emissions that erode the  $\text{CO}_2$  emission reduction benefit of ammonia fuel.
- The results of staged air testing showed that with even small amounts of staging in the upper sections of the furnace,  $\text{NO}_x$  emissions increased by  $\approx 25$  ppm. Therefore, air staging in the upper regions of the furnace may not be an effective  $\text{NO}_x$  reduction method. Moreover, this showed that for process heaters and other applications where the furnace operates at negative pressure, air leakage can have a significant impact on  $\text{NO}_x$  emissions in the field.
- Ammonia probing during FREE JET testing at 3.4 MMBtu/hr with main tips firing 10 vol% NG and 90 vol%  $\text{NH}_3$ , and with 20% heat release from natural gas in the auxiliary tips, resulted in 1100 ppm  $\text{NH}_3$  at 15' above the floor and 5.5 ppm in the stack. Adding  $\text{NH}_3$  above the flame to simulate selective non-catalytic reduction (SNCR) to reduce  $\text{NO}_x$  was not an option at high ammonia firing. Instead, the focus was to reduce the flame height.

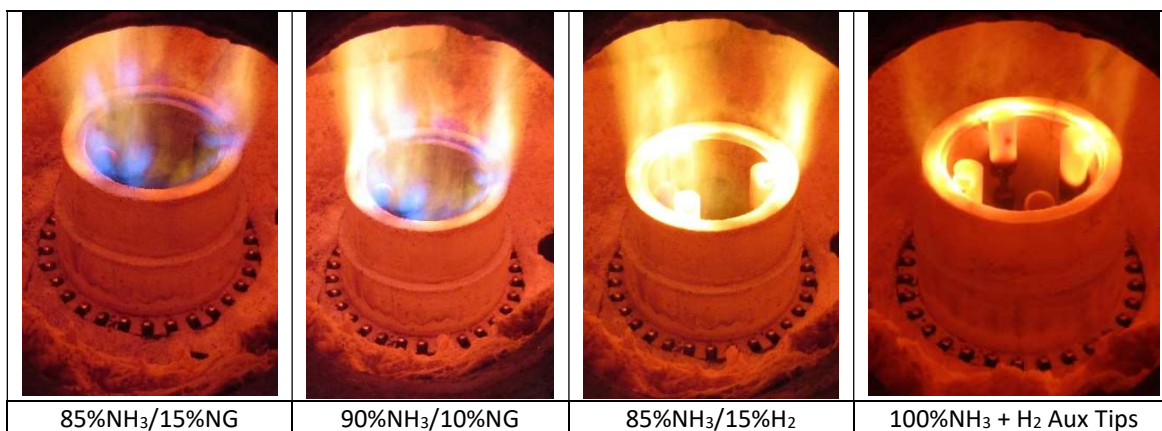


Figure 4 – Initial Testing of GLSF FREE JET with Main Tip Fuel Splits

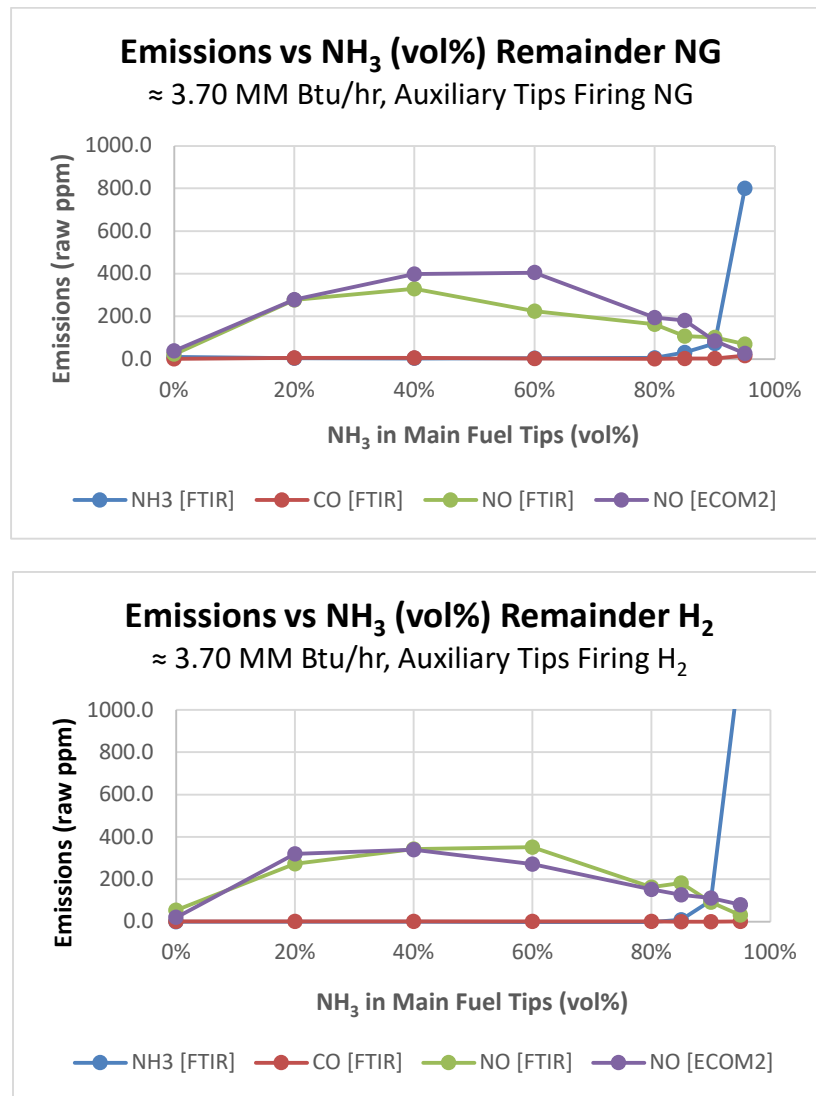


Figure 5: Comparison of stack emissions from the GLSF FREE JET burner for both natural gas and hydrogen used as support fuel

#### 4.0 OPTIMIZED NATURAL DRAFT GLSF FREE JET BURNER DEVELOPMENT AND TESTING

At the conclusion of the initial testing, it was evident that the improved GLSF FREE JET design had shown the most promise among the three concepts tested. The burner underwent additional development to improve the performance on ammonia firing. As stated before, the initial testing used either 100% NG or 100% H<sub>2</sub> in the auxiliary tips to provide flame stability. The main fuel tips used a blend of NH<sub>3</sub> and a support fuel (NG or H<sub>2</sub>).

In the improved burner development and testing, both the auxiliary and the main fuel tips were connected to the same supply, resulting in the same composition for both sets of tips. Design parameters examined/improved during initial development were further re-assessed so that the overall %NH<sub>3</sub> to the burner could be increased while trying to meet the target performance. Maintaining the auxiliary tip flame to provide robust ignition of the main fuel gas was found to be challenging, and several modifications were tested at the same furnace conditions used for the initial testing phase.

#### 4.1 Optimized Burner Performance Test Results

The maximum  $\text{NH}_3$  concentration achieved, while still meeting the desired target performance criteria, was 70%  $\text{NH}_3$  & 30% natural gas. While this overall  $\text{NH}_3$  content in the burner fuel was similar to the initial testing, eliminating the need for a separate 100% natural gas or 100% hydrogen supply for the auxiliary tips was a substantial improvement toward a burner suitable for industrial service deployment. At ammonia content above 70%, ammonia slip rapidly increased. The optimized natural draft burner performance with varying amounts of  $\text{NH}_3$  is shown in Figures 7 and 8 below.

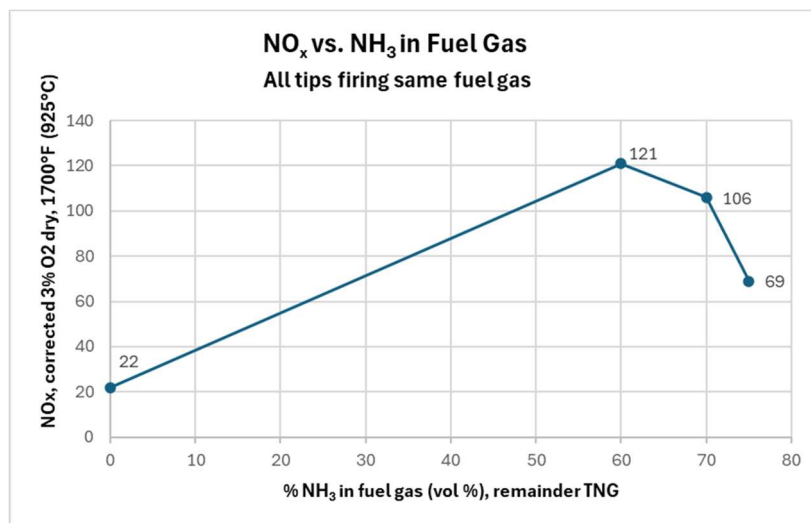


Figure 6:  $\text{NO}_x$  vs Fuel  $\text{NH}_3$  Content for Optimized Natural Draft GLSF FREE JET with Single Fuel Supply

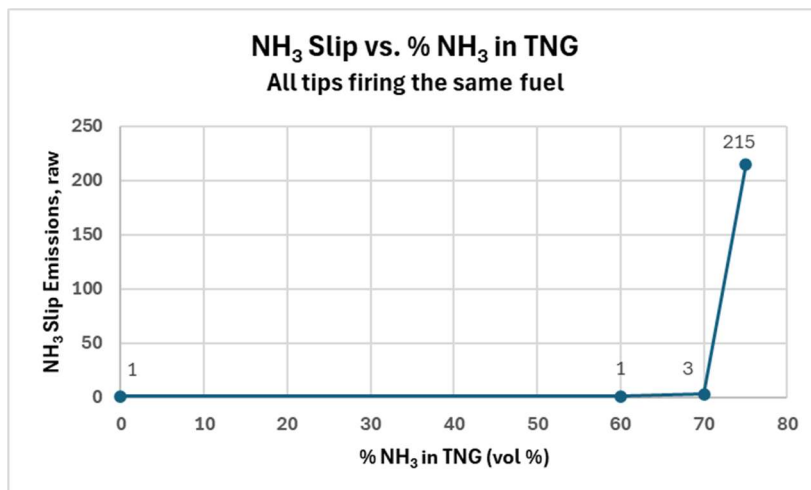


Figure 7:  $\text{NH}_3$  Slip vs Fuel  $\text{NH}_3$  Content for Optimized Natural Draft GLSF FREE JET with Single Fuel Supply

The optimized natural draft Free Jet burner on a single fuel supply has shown robust performance at high ammonia levels with reasonable levels of  $\text{NO}_x$  and  $\text{NH}_3$  emissions. This design needs further enhancement to allow higher levels of ammonia and finally reach 100% ammonia firing that is suitable for commercial application, which is the ultimate goal of this endeavor. Section *Future Work* in this paper elaborates on this.

## 5.0 DEVELOPMENT OF CFD MODELING TOOLS FOR BURNER PERFORMANCE PREDICTION

Using both combustion testing and computational fluid dynamics (CFD) is essential for the development of a burner for industrial service. Predicting burner performance (flame shape, emissions, flame-to-flame interactions, etc.) in a commercial application with reasonable certainty will be necessary to establish adoption in industry. While CFD tools for hydrocarbons and hydrogen fuels are very mature today, it is in a very early stage of development for ammonia. While single burners can be evaluated quickly in a test furnace, the value of CFD is in providing accurate performance predictions on multi-burner installations, especially for new or unusual applications.

CFD efforts focused on modeling furnace emissions of critical but hard-to-predict phenomena such as  $\text{NO}_x$  and ammonia slip. The CFD modeling method developed during this project provides a promising path forward for more challenging applications like ammonia combustion in multi-burner industrial equipment.

The key features of the model are as follows:

1. Realizable  $k-\varepsilon$ , steady-state RANS
2. The Eddy Dissipation Concept turbulence-chemistry interaction model (Magnussen & Hjertager<sup>1</sup>) with parameters tuned for this application
3. A reduced chemical kinetic mechanism based on the CRECK (Stagni *et al.*<sup>2</sup>) mechanism for natural gas and ammonia blends and mechanisms created by MIT for this project (Doner *et al.*<sup>3</sup>) for H-N-O kinetics, where no hydrocarbons are present

Some selected simulation results are shown below, with comparisons to physical test data.

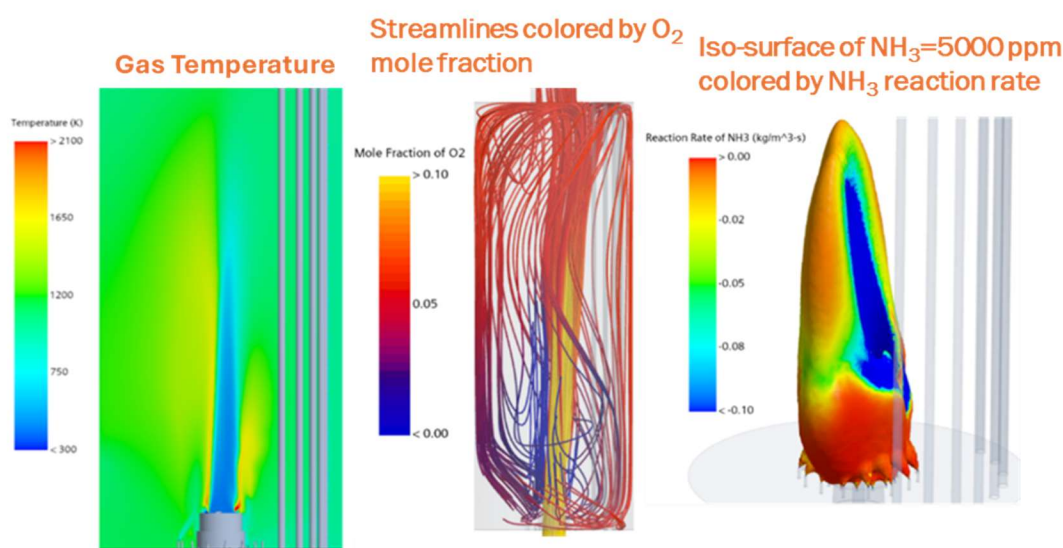


Figure 8: CFD results for 4 MMBtu/hr Heat Release with Main Fuel at 75%  $\text{NH}_3$ /25% NG and Auxiliary Fuel at 100% NG

Figure 9 shows typical CFD results for an ammonia-natural gas main fuel mixture in the GLSF FREE JET burner with a heat release of 4 MMBtu/hr. The cooling tubes situated on one side of the test furnace result in downward circulation of oxygen-rich gas near the tubes, resulting in faster fuel burnout on this side of the flame and the leaning of the flame toward the hotter side of the furnace.

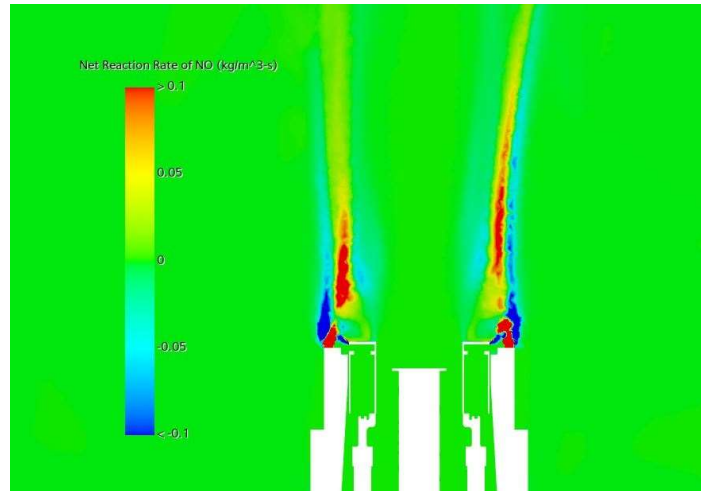


Figure 9 - Net Reaction Rate of NO with CRECK RM for GLSF Free Jet Burner at 4 MMBtu/hr with 75% NH<sub>3</sub>/25% NG Main Fuel and 100% NG Auxiliary Fuel

Figure 9 shows both the formation and destruction of NO in a flame burning 75% NH<sub>3</sub>, 25% natural gas. The model included enough chemical kinetic details to predict NO formation from fuel and thermal paths, as well as NO destruction by ammonia via selective non-catalytic reduction (SNCR) reactions. This model result is qualitatively consistent with Zeeco's understanding of how the fuel staging, flue gas entrainment and delayed air-fuel mixing work combined with current understanding of NH<sub>3</sub> oxidation and NO reduction chemistry. The combination of the delay in air-fuel mixing and the entrainment of lower O<sub>2</sub>, colder flue gas into the flame results in adjacent zones conducive for NO production from NH<sub>3</sub> oxidation and NO reduction from reaction with dissociated NH<sub>3</sub> and OH radicals.

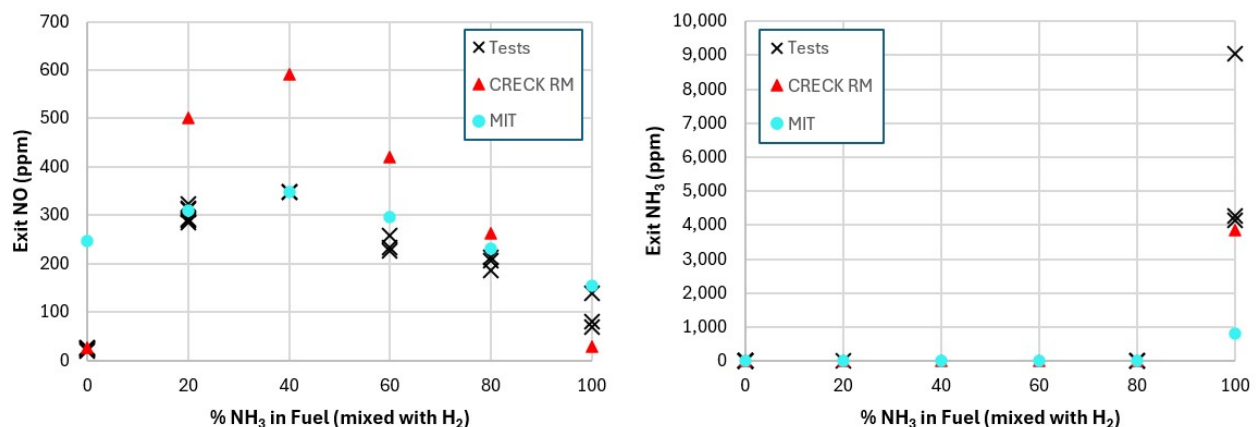


Figure 10: Comparison of Stack NO and NH<sub>3</sub> slip measurements for the Initial GLSF FREE JET NH<sub>3</sub>/H<sub>2</sub> fuel tests vs. CFD predictions using two kinetic models

Figure 10 compares measured and predicted stack emission for NO and ammonia slip. The CFD model that produced the predicted values used two different mechanisms:

1. 50-species reduced chemistry model based on the Stagni *et al.* detailed mechanism
2. Chemistry model developed by MIT for this project (Doner *et al.*)

The measured data in Figure 10 are from tests of the GLSF FREE JET burner firing various mixtures of ammonia and hydrogen in the main tips with 100% hydrogen in the auxiliary tips. The MIT mechanism gives excellent NO results for  $\text{NH}_3\text{-H}_2$  mixtures but overpredicts NO for pure  $\text{H}_2$ . CFD using both mechanisms predicts single-digit or fractional ppm ammonia slip for up to 80% ammonia but varies significantly at pure ammonia firing with the CRECK mechanism performing quantitatively better.

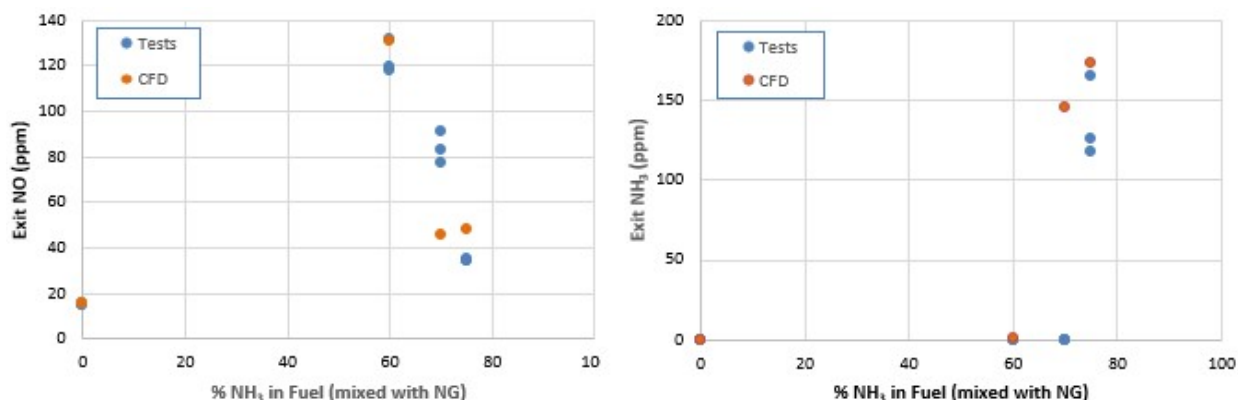


Figure 11 Comparison of Stack NO and  $\text{NH}_3$  slip vs. CFD Predictions using two models for Optimized Natural Draft FREE JET

Figure 11 shows CFD results for the optimized GLSF FREE JET burner. This burner was tested for 100% natural gas and fuel mixtures ranging from 60-75%  $\text{NH}_3$  (single fuel for both auxiliary and main tips). All simulations of these tests were done using the 50-species CRECK reduced mechanism because the MIT mechanism available during this work did not contain hydrocarbon chemistry.

NO is predicted reasonably well for this dataset. Ammonia slip is also predicted well. For the optimized natural draft FREE JET, the CFD model predicted ammonia slip breakthrough at 70% fuel  $\text{NH}_3$ , where the actual measurement showed breakthrough at 75%. The accuracy of the stack NO and  $\text{NH}_3$  concentration predictions is very encouraging, especially considering that experimental uncertainty quantification was not explored and kinetic model development remains a work in progress.

## 6.0 FUTURE WORK

Building on the initial success of the ammonia combustion results presented above, the following future work is planned.

### Burner Development

Design and test a prototype forced draft burner based on the GLSF FREE JET concept with the following characteristics:

- Capable of firing 100% ammonia and a backup fuel consisting of either natural gas or hydrogen
- Single fuel gas supply
- $\text{NO}_x$  emissions of less than 200 ppm (ideally under 100 ppm) and  $\text{NH}_3$  slip of less than 50 ppm (preferably under 10 ppm)

## CFD Tools Development

Future CFD work will continue the implementation of reduced and detailed kinetics. MIT and Stanford research groups will continue contributing expertise in advancing these goals.

## **7.0 CONCLUSIONS**

The initial burner development demonstrated that a natural draft ULNB can successfully combust 70% NH<sub>3</sub> in natural gas and achieve similar NO<sub>x</sub> performance at that ammonia concentration level as conventional raw gas burners firing conventional fuel gases. The work also demonstrated that staged fuel burners significantly outperform conventional burners when firing ammonia.

The combination of sub-models selected to achieve an ammonia combustion CFD capability gives acceptable NO and ammonia slip predictions for industrial applications and was demonstrated over different burner configurations and ammonia fuel blends with both hydrogen and natural gas. Among the chemical mechanisms tested, the reduced CRECK mechanism effectively modeled both ammonia and hydrocarbon combustion, showing reasonable agreement with experimental trends, though this will remain an area requiring further refinement.

Looking ahead, continued burner development closely coupled with advanced CFD modeling is expected to enable safe combustion of ammonia with even lower NO<sub>x</sub> emissions. The development of a forced draft burner will further expand the capabilities.

## **8.0 ACKNOWLEDGEMENTS**

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