Ammonia Combustion: Experiments and Modelling
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ABSTRACT: Ammonia is regarded as one of the most viable alternatives to produce carbon-free energy. However, scarcity of information on the emissions of burning ammonia inhibits its implementation as a fuel. As such, the present work focuses on quantifying the pollutant gas species, namely NO\(_x\), that are emitted from the combustion of ammonia and its mixtures with methane and hydrogen, and understanding how their concentrations are affected by several variables, such as equivalence ratio, constituents of the fuel mixture and amount of ammonia in the fuel mixture. Two different types of burners were used over a wide range of conditions, employing mixtures of ammonia/methane and ammonia/hydrogen under stoichiometry and lean conditions. The results were afterwards compared with recent chemical kinetic models that deal specifically with the combustion of ammonia. The experimental results showed that the NO\(_x\) concentration initially increases as the quantity of ammonia in the fuel mixture rises up to 50%, decreasing afterwards. Furthermore, NO\(_x\) emissions decrease as the equivalence ratio is reduced. Therefore, optimum combustion in terms of low NO\(_x\) emissions occurs for reduced equivalence ratios and high amounts of ammonia in the fuel mixture. The CO results indicate complete combustion of hydrocarbons. However, the presence of unburnt ammonia for high thermal inputs points towards incomplete combustion of ammonia under these conditions. Comparisons with the results from the chemical kinetic models show that the overall emissions patterns are reasonably captured.

Keywords: Ammonia, Combustion, Emissions, NO\(_x\), Experimental, Numerical.

1 INTRODUCTION

The global energy use has been steadily rising and the present demands are expected to increase 28% by 2040 [1]. Combustion processes constitute one of the major sources of the global energy supply. As of 2012, 90% of the energy used in electricity production, thermal energy and transportation results from the combustion of solid, liquid and gaseous fuels, with the overwhelming majority being of fossil origin [2]. However, the impacts of burning fossil fuels are well known: the flue gases that result from the combustion process greatly influence the biosphere and atmosphere in a negative manner [2].

As a proactive measure in decreasing carbon-based pollution, the UNFCCC created the Paris Agreement [3], which has been signed by 195 countries that are committed to limit the increase in global temperature. To achieve this goal, new technologies and resources must be developed and implemented, without resourcing to hydrocarbons.

Ammonia (NH\(_3\)) has been considered one of the most viable candidates for substituting fossil fuels, as it can be combusted in engines, gas turbines and burners, with slight or no modifications to existing ones, while also being compatible with fuel-cells [4]. Additionally, its long-lasting use as a refrigerant and component in the fertilizer industry has resulted in a robust infrastructure for handling, storage and transportation [5]. Therefore, the possible implementation of ammonia has an unmatched economic feasibility, when compared to other carbon-free alternatives [6].

The great potential of using ammonia is the possibility of its combustion resulting only in water and nitrogen. However, current applications also result in nitrogen oxides (NO\(_x\)), harmful pollutants that contribute to acid rain and smog [2]. Therefore, there is a necessity of understanding the mechanisms behind NO\(_x\) release and how it can be suppressed. Furthermore, since the implementation of ammonia should be gradual, fuel mixtures of ammonia and other additives (such as methane and hydrogen) should be thoroughly investigated in term of flammability conditions and emissions. Additionally, given the importance of numerical methods in developing future technologies in a cost-effective manner, experimental data is needed for validation of the simulations.

Several studies have focused on characterizing ammonia combustion in different scenarios. The first documented real-word application was in motor-buses, in 1945, in which a fuel mixture of ammonia and coal gas was used to power this transportation method for more than a year [7]. This successful application spawned some fundamental studies throughout the 1960’s [8], [9], which demonstrated the narrow flammability conditions of ammonia. More recently, researchers have related the difficulty of burning ammonia to the laminar flame velocity: ammonia presents a value of around 7 cm/s, which is rather low when compared with commonly used hydrocarbons, which recorded a maximum of 35 cm/s [10].

Ammonia-doped methane flames were investigated [11], [12], with the aim of understanding fuel-bound NO
emissions. Swirl burners employing pure ammonia [13], and mixtures of ammonia and methane [14] were also studied with the same goal. The results were in accordance amongst these researches, pointing to a peak of NO values in stoichiometric conditions. These values decreased as the equivalence ratio is reduced.

Other work was done to characterize mixtures of ammonia and methane in gas turbines [15], [16], measuring the effect that the quantity of ammonia in the fuel has on emissions. The results showed that, as the quantity of ammonia in the fuel mixture increases, the NO emissions rise until a peak is achieved. Afterwards, the NO values decrease. The same variation of NO with the quantity of ammonia in the fuel occurs for hydrogen-ammonia blends [17].

A number of numerical studies exist on the matter of burning ammonia, either alone or with other fuels. Some of these investigations spawned numerical chemical kinetics mechanisms that offer different descriptions of the species and reactions present in ammonia combustion [18]–[20].

Given that NOx emissions are the major concern inhibiting a wide acceptance of ammonia as fuel, the existing experimental research is not sufficient for thorough understanding of the processes behind their formation, nor for an extensive validation of the numerical mechanisms. Therefore, the principal aim of this work is to contribute with quantitative data on how several variables influence the gas species concentrations at the exhaust, namely NOx, when combusting fuel mixtures of ammonia with other constituents.

To achieve this goal, the experimental part of this investigation resourced to two burners: a flat-flame burner and a porous-media burner. The variables in study were the effect of equivalence ratio, the impact of different fuel constituents and the influence of amount of ammonia in the fuel mixture.

The second objective of this research is to evaluate how current numerical chemical kinetic mechanisms fare against the data gathered. Therefore, the experimental figures were interpreted against numerical simulations of the same conditions, employing relevant models in order to assess the quality of predictions.

The final objective is to understand the impacts of a feasible implementation of ammonia in the energy sector, while recognizing the potential contribution that the present work has in that regard. To do so, the benefits of ammonia completely substituting the fossil-fuels has been discussed.

2 MATERIALS AND METHODS

2.1 Burner Installations

The experimental work featured herein has been conducted at the Combustion Laboratory of IDMEC, at IST. Two distinct burners were employed: a flat flame burner and a porous-media burner. Figure 1 shows the diagram of the flat-flame burner.

![Schematic of the flat-flame burner.](image1)

This installation has been used for other studies [12], although with some differences. The base of the burner is an inverted cone fixed on a mount, with a hollow interior. It is made of stainless steel and it is actively cooled around the perimeter covering the flame position, resourcing to tap water. The interior is filled with small alumina spheres and several transversal stainless steel meshes, in order to achieve uniformity of flow in the cross-section. A hollow quartz cylinder sits on top of the base, allowing for entrainment of the flame and external observation. Along the perimeter of this tube, a ceramic wool has been tightly placed to reduce heat loss. On the top of the quartz tube rests a stainless steel chimney. Methane and ammonia, from gas cylinders, are fed to the intake of the burner, premixed with air from a compressor. All flow rates were measured with flow controllers.

Figure 2 shows the diagram of the porous-media burner.

![Schematic of the porous-media burner.](image2)

It consists of a cylindrical porous media at the core, surrounded by ceramic wool, which is in turn placed in a stainless steel cylindrical container. The ceramic core is characterized by 4 layers of porous foams made of alumina (Al2O3) and zirconia (ZrO2). Each layer has a diameter of 70 mm and a height of 20 mm, resulting in
a total of 80 mm of height. The two bottom layers have 40 pores per inch (ppi) while the top two have 10 ppi. Both regions have a volumetric porosity of 80%. In the bottom of the core, another insulating plate is placed, with a centre channel through which the gases enter premixed. In the top of the burner, a chimney is placed. Ammonia is fed to the intake of the burner, together with air and either methane or hydrogen. Flow rates were measured with flow controllers.

2.2 Measuring Techniques and Uncertainties

Temperatures measurements were taken with thermocouples with a Pt/Pt-13%Rh composition (type R). For the flat-flame installation, the thermocouple was deployed within a probe placed on a vertical slider, which could traverse the centreline of the quartz tube. For the porous-media, eight thermocouples are vertically stacked and positioned through the wall, measuring the temperature along the centreline.

The exhaust gas is collected at the exit of each burner using a stainless steel, water-cooled probe, placed at a fixed position above each burner.

The analysis of the composition of the gases was conducted by resourcing to different equipment. A chemiluminescent analyser was employed for NOx, a non-dispersive infrared gas analyser was used for CO and CO2, and a magnetic pressure analyser was utilized for O2. Finally, GASTEC detector tubes were employed to measure NH3 concentrations.

Table 1 summarizes the estimated average reproducibility uncertainties for the flue-gas data, expressed in percentages of the mean values.

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Average Reproducibility Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>± 4.7%</td>
</tr>
<tr>
<td>NOx</td>
<td>± 4.8%</td>
</tr>
<tr>
<td>CO</td>
<td>± 18.4%</td>
</tr>
<tr>
<td>CO2</td>
<td>± 5.3%</td>
</tr>
<tr>
<td>O2</td>
<td>± 4.1%</td>
</tr>
<tr>
<td>NH3</td>
<td>± 16.4%</td>
</tr>
</tbody>
</table>

Note that the higher values recorded for CO are due to the rather low concentrations. Additionally, the high uncertainty registered for NH3 measurements are related to the GASTEC analysis method, which is rather different from the other methods.

Bearing in mind the instrumental accuracies of the flow controllers used, there are also absolute errors involved with setting specific equivalence ratios or quantities of ammonia in the fuel mixtures.

Table 2 shows the average instrumental uncertainties related to those measurements, for each burner.

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Burner</th>
<th>Average Instrumental Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>% of NH3 in fuel mixture</td>
<td>Flat-flame</td>
<td>± 4.4%</td>
</tr>
<tr>
<td></td>
<td>Porous-media</td>
<td>± 4.3%</td>
</tr>
<tr>
<td>Equivalence ratio</td>
<td>Flat-flame</td>
<td>± 0.05</td>
</tr>
<tr>
<td></td>
<td>Porous-media</td>
<td>± 0.08</td>
</tr>
</tbody>
</table>

These instrumental uncertainties are constant for the respective burners. Therefore, they will not be represented in the graphs of chapter 3.

2.3 Numerical Method

The software employed in this work was Cantera [21], a code library for chemical kinetics calculations.

The programme employed is dependent on the installation geometry, and consists of a one-dimensional, laminar, premixed flame model, held in place by the burner. The script uses the experimental temperatures measured for the burners as input. For the flat flame, there is an extra step of calculating the adiabatic temperatures in the immediate vicinity of the flame, since there is no possibility of conducting experimental measurements in that region. These calculated temperatures are stitched with the experimental data.

Afterwards, the programme calculates the energy and mass transport equations along the vertical axis, yielding the final predictions for the concentrations of the products.

Chemical kinetics mechanisms are needed for the calculation of these energy and mass balances. Each of them includes a specific set of gas species and reactions, and, therefore, have different results and simulation times.

Due to the impracticality of investigating many different mechanisms, literature research and initial testing were conducted to select the most relevant. The three chosen mechanisms were Okafor [18], Dagaut [19] and Tian [20]. However, due to convergence constraints, they were used in two sets: the flat-flame burner results were compared with the Okafor and Dagaut models, while the results for the porous-media were contrasted against the Okafor and Tian models.

3 RESULTS AND DISCUSSION

3.1 Test Conditions

The flat-flame burner was used with ammonia-methane fuel blends premixed with air, with the objective of studying the effect of equivalence ratio on emissions.
Table 3 - Test conditions for the flat-flame burner.

<table>
<thead>
<tr>
<th>Power</th>
<th>Fuel mixture</th>
<th>Equivalence ratio</th>
<th>Ammonia in fuel mixture (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 W</td>
<td>CH₄-NH₃</td>
<td>$\phi = 0.8$</td>
<td>0, 10, 20, 30, 40, 50</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\phi = 0.9$</td>
<td>0, 10, 20, 30, 40, 50, 60</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\phi = 1.0$</td>
<td>0, 10, 20, 30, 40, 50, 60, 70</td>
</tr>
</tbody>
</table>

Table 4 - Test conditions for the porous-media burner.

<table>
<thead>
<tr>
<th>Power</th>
<th>Equivalence ratio</th>
<th>Fuel mixture</th>
<th>Ammonia in fuel mixture (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200 W</td>
<td>$\phi = 0.8$</td>
<td>H₂-NH₃</td>
<td>50, 60, 70, 80</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CH₄-NH₃</td>
<td>30, 50, 70, 80</td>
</tr>
</tbody>
</table>

Additionally, the fraction of ammonia in the fuel mixture was also varied to understand its effect. The thermal power was fixed to 300 W. Table 3 summarizes all test conditions for this installation.

The primary goal of the porous-media burner was to understand the influence that different fuel constituents may have on emissions when paired with ammonia. Therefore, two blends were employed: ammonia-methane and ammonia-hydrogen, both premixed with air. Furthermore, the quantity of ammonia in each blend was progressively changed, to gauge its effect. The power output was fixed to 1200 W, while the equivalence ratio was always 0.8. Table 4 summarizes these test conditions. The numerical simulations follow the same conditions specified for the experimental work.

3.2 Flat-Flame Burner

Photographs of the flames with different percentages of ammonia in the fuel mixture were taken to assess the colour-shift. Figure 3 shows the flames studied for the equivalence ratio of $\phi = 1$, without the insulation around the quartz tube. The pictures were taken at an angle of about 30° from the vertical centreline, with an SLR camera (Canon EOS 700D), with a focal distance of 50 mm, aperture of f/5, shutter speed of 1/20s and ISO of 6400. As the amount of ammonia in the mixture increases, the colour of the flame turns progressively whiter. Although reflections can be observed on the inside of the quartz tube, the flames are flat and above the burner. Note that varying the equivalence ratio does not change the colours significantly.

Temperature measurements were taken along the vertical centreline, at distances to the flame between 2.5 cm and 40 cm. Figure 4, Figure 6 and Figure 8 show the temperature measurements as a function of the axial distance, taken for the equivalence ratios of 0.8, 0.9 and 1, respectively. Each curve represents a different percentage of ammonia in the fuel mixture. The vertical bars represent the reproducibility uncertainties for each experimental point, based on the repetition of the samples.

The patterns show that temperature decreases along the axial distance, which is an expected behaviour due to heat loss.

The increase in ammonia fraction in the fuel mixture leads to an increase of the temperature across the complete profile. This pattern is consistent throughout the equivalence ratios. This is in contrast with the fact that the power input is the same. Furthermore, since the heat release of ammonia combustion per mole is less than that of methane, the temperature should decrease slightly, due to less specific internal energy for the same thermal input.

Additional comparisons between equivalence ratios with the same amount of ammonia in the fuel mixture show that, as the equivalence ratio decreases, the temperatures across the profile increase. This is not in accordance with the fact that peak temperature is commonly achieved around stoichiometry and decreases with the reduction of equivalence ratio.

![Figure 3 - Still photographs of the flames for various proportions of methane/ammonia in the fuel mixtures, for a thermal input of 300 W and $\phi = 1.0$. a) Pure methane, b) 20% of NH₃ in the fuel mixture, c) 40% of NH₃ in the fuel mixture, d) 60% of NH₃ in the fuel mixture, e) 70% of NH₃ in the fuel mixture.](image-url)
Figure 4 - Temperatures for NH₃-CH₄ fuel mixtures at 300 W and $\phi = 0.8$.

Figure 5 - NOₓ emissions for NH₃-CH₄ fuel mixtures at 300 W.

Figure 6 - Temperatures for NH₃-CH₄ fuel mixtures at 300 W and $\phi = 0.9$.

Figure 7 - CO and NH₃ emissions for NH₃-CH₄ fuel mixtures at 300 W.

Figure 8 - Temperatures for NH₃-CH₄ fuel mixtures at 300 W and $\phi = 1$.

Figure 9 - CO₂ emissions for NH₃-CH₄ fuel mixtures at 300 W.

Figure 5 shows the NOₓ emissions as a function of the amount of ammonia in the fuel mixture, for the different equivalence ratios. The presence of NOₓ in the exhaust is significant. The results increase as the percentage of ammonia in the fuel rises up to about 50%. The values peak at that point and start decreasing afterwards. This pattern is similar across the different equivalence ratios. However, the lower the equivalence ratio, the lower the NOₓ emissions are. Therefore, optimum combustion with low NOₓ occurs for low equivalence ratios and high amounts of ammonia in the fuel mixture. These results are in accordance with existing literature [15], [16].

Figure 7 shows the CO and NH₃ results as a function of the percentage of ammonia in the fuel mixture. NH₃ values were measured with the minimum detection limit of 2 ppm. They were sufficient to trigger the detection threshold, although not enough to be quantitatively measured. Therefore, the results are between 2 ppm and 10 ppm, which point towards complete combustion of ammonia. This is true for all equivalence ratios and amounts of ammonia in the fuel mixture.

The average CO concentrations are lower than 60 ppm, and no discernible difference is present between stoichiometry and the fuel-lean conditions. Therefore,
the combustion of the methane present in the fuel mixture is complete, regardless of equivalence ratio.

Figure 9 shows the CO₂ concentrations as a function of the amount of ammonia in the fuel mixture, for different equivalence ratios. The results are concordant with the equivalence ratios employed and the progressive withdrawal of methane.

Additionally, these values justify the contrasting differences found for the temperature results. It has been studied that a decrease in CO₂ concentration may significantly reduce the overall emissivity of the flue gases [22]. Therefore, as the CO₂ emissions decrease with the rise in quantity of ammonia in the fuel mixture, the heat lost through radiation is reduced, thus leading to higher temperatures. Analogous behaviour occurs when reducing the equivalence ratio.

The O₂ emissions were concordant with the equivalence ratios employed.

The NOₓ, NH₃ and CO results were compared with the numerical models Okafor and Dagaut for the same conditions. Figure 10 to 15 show the predictions and experimental data of CO and NOₓ as a function of the amount of NH₃ in the fuel mixture, for the different equivalence ratios. NH₃ predictions are not shown because both mechanisms calculated emissions of less than 1 ppm, thus agreeing with the experimental data in the completeness of ammonia combustion.
Numerical results for CO emissions in the fuel-lean conditions were less than 5 ppm for all conditions, which points to the complete combustion of methane. This agreement with the experimental data was not verified for stoichiometric conditions, where the mechanisms over-predicted the values by two orders of magnitude.

NO\textsubscript{x} numerical results captured the experimental patterns reasonably, except for an outlier with the Dagaut model for \( \phi = 0.8 \). However, the numerical results over-predicted the experimental counterparts by around 100%. The results between both mechanisms were very close for the majority of conditions.

3.3 Porous-Media Burner

Figure 16 and Figure 18 show the temperature profiles along the centreline of the burner, for blends of NH\textsubscript{3}-CH\textsubscript{4} and NH\textsubscript{3}-H\textsubscript{2}, respectively. Each curve represents different amounts of ammonia in the fuel.

The differences observed between fuel constituents relate to flame front position and maximum temperature. The position of the flame front is more upstream in the case of NH\textsubscript{3}-H\textsubscript{2}, which is due to the increased reactivity of hydrogen, when compared to methane. Therefore, the flames that contain hydrogen are much more susceptible to flashback. In regard to the higher maximum temperature registered for NH\textsubscript{3}-H\textsubscript{2}, the CO\textsubscript{2} is once more the culprit. The absence of carbon in these blends lead to less emissivity of the flue gases, thus decreasing the heat lost through radiation.

Figure 17 shows the NO\textsubscript{x} emissions as a function of the quantity of NH\textsubscript{3} in the fuel mixture, where each curve represents different combinations of fuel constituents.

The NO\textsubscript{x} pattern for NH\textsubscript{3}-CH\textsubscript{4} is concordant with the data gathered for the flat-flame burner. The results for NH\textsubscript{3}-H\textsubscript{2} are similar in value, although they increase with the rise of ammonia quantity in the fuel, thus exhibiting a contrasting. However, the values are of the same order of magnitude as in the literature [17].

Figure 19 shows the CO and NH\textsubscript{3} emissions as a function of the quantity of NH\textsubscript{3} in the fuel mixture.

The unburnt NH\textsubscript{3} concentration is significant. For NH\textsubscript{3}-CH\textsubscript{4}, linearity with quantity of ammonia in the fuel is observed. For NH\textsubscript{3}-H\textsubscript{2}, the NH\textsubscript{3} emissions are lower. Comparisons between the NO\textsubscript{x} and NH\textsubscript{3} patterns point towards the occurrence of SNCR of the NO\textsubscript{x}.

The low CO results for NH\textsubscript{3}-CH\textsubscript{4} prove complete combustion of methane. The values for NH\textsubscript{3}-H\textsubscript{2} are below the detection threshold of the analyser, thus constituting background noise. This agrees with the absence of carbon in this fuel mixture.

The O\textsubscript{2} results were concordant with the equivalent ratio employed.

The results for NO\textsubscript{x}, NH\textsubscript{3} and CO were compared with the numerical models Okafor and Tian for the same conditions. Figure 20 to 23 show the predictions and experimental data of CO and NO\textsubscript{x} as a function of the amount of NH\textsubscript{3} in the fuel mixture, for the different combinations of fuel constituents.
NH₃ predictions are not shown because both mechanisms calculated emissions of less than 1 ppm. This does not agree with the significant concentrations found in the experimental data.

The inexistence of CO in the predictions for NH₃-H₂ is in accordance with the lack of carbon in this combustion. Although the CO emissions were over-predicted by an order of magnitude for NH₃-CH₄, they correctly portray the progressive withdrawal of methane.

The NOₓ patterns are captured fairly well, although Okafor proved to be a better fit than Tian. Nevertheless, the numerical results over-predicted the results by more than 300%.

### 3.4 The Path for an Ammonia-Based Economy

The research conducted here leads to believe that there are optimum conditions for combusting mixtures of ammonia with low NOₓ. Thus, the potential of ammonia substituting fossil-fuels in combustion processes is demonstrated. However, development is still needed to fully eliminate pollutants. To understand where research is needed the most, the full potential of ammonia in future energy production processes must be discussed.

Figure 24 represents the possible uses of ammonia in the near-future.

For ammonia to be considered a clean fuel, carbon-pollution must be removed at the very start. Synthesis of NH₃ can occur resourcing to steam reforming coupled with carbon capture and storage (CCS) [23]. On the other hand, it can be produced without hydrocarbons, by employing wet air and renewable energies [24]. The CCS process can be standalone to withdraw CO₂ from the atmosphere or from other industries. The steel industry is an example where ammonia is a known by-product that can be either purified for other uses, or employed in reducing the carbon-footprint [25]. Note that the captured carbon can be used in the production of synthetic hydrocarbons that can be implemented in systems with net-zero emissions or even in a dual-fuel approach with ammonia, where needed.

The long-standing use of ammonia in the fertilizer, refrigerant and chemical industries has allowed for a robust infrastructure that can facilitate its introduction in any sector [4]. Therefore, ammonia can have many uses regarding the production and storage of energy. It can be used as a liquid fuel for light- and heavy-duty transportation [5] or in the production of electricity through gas-turbines [15]. There are already examples of its use in the aerospace industry [26]. Moreover, it can be employed in fuel-cells [27], power cycles [25] and as an energy vector for facilitating storage and transportation [4]. Multiple symbiosis between these use-cases are viable.
The possible widespread use of ammonia as an energy source is a serious contender for meeting the growing global energy demands while promoting the active reduction of carbon-pollution. Experimental results on its emissions – like the ones presented in this work – are of utmost importance to improve numerical tools, so that they are able to correctly predict the properties of ammonia combustion across a range of conditions. This contributes to a gradual development of cost-effective manners to assess the characteristics of future reactors, so that they may be optimal in maximizing efficiency and minimizing emissions. The following decades may give way to a significant change in the management of energy resources, so that ammonia may finally be regarded as an important player in the energy sector, capable of supporting a sustainable and carbon-free society.

4 Closure

4.1 Conclusions

The combustion of mixtures of ammonia with methane and hydrogen has been investigated with the objective of understanding the resultant emissions. The experimental work in two different burners allowed for evaluation on the impacts of equivalence ratio, quantity of ammonia in fuel, and different fuel constituents. Afterwards, the experimental data was compared with relevant numerical chemical kinetics mechanisms.

Temperatures for low power inputs were observed to increase as the amount of ammonia in the fuel rises. The same behaviour occurs when the equivalence ratio is reduced. The cause was found to be the decrease in emissivity of the flue gases, due to reduced concentrations of CO\(_2\), which reduced the heat lost through radiation. Temperatures for high thermal inputs did not exhibit this behaviour.

CO concentrations proved complete combustion of methane, when present, and O\(_2\) results were concordant with the equivalence ratios employed.

NH\(_3\) results for low power inputs point towards the complete combustion of ammonia, although the same cannot be said for higher thermal inputs, where the concentrations are significant and warrant post-combustion treatment.

NO\(_x\) results for NH\(_3\)-CH\(_4\) quickly rise as ammonia is introduced up to 50%, where they peak. The values decrease afterwards. The reduction of equivalence ratio decreases NO\(_x\) emissions. Therefore, combustion of NH\(_3\)-CH\(_4\) blends with low NO\(_x\) in the exhaust may occur for low equivalence ratios and high percentages of ammonia in the fuel mixture. The same is not true for NH\(_3\)-H\(_2\), since NO\(_x\) emissions increase for very high amounts of ammonia in the fuel. Nevertheless, this blend combusts without the presence of carbon.

Overall, although the numerical simulations captured the NO\(_x\) patterns reasonably well, the experimental results were over-predicted by a substantial margin. CO data was modelled well, except for stoichiometry. Simulations of NH\(_3\) emissions were only concordant with the experimental data for low power inputs.

Conclusively, ammonia combustion with other constituents has been proven feasible. Therefore, ammonia presents high potential of substituting fossil fuels, although research is still needed in eliminating nitrogen-based pollutants.

4.2 Future Work

Research should be conducted on burners that offer great potential for low emissions, such as swirl burners.
Emissions suppression should also be developed, especially post-combustion treatment. Scalability of these processes for industrial applications must be taken into account.

Finally, numerical mechanisms still need extensive development. Efforts should be made towards a common model, because present investigations are segregated among many different mechanisms.

5 References


