LOW-NOX AMMONIA COMBUSTION: CHEMICAL REACTOR NETWORK SIMULATIONS VS EXPERIMENTS

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ABSTRACT

Decarbonization policies offer the opportunity to consider energy carriers that previously had not been considered viable. Ammonia (NH_3) is a carbon-free energy carrier with great potential for industry, as well as other sectors such as shipping, but primarily as a molecular-based hydrogen (H_2) carrier. As NH_3 has significant advantages over H_2 in terms of liquefaction, storage and transport, NH_3 seems well-suited for global trade and long-term storage of renewable energy on a large scale. While most strategies aim to separate hydrogen from ammonia at the terminal and then distribute H_2 locally in dedicated grids, another option could be to use ammonia directly as a fuel, for example to produce high temperature process heat. This could make NH_3 particularly interesting for combustion processes at industrial sites without a direct connection to a decarbonized energy infrastructure. In Germany this energy demand today accounts for more than 20 % of Germany's final energy demand, the situation is likely similar in other industrialized countries.

However, the combustion of NH_3 poses its own challenges: NH_3 is far less reactive than natural gas or hydrogen, which significantly affects combustion stability, and nitrogen oxide emissions (NO_X) are likely to be higher than with natural gas or even hydrogen.

This contribution presents the results of chemical kinetics simulations and compares them with ammonia combustion experiments on laboratory scale, carried out at Gas- und Wärme-Institut Essen e.V. (GWI). A first chemical reactor network (CRN) was developed which can be used to predict the formation of nitrogen oxides under different operational conditions and assess the efficacy of various primary measures to reduce nitrogen oxide emissions. As the numerical model is parametrized with geometric data of a real burner system, the results of these simulations need to be compared with the experimental data from a lab-scale burner developed at GWI. The results of these investigations serve to analyze the combustion of ammonia and ammonia / hydrogen in the context of industrial process heating and to design and optimize industrial burners able to use this challenging fuel. The focus lies on combustion stability, flame shape and minimization of NO_X emissions.

1   INTRODUCTION

The need to reduce greenhouse gas emissions as far as possible is one of the key challenges of the 21st century. After the Fuel Emissions Trading Act was passed in December 2019, the German Federal Ministry of Justice and Consumer Protection (2019) laid another cornerstone for achieving climate protection targets with the National Hydrogen Strategy in June 2020. It sees hydrogen as one of the most important energy carriers of the future. However, it is becoming increasingly apparent that parts of the required energy quantities will have to be imported in the future, especially for European manufacturing industries. One way of transporting large quantities of hydrogen will be ammonia. The first agreements for the construction of import terminals for green ammonia have already been concluded and are scheduled to go into operation from 2026 (German Federal Ministry for Economic Affairs and Climate Protections, 2022).

The advantage of ammonia over hydrogen is the lower energy intensity of the phase change from gas to liquid. Under ambient pressures, ammonia liquefies at a higher temperature (approx. -33 °C). This means that strong cooling as with hydrogen (approx. -252 °C) is not necessary. In addition to better store of ammonia, it also has a major advantage over hydrogen in terms of transportability. In liquid form, larger quantities of energy can be stored and transported with the same container volume. Due to the fact that ammonia is used as a primary fertilizer in agriculture, existing transport infrastructures and the necessary regulations and standards could be used. In this context, the question of the direct use of ammonia in industrial combustion plants also arises in order to avoid further energy losses, e.g. through a cracking process, and to be able to offer companies with industrial sites that are not close to H_2 backbones an economical decarbonized fuel supply. However, ammonia differs significantly from natural gas and hydrogen in terms of its combustion properties; the flame stabilization and the resulting pollutant emissions (NO_X, unburned NH_3 and N_2O) from combustion currently are very challenging. In addition to the experimental investigations, numerical analyses using chemical kinetics offer an option to better understand the formation of relevant pollutants, to identify effective pollutant reduction measures and finally to optimize the burner technologies to be used in industrial furnaces.

2 CHALLENGES FOR INDUSTRIAL USAGE OF AMMONIA-BASED FUELS

Today, industrial gas-fired processes are usually operated using natural gas. Compared to this conventional fuel or hydrogen as a promising green fuel, burning ammonia is more difficult due to its combustion characteristics. Compared to hydrogen, ammonia has a significantly lower adiabatic flame temperature, much narrower flammability limits and, in addition, a minimum auto-ignition temperature that is 130 °C higher, as shown in table 1.

Table 1: Comparison of basic combustion characteristics of ammonia, hydrogen and methane
(Kobayashi *et al.*, 2018)

	NH_3	H_2	CH_4
Lower heating value (MJ/m^3)	14.35	10.8	35.89
Flammability limit (Equivalence ratio)	0.63 – 1.4	0.1 – 7.1	0.5 – 1.7
Adiabatic flame temperature in air (°C)	1800	2110	1950
Minimum auto ignition temperature (°C)	650	520	630
Minimum ignition energy (mJ)	14	0.019	0.28

In addition to the previously mentioned fundamental combustion characteristics the laminar combustion velocities and the ignition delay times for ammonia, hydrogen and different NH_3-/H_2-blends are shown in figure 1.
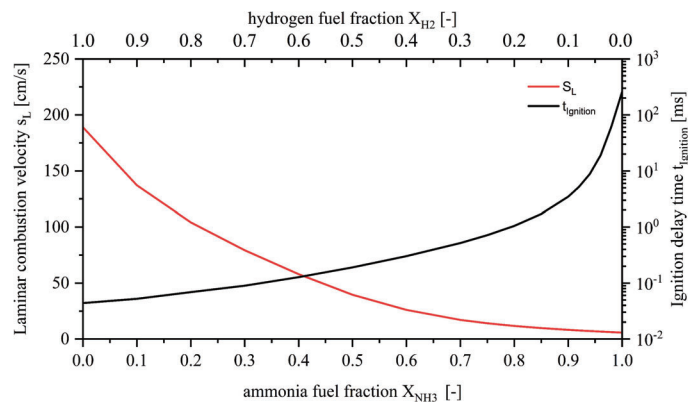

Figure 1: Impact of different hydrogen contents in NH_3-/H_2-blends on the laminar combustion velocities (p = 1 bar, $T_{Initial}$ = 300 K, Φ = 0.91) and the ignition delay time (p = 1 bar, $T_{Initial}$ = 1200 K, Φ = 0.91), calculated with the mechanism of Stagni *et al.* (2020)

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With regard to the stabilization of technically relevant flames, the combination of low laminar combustion velocity and high minimum ignition delay time is a major challenge in relation to ammonia. In comparison to hydrogen, these behave in almost completely opposite ways. For the design of industrial ammonia burner systems, this means not only that an unstable condition or flame lift-off is more likely to occur, but also that combustible mixtures are more difficult to ignite.

The combustion of ammonia presents other unique challenges as well, particularly regarding the production of nitrogen oxides (NO_X). Unlike conventional gaseous fuels, where thermal mechanisms dominate NO_X formation, burning ammonia introduces a significant role for fuel-bound nitrogen in NO_X formation, especially in high-temperature applications (MacLean *et al.*, 2012). This would lead to considerable problems with regard to compliance with the emission limits currently applicable to industrial processes. Additionally, the high water vapor content in the flue gas of hydrogen-rich fuels like ammonia must be considered when quantifying and comparing emissions. Flue gas sample drying during the combustion of hydrogen-rich fuels can distort comparability with emissions from more traditional fuels such as natural gas (Leicher, 2022).

In contrast to gas-fired applications in the residential or power sectors, combustion systems used for industrial processes are typically non-premixed to facilitate air preheating or oxy-fuel combustion (Leicher, 2022; Baukal, 2004). In non-premixed combustion, where fuel and oxidizer are not mixed prior to entering combustion space, the mixing process becomes crucial for industrial burner performance. This approach, prevalent in industrial process heating, offers better combustion stability when compared to premixed flames, as found in gas turbines. This might make it potentially advantageous for challenging fuels.

Ammonia's recent introduction as an industrial process heating fuel raises several unanswered research questions regarding its combustion behaviour and how to address its specific challenges best. Given the growing interest and relevance, further research and understanding are necessary to optimize the use of ammonia in industrial combustion processes.

3   EXPERIMENTAL INVESTIGATION OF FLAME STABILITY THROUGH SWIRLED COMBUSTION

In addition to some first experimental investigation with an industrial burner system the research on ammonia started at Gas- und Wärme-Institut Essen e.V. (GWI) with a lab-scale non-premixed burner developed in-house. As the stability of flames is a main requirement for industrial burner systems, a swirl-stabilized burner was additively manufactured from stainless steel by Kueppers Solutions GmbH, using the SLM process (selective laser melting). Compared to a conventionally manufactured component, 3D-printing enables a lot of degrees of freedom in the construction of new geometries and designs (Bähr, 2020).

The main objective of the conceptual design for the laboratory burner was to stabilize ammonia flames and flames of ammonia blends. Therefore swirl was used, which is a proven method to stabilize flames, especially technical flames with ambient air as oxidizer (Merkle, 2006; Fokaides, 2009; Maier, 1967, Leukel, 1967). When the intensity of the swirl is sufficiently high, a recirculation zone established inside or at the end of the flametube, which is characterized by low local flow velocities. At this position, hot flue gases are conveyed back into the reaction zone and mixed with the fuel and combustion air (Biebl *et al.*, 2024). The intensity of the swirl can be characterized by the dimensionless swirl number S. According to Leukel (1967), it is calculated by the ratio of the angular momentum flux to the product of the axial momentum flux and a reference radius (Biebl *et al.*, 2024). The design of the laboratory burner allows to choose between four different types of swirled or non-swirled inlet flows of the combustion air (S = 0. S = 0.3, S = 0.5, S = 1.1) by using swirl vanes which were set at different angles. In addition to swirl stabilization, the influence of adding hydrogen to stabilize flames was also investigated during the experimental studies (Biebl *et al.*, 2024). As shown in figure 1, the combustion properties of the fuel gas blends are directly and massively influenced by the admixture of hydrogen. With a volumetric proportion of 20 % H_2, the laminar combustion velocity is doubled while the ignition delay time is reduced by more than 99 %.

Figure 2 shows the photographic images of the flames of H_2-/NH_3-fuel gas blends in the range $0 \leq X_{NH3} \leq 1$, where X_{NH3} indicates the volumetric amount of ammonia in the H_2-/NH_3-fuel gas blend.

The equivalence ratio Φ remains constant across all measurement series presented at Φ = 0.95, i.e. a slightly super-stoichiometric combustion which is common for many combustion processes in the thermal processing industries. Along the varying content of NH_3 in the fuel gas blend, the swirl number S was changed. With this setup, the devised burner system successfully achieved pure ammonia combustion. Besides the fuel gas composition, the swirl intensity significantly impacts the flame shape and flame stability.
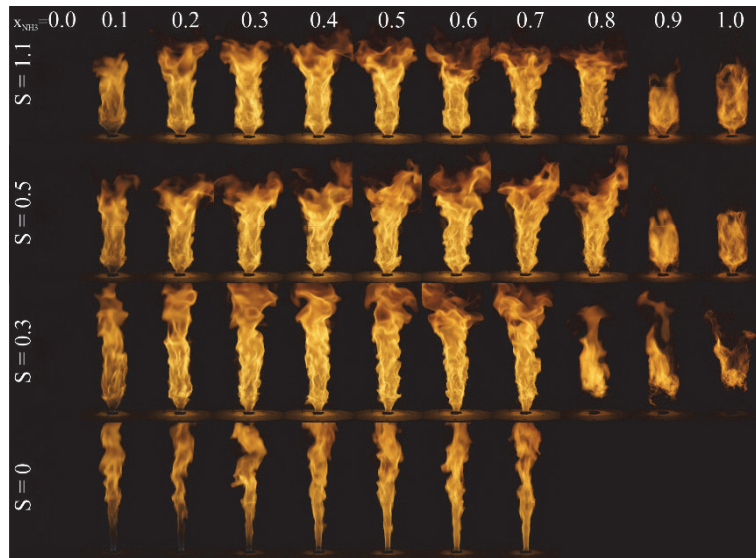

Figure 2: Images of ammonia-hydrogen-air flames for different ammonia contents and different swirl numbers (Q_{th} = 8 kW; Φ = 0.95) (Biebl *et al.*, 2024)

The photographic images show a yellow-glowing flame in all series of experiments presented (S = 0 – 1.1). Starting with a V-shaped flame located at the burner mouth, the flame shows variations in the visible radiation intensity and length with increasing NH_3 content up to X_{NH3} = 0.7. With increasing swirl number from bottom to top, a broadening of the flame front can also be seen, which is clearly torn open at the end by the swirl. For S = 0.5 and S = 1.1 higher ammonia contents above 80 % an abrupt transition in the shape and composition of the flame was observed, when the flame transformed into a compact swirl flame. In contrast, for the moderate swirl number S = 0.3, a lifted flame can be established, even this flame shape is technically rather irrelevant due to its instability. Without swirl (S = 0), a flame can no longer be stabilized, and the reaction extinguishes.

Based on figure 2, swirl can be identified as an effective measure for stabilizing ammonia flames. Up to ammonia contents of X_{NH3} = 0.7 the flame gets chemically stabilized through the reaction-promoting combustion properties such as high laminar combustion velocity, wide flammability limits and low ignition delay time of hydrogen (Biebl *et al.*, 2024).

4   NUMERICAL MODELING OF BURNER SYSTEMS THROUGH REACTOR NETWORKS AND VALIDATION

After the successful experimental demonstration of the stabilization of ammonia and ammonia-hydrogen flames, the next step is to understand the formation of pollutant emissions and approaches of avoiding them.

Even though the combustion of NH_3 is a promising future option for the decarbonization of various industries, the modelling of the fundamental chemistry is still under development. According to Alnasif *et al.* (2023) there are a variety of reaction mechanisms, each of them having been developed for specific conditions and thus delivering meaningful results in the context of the developed application. However, there is still no mechanism that provides completely reliable results for all combustion characteristics

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and the formation of specific species such as NO (Alnasif *et al.* 2023). As part of the model development, different reaction mechanisms were investigated and compared with each other and with experimental measurements. Since the mechanism of Stagni *et al.* (2020) provided the best results under the investigated boundary conditions, only these results are presented below. The mechanism of Stagni *et al.* (2020; Stagni *et al.*, 2023) includes 31 species and 210 reactions and was developed for the oxidation and pyrolysis of ammonia at atmospheric pressure in the temperature range of 500 – 2000 K, which makes it particularly interesting for the description of NH_3 combustion for industrial process heating.

The primary target of the model development was to be able to make predictions about the effectiveness of primary NO_x-reducing measures depending on the respective burner design with the help of a coupled chemical reactor network consisting of several PSR's (Perfectly Stirred Reactor) (Glaborg *et al.*, 1986). Within a Python-based program, the chemical kinetics were solved using the open-source library Cantera (Goodwin *et al.*, 2022). Figure 3 shows the basic functionality of the developed reactor network.
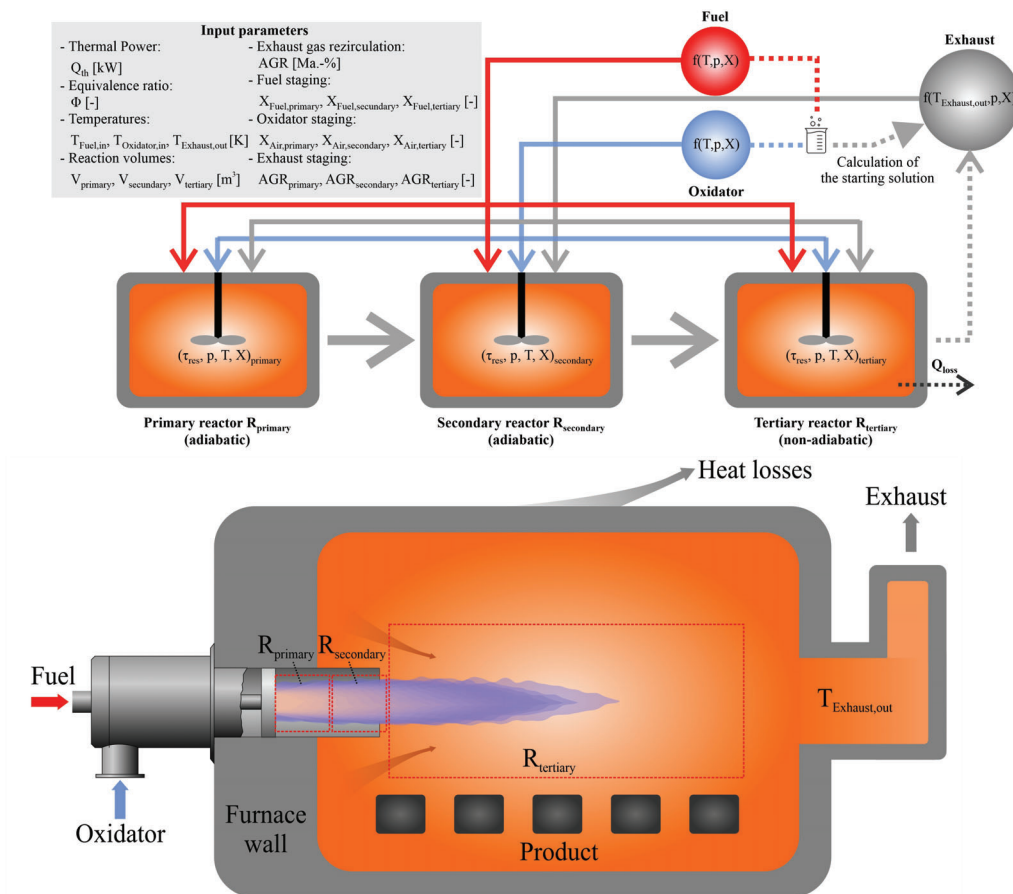

Figure 3: Chemical reactor network for the numerical description of a burner inside a furnace chamber based on the open-source library Cantera (Goodwin *et al.*, 2022) (top) and schematic description of a burner system inside an industrial furnace (bottom)

A chemical reactor network consists of several PSRs. In this case, three of them are used to describe the different reaction zones. The variable input parameters, which are also listed in figure 3 on the top left, are specified at the beginning as the boundary conditions of the simulation. To enable transferability to industrial burner systems in the future, the reaction volumes of the individual reactors are calculated based on the real geometric dimensions of the burner. A schematic description of a burner firing into

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an industrial furnace is shown in figure 3 at the bottom. The thermal energy input of the burner is used to heat up a product. In addition to the heat-absorbing product, some of the energy is wasted through heat losses. The rest of the energy input exits the process again via the exhaust gas and is utilised further in various applications. While the primary reactor ($R_{primary}$) and the secondary reactor ($R_{secondary}$) describe the area close to the burner within the flame tube, the tertiary reactor ($R_{tertiary}$) corresponds to the furnace chamber that is heated by the burner. Since the flame tube is usually positioned in the insulated furnace wall or partially enters the furnace chamber, $R_{primary}$ and $R_{secondary}$ are assumed to be adiabatic. As already mentioned before, the dominant heat losses occur within the furnace chamber and in a real furnace application heat is absorbed by the heated product. Therefore, $R_{tertiary}$ is designed as non-adiabatic and a corresponding loss is taken into account via the specified flue gas outlet temperature $T_{Exhaust,out}$.

There are already a large number of known primary NO_x reduction measures that are also used with conventional fuels. The most common of these for atmospheric burner systems include flue gas recirculation, staging of combustion gas and staging of combustion air (Baukal, 2004). As the staging of the combustion air had the greatest influence on the resulting NO_x-emissions in the numerical and experimental investigations, these results are presented below and compared with the experimental values for validation (see figure 4).

By staging the combustion air at least two combustion zones are created. Due to the sub-stoichiometric conditions ($\phi > 1$) the local oxygen concentration in the primary combustion zone is reduced and so the formation of NO_x is reduced as well. To reach the overall super-stoichiometric conditions, the remaining air is added in the second combustion zone and the incomplete combustion products are fully reacted with low emissions of pollutants. As per Alliat *et al.* (2015) and Fleischmann *et al.* (2005) the effectiveness of air staging is not only determined by the air distribution ratio, but also by the distance between the different zones. In particular, the injection location has a significant influence on the effectiveness of the air staging.

Figure 4 below shows the influence of air staging on the resulting pollutant emissions, measured based on NO-, N_2O- und NH_3-emissions. All measurement points on display as well as the numerical simulations were carried out at a constant thermal power of 8 kW and a global equivalence ratio of $\Phi_{Overall} = 0.85$. The simulated exhaust gas outlet temperature in the tertiary reactor was selected according to the average furnace chamber temperature of the experimental investigations and set to $T_{Exhaust} = 1023$ K. The detailed description of the experimental burner tests, including the measured values obtained, has already been published (Biebl *et al.*, 2024).
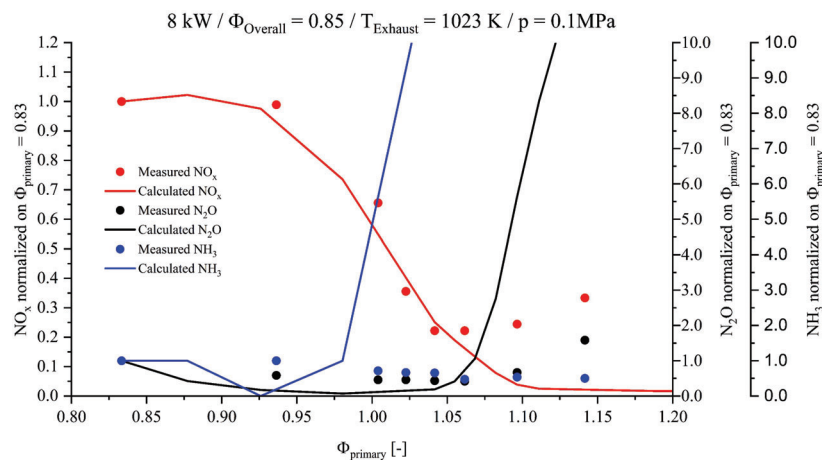

Figure 4: Influence of air staging on the resulting emissions of an ammonia fired lab-scaled burner as a comparison between measured (Biebl *et al.*, 2024) and calculated values with the mechanism of Stagni *et al.* (2020)

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As the calculated emission values were significantly higher than the experimentally determined values, the values were each normalized to the unstaged operating point, which is when $\Phi_{Primary} = \Phi_{Overall}$. It should be mentioned that the overall equivalence ratio remains constant across all operating points considered, both for the measurements and for the simulations.

The equivalence ratio of the primary stage is shown on the x-axis. According to the experimental investigation the stabilization of a flame was possible up to a primary equivalence ratio of $\Phi_{Primary} = 1.14$. If the primary air volume was reduced further, the ammonia flame became unstable and the flame was extinguished. From $\Phi_{Primary} = 0.93$, the NO_x emissions drop significantly to a local minimum in the range between $1.04 \leq \Phi_{Primary} \leq 1.06$. There, a NO_x reduction of approx. 80 % is achieved. A renewed increase in NO_x emissions was observed beyond the range ($1.06 \leq \Phi_{Primary}$). In the simulation, the NO_x values are running towards zero, which is strongly related to formation of other species.

In particular, N_2O proved to be a good indicator of flame extinction in both the experimental and numerical investigations. By reducing the oxygen supply in the primary combustion zone to $\Phi_{Primary} = 1.06$, N_2O falls steadily. As soon as the primary combustion air is reduced further, a significant increase in N_2O can be observed. The calculated values are by orders of magnitude larger than the measured values. During all of the measurements, there was no NH_3 slip until the flame was extinguished (Biebl *et al.*, 2024). In the chemical kinetics investigations, however, an exponential increase in the NH_3 emissions contained in the exhaust gas can already be seen from $\Phi_{Primary} = 0.98$. Qualitatively, the NH_3 curve thus runs parallel to the N_2O curve.

With the help of the developed chemical kinetics model, the trends of the measured pollutant emissions could be reproduced very well and the numerical model for this burner could be validated. In particular, the very good agreement with regard to the NO_x curves, which are the primary focus of the investigation, confirms the implementation of an extensive parameter study in order to also vary other parameters, such as the recirculation of exhaust gases, and to identify their influence on the nitrogen oxides. The extended results of the parameter study on the influence of air staging on nitrogen oxide emissions are presented below and the reduced formation is explained.

5   PARAMETER STUDY ON AIR STAGING AND OPTIMIZED OPERATING POINT

The requirements for industrial burner systems are manifold and depend on many factors, such as the area of application, temperature level and also the geometry of the furnace chamber. The search for the optimum operating point is therefore highly specific and dependent on the burner. In the laboratory burner used here, the focus was on the stabilization of a flame in combination with the lowest possible nitrogen oxide emissions, with simultaneously low N_2O emissions and as little ammonia slip as possible. For the sake of clarity, these explanations will focus on the species NO and NO_2 (summed up to NO_x) as well as N_2O.

The thermal power ($Q_{th} = 8$ kW), the equivalence ratio ($\Phi_{Overall} = 0.85$), the pressure ($p = 0.1$ MPa) and the exhaust gas outlet temperature at the tertiary reactor ($T_{Exhaust} = 1023$ K) were kept constant for the entire parameter study. Only the volumetric air fractions of the primary ($X_{Air,primary}$), secondary ($X_{Air,secondary}$) and tertiary ($X_{Air,tertiary}$) reactors were varied. The relationship between the air fractions is described by equation (1):

$$X_{Air,primary} + X_{Air,secondary} + X_{Air,tertiary} = 1 \qquad (1)$$

Figure 5 below shows a ternary diagram which illustrates the relationship between the three air fractions described by equation (1) for the resulting emissions of a particular species at the outlet of the tertiary reactor.
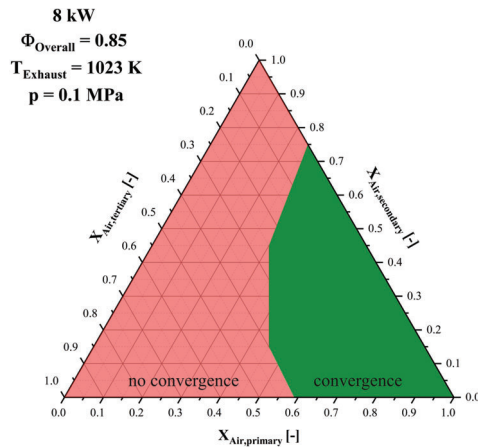
Figure 5: Calculated influence of different levels of air staging on the stability of ammonia combustion using mechanism of Stagni *et al.* (2020)

Two basic areas can be recognized in the figure. The first area (red) represents the range within which the numerical model no longer converges. In the context of the burner operation, this can be assumed to indicate that a stable flame can no longer be established. Accordingly, the green area indicates converged simulations, where the resulting concentrations can be interpreted.

For a dual-stage system, as also investigated in the experimental studies, the minimum primary air fraction at which the model still converges is approx. $X_{Air,primary} = 0.6$. In terms of the equivalence ratio, this corresponds to $\Phi_{Primary} = 1.39$, which, according to Kobayashi *et al.* (2018), is consistent with the literature values for the ignition limits in the range $0.63 \leq \Phi \leq 1.4$. By adding a third air stage, this range can be extended to $X_{Air,primary} = 0.3$. However, whether this condition is relevant for technical applications must be validated by means of experimental investigations. Therefore, for the following considerations, the showed air ratios are reduced following $0.6 \leq X_{Air,primary} \leq 1.0$.
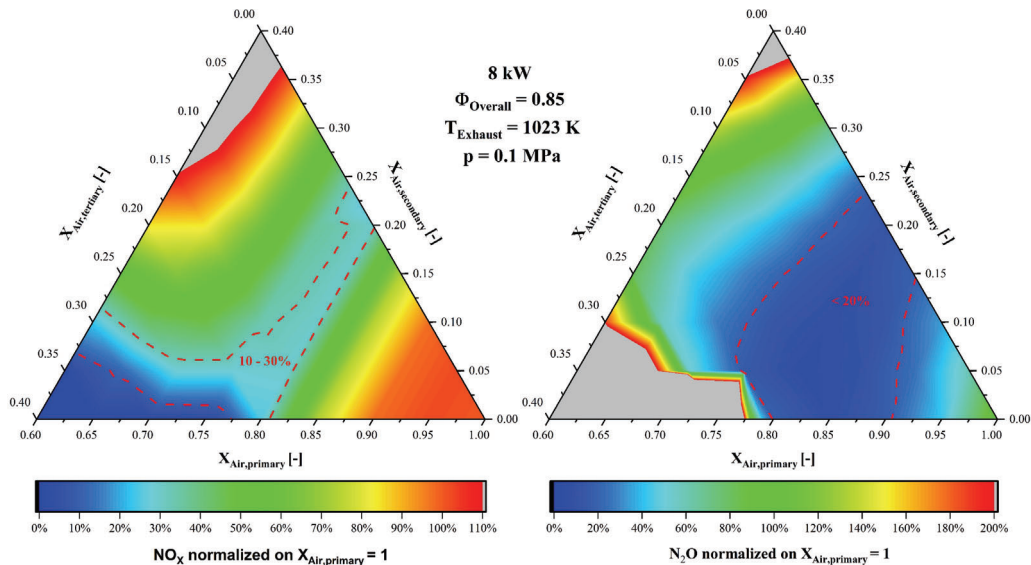

Figure 6: Calculated influence of air staging on NO_x (left) and N_2O emissions (right) in the exhaust of ammonia combustion using mechanism of Stagni *et al.* (2020)

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The emission values shown in figure 6 are normalised to the value for $X_{Air,primary} = 1$. While the emission map for NO_X is shown on the left, the map for N_2O is shown on the right. Values above the maximum limit are shown in light grey and values equal zero in black. In addition, red lines in both graphs indicate areas where emissions are within an acceptable range. With dual staging, taking into account $X_{Air,secondary} = 0$, the primary air fraction should be below $X_{Air,primary} = 0.81$ in order to achieve a significant NO_X reduction. At the same time, there is a range of minimal N_2O values for $0.8 \leq X_{Air,primary} \leq 0.91$. Although the third air stage in the secondary reactor tends to lead to higher NO_X values, it also leads to lower N_2O values.

The local NO_X minimum considered in figure 4 can be found here at the point $X_{Air,primary} = 0.8 / X_{Air,tertiary} = 0.2$ and can be regarded as a "sweet spot" from various points of view. On the one hand, both the emission requirements and the requirements for the stability of the flame, which has been proven experimentally (figure 4) (Biebl *et al.*, 2024), are met. Secondly, a two-stage system is much easier to transfer to an industrial burner system than a three-stage system. For certain applications, however, it can also make sense to provide a three-stage air staging system. This means that more fuel is converted in the area close to the burner, which ultimately widens the stability range of the reaction and thus of the flame. This needs further validation by experimental investigations.

Parallel to the simulations with the developed CRN, reaction path analyses were carried out with ammonia and for different stoichiometries in order to better understand the inhibited formation of NO as a result of staged combustion.

Figure 7 shows qualitative reaction path analyses for sub-stoichiometric (top) and super-stoichiometric ammonia combustion (bottom). The element flow charts were created based on the kinetics software Cosilab (Cosilab Collection, 2021) and then analyzed mathematically and graphically.
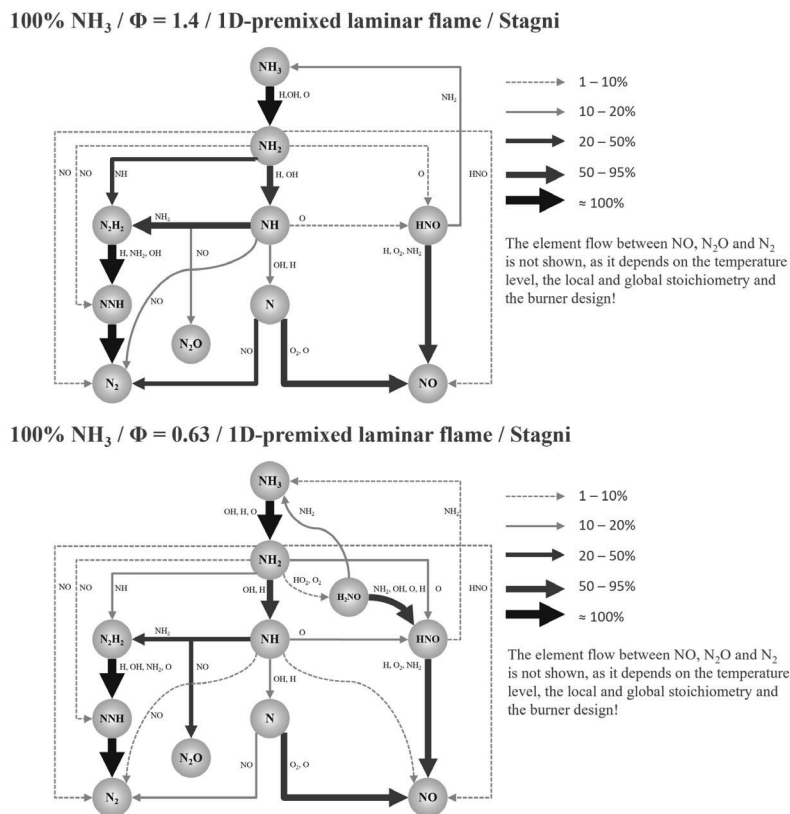

Figure 7: Element flux analysis of ammonia combustion with an equivalence ratio of $\Phi = 1.4$ (top) and $\Phi = 0.63$ (bottom) modeled as 1D-premixed laminar flame, using the mechanism of Stagni *et al.* (2020) with the software Cosilab (Cosilab Collection, 2021) and showing the element flow just in one direction.

The species NH_2, NH, NNH und N_2H_2 are primarily responsible for the reduced formation of NO through air staging. Mashruk *et al.* (2020) already identified NH_2 as a key species for reducing NO within the flame. Within the primary reactor, increased concentrations of NO and NH_2 are initially produced due to the lack of oxygen. These are converted via the reaction equations $NH_2 + NO \leftrightarrow NNH + OH$ and $NH_2 + NO \leftrightarrow H_2O + N_2$ (Mashruk *et al.*,2020), whereby the resulting NNH reacts further via the equation $NNH \leftrightarrow N_2 + H$ to form molecular nitrogen. Another relevant intermediate for the formation of N_2 is N_2H_2, which is formed via the reaction of NH_2 with NH to produce a free H-atom ($NH_2 + NH \leftrightarrow N_2H_2 + H$). A negligible proportion of the N_2H_2 is recombined to form NH_3. However, over 95 % of N_2H_2 reacts with H and OH to form NNH and then back to N_2. As a result of a chain reaction, the increased formation of NH_2 also produces more NH, which is degraded with NO to N_2O. According to Mashruk *et al.* (2020), the reaction equation $NH + NO \leftrightarrow N_2O + H$ shows a direct correlation between the avoidance of NO_x and the formation of N_2O, which is reflected in both the experimental and numerical investigations. With sufficient reactivity and the presence of H, the resulting N_2O reacts in the tertiary reaction zone via the endothermic reaction equation $N_2O + H \leftrightarrow N_2 + OH$ to form N_2.

Applied to the observations made during the experimental investigations, this means that if there is too little oxygen in the primary combustion zone, there is no longer sufficient reactivity or radicals to allow N_2O to react to N_2. The result is the extinguishing of the flame.

6   CONCLUSION

In addition to the experimental investigation of the flame stability of NH_3-/H_2-flames, the influence of air-staging on the resulting NO_x and N_2O emissions was also analyzed. In addition to that, a CRN model was developed and validated with the experimentally determined values to reliably identify optimized operating points. Within the considered model, real burner geometries can also be considered by input parameters so that they can be transferred to other burner geometries. The most important results are briefly described below:

-    Stable flames of pure ammonia could be established at swirl numbers between S = 0.5 to S = 1.1 with equivalence ratios of $0.83 \leq \Phi \leq 1$.
-    With the help of chemical reactor networks, it is possible to mathematically describe real burner systems and thus obtain burner-specific, reliable tendencies for resulting pollutant emissions and, in addition, trends in the stability behavior of ammonia flames based on defined criteria.
-    Staging the combustion air was identified as a very effective method of reducing NO_x emissions from NH_3 flames. A numerically determined and experimentally confirmed optimum operating point of dual-stage air staging is available for $X_{Air,primary} = 0.8$ and $X_{Air,tertiary} = 0.2$ at which NO_x emissions were reduced by approx. 80% with simultaneously low N_2O emissions.
-    The formation of higher concentrations of NH_2 in the primary reactor is one of the main reasons for the low NO_x emissions of staged combustion. A reburn to NNH is achieved via the reaction with NO, which in turn reacts to form N_2.
-    There is a direct connection between NO and N_2O via the reaction $NH + NO \leftrightarrow N_2O + H$. Due to a reduced concentration of radicals within the secondary and tertiary reactor, only a lower reaction of N_2O to N_2 takes place, so that the N_2O emissions can be a reliable indicator for evaluating the reaction stability.

It was proven that it is possible to stabilize burner flames with ammonia, despite its difficult combustion properties. Although the resulting pollutant emissions require modifications in the design of the burners, known primary measures appear to be an effective reduction method. Grading the combustion air seems to be the most effective method so far and also offers the advantage that it is technically comparatively easy to implement. Further primary measures to reduce emissions and further stabilization measures will be investigated in the future using a similar approach based on simulations and experiments. Therefore, CRNs offer valuable support for burner development, by providing reliable, qualitative insights with moderate effort. By coupling the geometric data of the burner system, the functionality can also be transferred to other systems. In combination with the subsequent reaction path analysis,

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relevant formation paths can be identified, and the modeling of ammonia combustion can be further improved in the future.

NOMENCLATURE

Roman symbols

AGR	Exhaust recirculation rate	(Ma.-%)
P	Pressure	(Pa)
Q	Thermal Power	(kW)
T	Temperature	(K)
V	Reaction volume	(m^3)
X_i	Volume fraction	(-)
X	Composition of the gas	(Vol.-%)

Greek symbols

τ	Residence time	(s)
Φ	Equivalence ratio	(-)

Subscripts

res	Residence
th	Thermal

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