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Assessing the potential of a chemiluminescence and machine learning-based method for the sensing of premixed ammonia-hydrogen-air turbulent flames

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Abstract

The potential of chemiluminescence to develop non-intrusive sensors for the monitoring and control of turbulent ammonia-hydrogen flames is here investigated experimentally. This study looks into the impact of equivalence ratio ($0.35 \leq \phi \leq 1.70$), NH_3 fuel fraction ($0.55 \leq X_{\text{NH}_3} \leq 0.90$) and Reynolds number ($4000 \leq \text{Re} \leq 7000$) on UV, visible and infrared chemiluminescence signatures and NO_x emission of NH_3/H_2 turbulent flames within an atmospheric tangential swirl burner. Chemiluminescence spectroscopy is employed to provide detailed information about the excited species (e.g., NO^* , OH^* , NH^* , NH_2^* , and NO_2^*) in both *in-flame* and *post-flame* zones. Findings are compared to previous measurements in laminar flames and similar trends are observed. Many chemiluminescence intensity ratios are investigated but none are found to be potential surrogates of equivalence ratio and NH_3 fuel fraction across all the conditions considered. Therefore, a more advanced method based on machine learning is used to infer equivalence ratio and NH_3 fuel fraction from the chemiluminescence intensities of more than just two excited radicals at once. This method referred to as Gaussian Process Regression (GPR) is found to provide predictions of equivalence ratio and NH_3 fuel fraction with an accuracy better than 0.1 and 0.02, respectively, across the whole range of conditions. GPR is also able to predict the measured NO , N_2O and NO_2 emissions using only measured chemiluminescence intensities, confirming the potential of chemiluminescence sensors coupled with a machine learning-based method for the monitoring and control of practical NH_3/H_2 flames.

Keywords: Carbon-free; Spontaneous Emission; Swirl Flame; NO_x ; Gaussian Process Regression.

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1. Introduction

Ammonia (NH_3) has emerged as a promising alternative fuel due to its relatively high energy density, low carbon footprint, and high efficiency in storage and transportation [1–4]. However, NH_3 is a weakly reactive fuel [5]. Adding hydrogen (H_2) can significantly enhance reactivity while maintaining the carbon-free nature of the fuel mixture [6, 7]. Combustion diagnostics have also been employed to monitor combustion characteristics [8–10], such as combustion instabilities [11] and heat release rate [12, 13]. Chemiluminescence-based diagnostics techniques have been widely used for combustion measurements in laboratory and industrial applications [14], providing a non-invasive and sensitive method for measuring combustion characteristics, due to its cost-efficient and simple set-up. The close relationship between combustion characteristics and chemiluminescence allows to better understand the combustion process to optimize reactive systems for efficiency and emissions reduction. Zhu et al. [15] measured the chemiluminescence spectra of laminar premixed NH_3/CH_4 flames for various equivalence ratios ($0.60 \leq \phi \leq 1.30$), NH_3 fuel fractions and strain rates ($55/\text{s} \leq \alpha \leq 300/\text{s}$). They identified the relevant excited radicals, including NO^* , OH^* , NH^* , CN^* , CH^* and CO_2^* , and examined the relationship between chemiluminescence intensity ratios and the flames' inlet conditions. Mashruk et al. [16] explored the chemiluminescence of more practical, turbulent premixed NH_3/CH_4 flames for wide ranges of equivalence ratio, NH_3 fraction in the fuel blend ($0 \leq X_{\text{NH}_3} \leq 0.70$) and Reynolds number ($10,000 \leq \text{Re} \leq 40,000$). They found that conclusions drawn by Zhu et al. [15] for laminar flames also applied to turbulent swirl flames.

The main differences in chemiluminescence between laminar and turbulent flames can be attributed to variations in flame structure [17], the influence of stretch and strain [18], and the characteristics of mixing dynamics [19]. Laminar flames are characterised by the presence of smooth, well-defined reaction zones with minimal mixing between reactants and products [20]. This results in the generation of chemiluminescence signals that are stable and spatially concentrated. These signals are strongly correlated with global flame parameters, such as equivalence ratio and heat release rate, which facilitates their interpretation. In contrast, turbulent flames are distinguished by irregular and dynamic flame fronts, which are shaped by turbulence-induced wrinkling [21]. The interaction between turbulence and flame structure gives rise to considerable effects on flame stretch and strain, which in turn affect radical formation and quenching processes [22], thereby reducing chemiluminescence intensities in regions of high strain or local extinction [23]. The enhanced mixing that occurs in turbulent flames introduces further variations in temperature, equivalence ratio and radical concentrations [24], thereby broadening the spatial and spectral distribution of chemiluminescence, while enhancing NO formation in lean regions and suppress it in fuel-rich zones, further complicating the relationship between chemiluminescence and NO_x emissions. While laminar flame chemiluminescence reflects steady-state conditions [20], allowing predictable kinetics, turbulent flames exhibit unsteady and fluctuating signals. As a result, advanced diagnostic techniques, such as machine learning approaches, are required to extract meaningful insights.

The application of machine learning (ML) in combustion research has gained significant momentum in recent years, revolutionizing the way complex combustion phenomena are analyzed and controlled [25, 26]. Machine learning techniques, with their ability to process and learn from large datasets, offer unprecedented capabilities in measuring, modeling, predicting, and optimizing combustion processes. Due to the application of ML techniques to enhance the accuracy and speed of data interpretation, the diagnostics of combustion can be significantly improved as found for example by Chen et al. [27] and Wan et al. [28]. In wildfire management, ML models predict fire behavior and assess risk by analyzing historical data, weather patterns, and vegetation indices, aiding in prevention and mitigation efforts [29]. Additionally, ML-driven computational simulations and kinetic modeling offer more accurate and efficient models for predicting combustion processes and reduce the computational cost [30]. Recently, Guiberti et al. [31] used data recorded by Zhu et al. [15] to train a machine learning-based regression algorithm (Gaussian Process Regression, GPR) and showed that the equivalence ratio and the NH_3 fuel fraction could be recovered accurately using only OH^* , NH^* , CN^* and CH^* intensities as inputs. The GPR algorithm still performed well when applied to turbulent swirl NH_3/CH_4 flames. However, there are no equivalent studies to that of Mashruk et al. [16] and Guiberti et al. [31] for carbon-free, NH_3/H_2 turbulent swirling flames.

Pugh et al. [32] examined the chemiluminescence of partially premixed NH_3 and 70% NH_3 /30% H_2 flames as a function of the inlet gas temperature to identify the flame configuration with the lowest combined emissions concentration. In a follow-up to their original study, Zhu et al. [33] explored the chemiluminescence of laminar premixed NH_3/H_2 flames and identified ratios OH^*/NO^* and $\text{OH}^*/\text{Violet}$ as potential surrogate of equivalence ratio. Lately, the experimental data obtained by Zhu et al. [33] were used by Konnov [34] to build a new model focusing on $\text{H}/\text{N}/\text{O}$ sub-mechanisms, in particular in the formation and consumption of excited NO_2^* , $\text{NO}(\text{A})$, NH^* , and NH_2^* . The detailed experimental data derived by chemiluminescence intensity were crucial for the validation of the mechanism for this type of flame. However, their investigation was limited to laminar flames, and the effects of turbulence couldn't be studied. Considering that most industrial combustion devices operate in turbulent regions and the effects of strain effect, curvature, local extinction and turbulence/flame interaction and so forth, may significantly influence the combustion characteristics and the chemiluminescence of the flame, investigation of the chemiluminescence signature of turbulent NH_3/H_2 flames is desired to develop chemiluminescence-based sensors.

The current study builds upon these previous investigations by examining the influence of equivalence ratio, NH_3 fuel fraction, and Reynolds number on the chemiluminescence signature and NO_x emission of turbulent premixed NH_3/H_2 flames using UV-visible-IR chemiluminescence spectroscopy. Specifically, this study aims to uncover the potential of chemiluminescence as a tool for the monitoring and control of NH_3/H_2 turbulent flames. As such, the main objective is to identify how the flames' chemiluminescence signature alone can be recorded and post processed to infer critical properties such as equivalence ratio, fuel composition and harmful NO_x emission. To achieve this, the machine learning-based method, specifically Gaussian Process Regression (GPR), will be employed. This approach leverages chemiluminescence data derived from the experimental database to demonstrate the feasibility of accurately predicting equivalence ratio, fuel composition, and NO_x emissions, paving the way for non-intrusive diagnostic tools for NH_3/H_2 turbulent flames.

2. Experimental setup

2.1. Burner configuration

Figure 1 shows a schematic of the atmospheric industrial scale tangential swirl burner used in this study. Flow rates are prescribed using Bronkhorst flow controllers (accuracy better than $\pm 0.5\%$ within 15–95% of the full scale). Ammonia and air were injected at the base of the mixing chamber, while hydrogen was injected through 6 equispaced holes, located 40 mm below the burner exit, angled at 45° . Before entering the combustion chamber, fuels and air pass through a radial-tangential swirler, which is equipped with a 31.5 mm outer diameter nozzle. To promote flame stabilization, the burner is also equipped with a central bluff-body of 22.5 mm diameter. In the current study, the burner features a swirl number of $S_g = 1.05$. The swirl number is defined as follows:

$$S_g = \frac{A_{\text{noz}} r_{\text{tan}}}{A_{\text{tan}} r_{\text{noz}}} \left(\frac{Q_{\text{tan}}}{Q_{\text{tot}}} \right)^2 \quad (1)$$

where A_{noz} is the exit area of the burner exit nozzle, A_{tan} is the area of the tangential inlet, r_{tan} is the effective radius of the tangential inlet, r_{noz} is the radius of the burner exit nozzle, Q_{tan} is the tangential flow rate, and Q_{tot} is the total flow rate. The combustion chamber is made of a transparent cylindrical GE214 quartz tube of 156 mm diameter. A permanent CH_4 pilot flame is used for ignition and avoids total extinctions during blow-off events. The pilot flame was positioned out of the focal areas of both the spectrometers employed in this study. Background spectra were taken with the pilot flame on and subtracted from each experimental points. Removing background emission enables the isolation of chemiluminescence signals of single excited radicals, as further described later. This practice is a standard procedure in pre-processing chemiluminescence measurements, aimed at excluding interference from background emission. Additionally, this process facilitates the creation of a comprehensive and high-quality database, useful to validate numerical simulations.

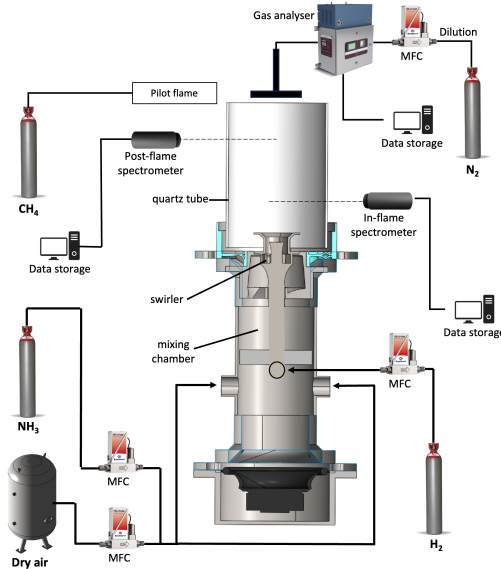


Fig. 1: Schematic of the experimental setup.

2.2. Operating conditions

In this work, different volume fractions of NH_3 in the NH_3/H_2 fuel blend ($0.55 \leq X_{\text{NH}_3} \leq 0.90$), different equivalence ratios ($0.35 \leq \phi \leq 1.70$) and bulk Reynolds numbers ($4000 \leq \text{Re} \leq 7000$) are analysed, corresponding to a total of 252 tested operating conditions. The lean blowout (LBO) and rich blowout (RBO) set the limits for equivalence ratios and NH_3 fuel fractions accessible for each Reynolds number [35, 36]. Fuels and air are injected at constant temperature and pressure, $T_{\text{in}} = 288 \text{ K} (\pm 3 \text{ K})$ and $0.1 \text{ MPa} (\pm 1 \times 10^{-3} \text{ MPa})$, respectively.

2.3. Chemiluminescence measurements

Two compact bench spectrometers are used simultaneously to record chemiluminescence in the in-flame zone (Avantes AvaSpec-ULS4096CL-RS-EVO) and the post-flame zone (StellarNet Inc BLUE-Wave), positioned at $\sim 0.03 \text{ m}$ and $\sim 0.12 \text{ m}$ height from the burner exit, respectively. These specific locations were chosen to capture distinct spectral processes: the in-flame zone measures chemiluminescence from radicals actively involved in combustion reactions, while the post-flame zone captures emissions from reaction products and intermediates that persist downstream. The spectrometer used for the in-flame zone features a high spectral resolution of 0.3 nm and sensitivity from 200 nm to 1100 nm to ensure precise detection of narrow spectral signals and excited radicals. The post-flame zone spectrometer, with a resolution of 0.5 nm and sensitivity

from 200 nm to 1150 nm, balances resolution with coverage, accommodating broadband emissions typical of exhaust gases. Both spectrometers are installed at a distance of ~ 0.15 m from the quartz cylinder to minimize heat exposure and optical distortion caused by high-temperature gradients near the burner while maintaining an adequate signal-to-noise ratio (SNR). The exposure time is set to 1 s, and 20 scans are averaged to enhance statistical convergence and improve the SNR, which is critical for resolving weak chemiluminescence signals. The Y-axis calibration using a standard light source (SL1 Tungsten Halogen) ensures quantitative accuracy and consistency across measurements. Contributions from different species or specific spectral ranges are quantified by integrating the chemiluminescence spectra over defined wavelength ranges, as discussed in subsequent sections.

2.4. Emissions measurements

Important species in the wet exhaust gases, such as NO, N₂O, NO₂, NH₃, H₂O, and O₂, are measured using an Emerson CT5100 quantum cascade laser analyzer, as in [24, 37]. The analyzer's sampling temperature of 463 K and a frequency of 1 Hz ensure accurate detection in high-moisture environments typical of combustion exhaust. The device's high linearity (0.999) and repeatability ($\pm 1\%$) are crucial for reliable quantification of trace species. Where necessary, dilution with N₂ [37] is employed to ensure that species concentrations remain within the detection range, thus avoiding saturation of the detector. Data are recorded over a 120 s period to capture transient fluctuations in emissions and time-averaged to provide a representative measure of steady-state combustion conditions. For this study, the analysis focuses on NO, NO₂, and N₂O emissions, which are critical indicators of combustion efficiency and environmental impact.

3. Machine Learning Regression Methodology

This work implements a Gaussian Process Regression (GPR) algorithm to predict key combustion parameters, including equivalence ratio, ammonia fuel fraction, and emissions of NO, NO₂, and N₂O, in NH₃/H₂ swirl flames. A step-by-step simplified schematic of the GPR methodology is shown in Fig. 2. The process begins by defining a prior distribution over functions, characterized by a mean function and a kernel (covariance function) that encodes assumptions about smoothness or other function properties. Observed data, consisting of input-output pairs, is then incorporated to update the prior using Bayes' theorem, producing a posterior distribution. The posterior provides predictions for new inputs, represented by a mean and variance (uncertainty estimation).

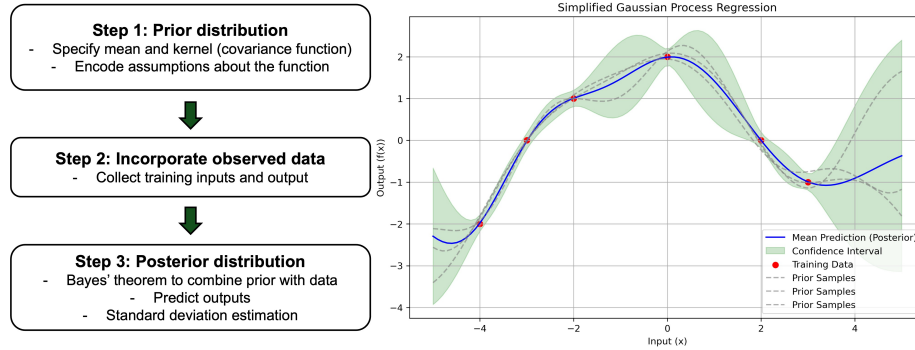


Fig. 2: Simplified schematic of Gaussian Process Regression (GPR): training data (red symbols); posterior mean (blue line); confidence interval (shaded region) equal to 95%; prior samples (gray dashed lines).

GPR was selected due to its strengths in modelling non-linear relationships and its probabilistic framework, which provides not only predictions but also an associated uncertainty measure; this implies that the true value is typically distributed around the predicted mean value. Consequently, it offers an estimate of the corresponding standard deviation, aiding in the assessment of the reliability of the model outputs. This characteristic is especially relevant in combustion studies where experimental variability can be significant. In addition, its non-parametric nature allowed flexibility without requiring explicit functional forms, and the ability to incorporate prior knowledge through kernel functions enhanced its adaptability to the dataset. In this study, GPR demonstrated superior performance compared to alternative regression approaches, such as ordinary least squares regression, lasso linear regression, and support vector regression. While these alternatives often require extensive data and parameter tuning, GPR proved more robust and effective for the given application. As a result, it emerged as the most suitable choice for achieving the research objectives. The methodology builds on prior work by Guiberti et al. [31], who successfully applied GPR to NH₃/CH₄ laminar flames to predict equivalence ratio and NH₃ fuel fraction using chemiluminescence data (OH*, NH*, CN*, CH* intensities). Here, the same approach is adapted for turbulent NH₃/H₂ swirl flames, extending its application to predict NO, NO₂, and N₂O emissions as well. This represents a novel contribution, as emissions prediction was not addressed in [31]. To implement the GPR algorithm, the scikit-learn library in Python is used [38]. The kernel function, k , which defines the covariance between data points, is constructed as a combination of a rational quadratic kernel (k_{rq}) and a white noise kernel (k_{w}). This design introduces three hyperparameters: the length scale (l), scale mixture (α), and noise level (n). The rational quadratic kernel k_{rq} is defined as:

$$k_{\text{rq}}(x_i, x_j) = \left(1 + \frac{d(x_i, x_j)^2}{2\alpha l^2} \right)^{-\alpha} \quad (2)$$

Table 1: Hyperparameters used for the GPR.

	Length Scale, l	Scale Mixture, α	White Noise Level, n
ϕ	1.12	1	1.62×10^{-3}
X_{NH_3}	1.38	0.162	2.53×10^{-4}
NO	0.74	0.0239	4.06×10^{-3}
N ₂ O	0.333	10	1.95×10^{-3}
NO ₂	0.3	10	5.68×10^{-3}

where x_i and x_j are datapoints, and $d(x_i, x_j)$ is their Euclidean distance. The white noise kernel accounts for measurement noise and is defined as:

$$k_w(x_i, x_j) = \begin{cases} n & \text{if } x_i = x_j \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

The dataset from the experimental campaign includes equivalence ratio, ammonia fuel fraction, and emissions of NO, NO₂, and N₂O. To train the GPR model, 75% of the data (121 points) is randomly selected, excluding unstable flame conditions. The remaining 25% is reserved for validation. Optimal hyperparameters are determined by maximizing the coefficient of determination (R^2) for the regression of predicted versus true validation data. Details of the optimized hyperparameters are provided in Table 1.

Once trained, the GPR algorithm’s performance is evaluated on an independent test dataset to assess its predictive capability for equivalence ratio, ammonia fraction, and emissions. This approach ensures robust validation of the algorithm in a context distinct from the training and validation phases. Further details about the GPR algorithm can be found in [31].

4. Results and discussion

The chemiluminescence spectra and intensities of single species are analysed in this section. Fig. 3 shows an example of chemiluminescence spectrum for $X_{NH_3} = 0.60$, $\phi = 1.20$ and $Re = 6000$. Fig. 3a and Fig. 3b respectively show the UV and UV-visible spectra of the *in-flame* zone. Figure 3c focuses on the visible-IR range and also includes the spectrum recorded in the *post-flame* zone. The *in-flame* UV-visible spectra are consistent with that recorded by Zhu et al. [33] for equivalent laminar flames. Specifically, contributions from NO*, OH* and NH* excited radicals are apparent and a broadband background which is mainly produced by H₂O*, H₂O₂* and NO₂* [16], is observed between 220 and 350 nm. There is also an intense broadband emission covering the whole visible range and it is attributed to multiple excited radicals including NO₂* and NH₂*. Although spectral contributions from NO₂* and NH₂* are overlapping and cannot be strictly separated, for simplicity and nomenclature sake, dedicated wavelength ranges are attributed to NO₂* and NH₂* in this study. Here, wavelength ranges selected for the different excited radicals are: 221.5-261.5 nm for NO* [39], 302-326 nm for OH* [39], 335-346 nm for NH* [39, 40], 450-500 nm for NO₂* and 620-645 nm for NH₂* [39, 41]. Before spectral integration, the unwanted broadband background between 220 and 350 nm is removed from NO*, OH*, NH* peaks using the subtraction procedure already described by Zhu et al. [33] and Mashruk et al. [16]. The broadband contribution between 350 and 400 nm is here identified as *Violet*. Additionally, *IR1* and *IR2* are defined to include contributions in the IR, in the ranges 800-900 nm and 900-1000 nm, respectively. Nitrous oxide excited radicals (N₂O*) may also contribute to chemiluminescence but cannot be featured here because the associated wavelength range is out of the detectable range (172-197 nm) [42] of the spectrometers. The chemiluminescence intensity of each species is normalised by the highest value detected for this species across all conditions tested in this study. The highest intensity value detected is OH* in the UV spectrum and NH₂* in the visible one, as expected from [33]. For the *post-flame* zone, 10 different spectral ranges are defined, namely: 500-550 nm for *P1*, 550-600 nm for *P2*, 600-650 nm for *P3*, 650-700 nm for *P4*, 700-750 nm for *P5*, 750-800 nm for *P6*, 800-850 nm for *P7*, 850-900 nm for *P8*, 900-950 nm for *P9* and 950-1000 nm for *P10*, covering the visible and IR ranges. To give an idea of the precision of the chemiluminescence measurements, many spectra were recorded for the same flame ($\phi = 1$, $X_{NH_3} = 0.55$ and $Re = 6000$) and the following coefficient of variations of chemiluminescence intensities were found: 1.37% for NO*, 1.46% for OH*, 1.48% for NH*, 0.84% for NO₂, 1.46% for NH₂, 0.77% for *Violet*, 0.67% for *IR1* and 0.41% for *IR2*.

4.1. Chemiluminescence spectra and intensity of single excited radicals

Figure 4 shows the measured chemiluminescence intensities as a function of equivalence ratio for various NH₃ fuel fractions and a constant Reynolds number of $Re = 6000$. Trends are in very good agreement with that measured by Zhu et al. [33] in laminar flames for comparable ranges of equivalence ratio and NH₃ fuel fraction. Specifically, curves of OH*, NO*, NH*, *Violet* vs. equivalence ratio feature only one peak, somewhat close to stoichiometric, and increasing the NH₃ fuel fraction decreases the intensity. Also consistent with Zhu et al. [33], curves of NO₂, NH₂* vs. equivalence ratio feature two local maxima (one for lean equivalence ratios and another for rich equivalence ratios) if the NH₃ fuel fraction does not exceed $X_{NH_3} \simeq 0.70$. Such non monotonic trends are the manifestation of multiple excited radicals contributing in the same spectral range, each with a different sensitivity to equivalence ratio. In the IR, which was not investigated by Zhu et al. [33], trends of *IR1* with equivalence ratio and NH₃ fuel fraction resembles that of NO₂. Conversely, *IR2* has a similar monomodal profile as that of OH*, NO*, NH* radicals, but the peak *IR2* intensity is somewhat shifted towards leaner equivalence ratios. For the *post-flame* zone, the curve of *P10* intensity in the IR vs. equivalence ratio features only one peak, at stoichiometry. The *P10* intensity decreases when the NH₃ fuel fraction is increased and the decrease is much less pronounced than for the excited radicals in the UV. This behavior is consistent with the radiation of hot water vapor with an intensity strongly dependent on temperature. Indeed, temperature is maximal at stoichiometry and decreases, albeit not too quickly, when more NH₃ is introduced in the fuel.

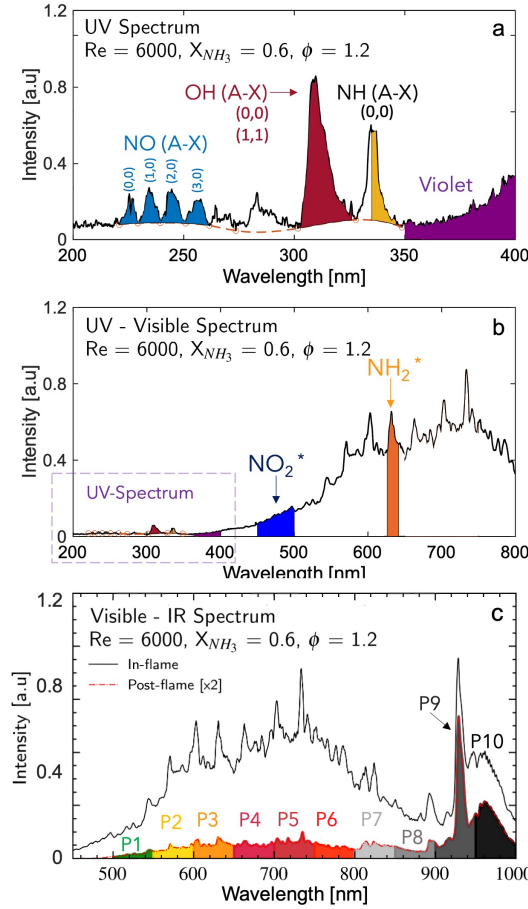


Fig. 3: Chemiluminescence spectrum recorded for $X_{NH_3} = 0.6$, $\phi = 1.20$ and $Re = 6000$ in the UV range (a), UV-visible range (b) and visible-IR range (c). A comparison between *in-flame* (black) and *post-flame* (red) spectra is shown in panel c. Colour labels indicate the features assigned to various excited radicals. The intensity of the *post-flame* spectra is doubled to facilitate comparison.

4.2. Chemiluminescence intensity ratios

One of the goals of this study is to identify spectral bands that can be monitored and used to infer important flame properties such as equivalence ratio, NH_3 fuel fraction or NO emission. To eliminate intensity fluctuations due to flame surface area modulation in turbulent flames, this is typically achieved by considering chemiluminescence intensity ratios instead of intensities from single species or isolated spectral ranges (see for example [15] or [16]). Many ratios may be created with the aforementioned spectral ranges and these were all tested. However, only the most promising ratios featuring meaningful trends are discussed here, and the others are left for supplementary material. The eight most promising ratios are shown in Fig. 5 as a function of equivalence ratio for different NH_3 fractions and a constant Reynolds number of $Re = 6000$. Additionally, Fig. 6 shows seven of these ratios measured as a function the Reynolds number for different equivalence ratios and NH_3 fuel fractions. These ratios are now analysed using previous work (Zhu et al. [33] for NH_3/H_2 laminar flames and Mashruk et al. [16] for NH_3/CH_4 turbulent flames) as reference and on the premise that, to be most useful by itself, a ratio should feature a large sensitivity to a desired property (e.g., equivalence ratio) while being insensitive to the others (e.g., NH_3 fuel fraction and Reynolds number).

- NH^*/OH^* : Trends of this ratio match that previously observed for laminar flames. It increases monotonically with equivalence ratio and is not too sensitive to the NH_3 fuel fraction if $\phi \leq 1.0$, making it a surrogate candidate for equivalence ratio in lean flames. However, monotonicity with equivalence ratio and insensitivity to the fuel composition are lost if rich flames are considered. In addition, the NH^*/OH^* is quite sensitive to the Reynolds number (c.f., Fig. 6a). For this reason, this ratio is not an ideal standalone surrogate of equivalence ratio.
- $OH^*/Violet$: Qualitatively, trends of this ratio also match that observed for laminar flames. It is too sensitive to both equivalence ratio and NH_3 fuel fraction to be useful for lean equivalence ratios. However, the insert in Fig. 5b as well as Fig. 5d of [33] show that this ratio may be an appropriate surrogate of rich equivalence ratios. Unfortunately, the $OH^*/Violet$ ratio decreases monotonically with the Reynolds number, suggesting that equivalence ratio predictions

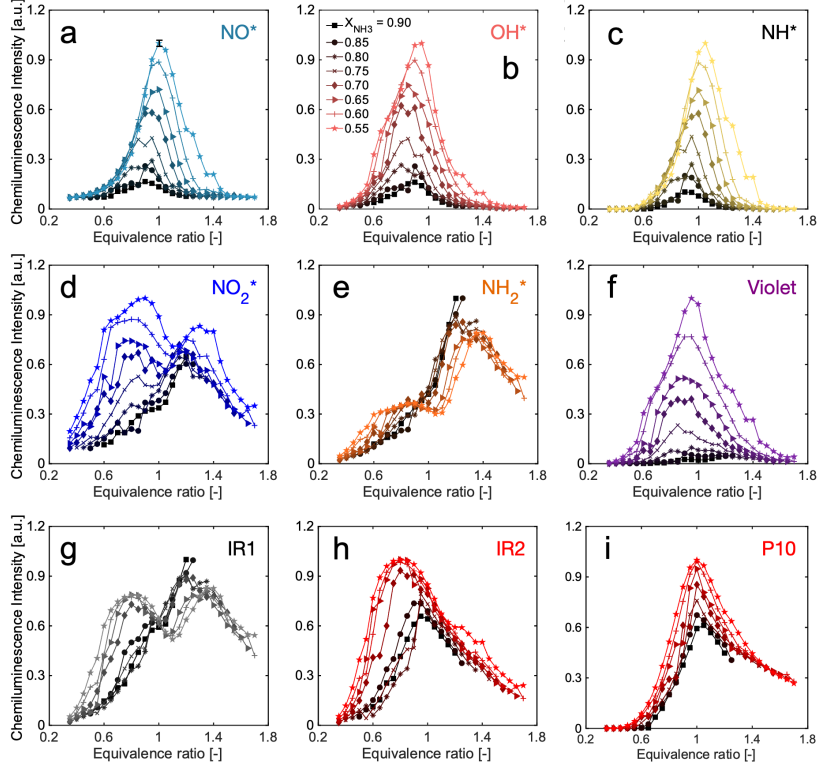


Fig. 4: Chemiluminescence intensities of single excited radicals or spectral ranges as a function of equivalence ratio for different NH_3 fuel fractions and a constant Reynolds number of $\text{Re} = 6000$.

with this ratio could become insufficiently accurate if applied to flames with unknown or significantly varying Reynolds number. Given that it shows potential for rich NH_3/H_2 flames, i.e., those relevant to the first stage of two-stage, rich-lean combustors, the $\text{OH}^*/\text{Violet}$ ratio may be worth considering for some applications.

- $\text{NH}_2^*/\text{NO}_2^*$: Trends of this ratio agree with that observed for laminar flames (labelled as Red/Blue in [33]). Although it is virtually insensitive to the Reynolds number, it increases monotonically with both the equivalence ratio and the NH_3 fuel fraction. Monotonicity is a good asset but sensitivity to multiple properties disqualifies the $\text{NH}_2^*/\text{NO}_2^*$ ratio as a useful standalone surrogate.
- $\text{IR2}/\text{NH}_2^*$: This ratio was not considered for laminar flames in [33]. It is somewhat sensitive to the Reynolds number and, more important, it varies non-monotonically with both the equivalence ratio and the NH_3 fuel fraction. Consequently, the $\text{IR2}/\text{NH}_2^*$ is not a useful surrogate.
- $\text{NO}_2^*/\text{IR1}$: This ratio was not considered for laminar flames in [33]. It is somewhat sensitive to the Reynolds number, and it decreases very rapidly as the equivalence ratios decreases for far lean equivalence ratios. However, it varies non-monotonically with both the equivalence ratio and the NH_3 fuel fraction for most equivalence ratios considered. It is not a useful surrogate.
- $\text{NO}^*/\text{IR1}$: This ratio varies non-monotonically with both the equivalence ratio and the NH_3 fuel fraction. It is not a useful surrogate.
- $\text{NH}^*/\text{IR1}$: Trends of this ratio agree with that observed for the ratio labelled NH^*/Red for laminar flames in [33]. It increases monotonically and very rapidly when the NH_3 fuel fraction is increased, but it varies non-monotonically with the equivalence ratio. If paired with the $\text{NH}_2^*/\text{NO}_2^*$ ratio, the $\text{NH}^*/\text{IR1}$ ratio may perhaps be used to achieve combined predictions of equivalence ratio and NH_3 fuel fraction. Unfortunately, the $\text{NH}^*/\text{IR1}$ ratio is strongly sensitive to Reynolds number, limiting its application to flames with known and constant Reynolds number.
- $\text{P10}/\text{P1}$: This ratio is tested because it involves contributions measured in the *post-flame zone* only, and it relies on emissions that are very far apart spectrally, namely the green and IR ranges. Close to stoichiometric, this ratio has the useful property of increasing monotonically and very rapidly when the NH_3 fuel fraction is increased up to $X_{\text{NH}_3} = 0.7$. However, maximum intensity is reached when $0.55 \leq X_{\text{NH}_3} \leq 0.65$. It also varies non-monotonically and very rapidly with the equivalence ratio. It is not a useful surrogate.

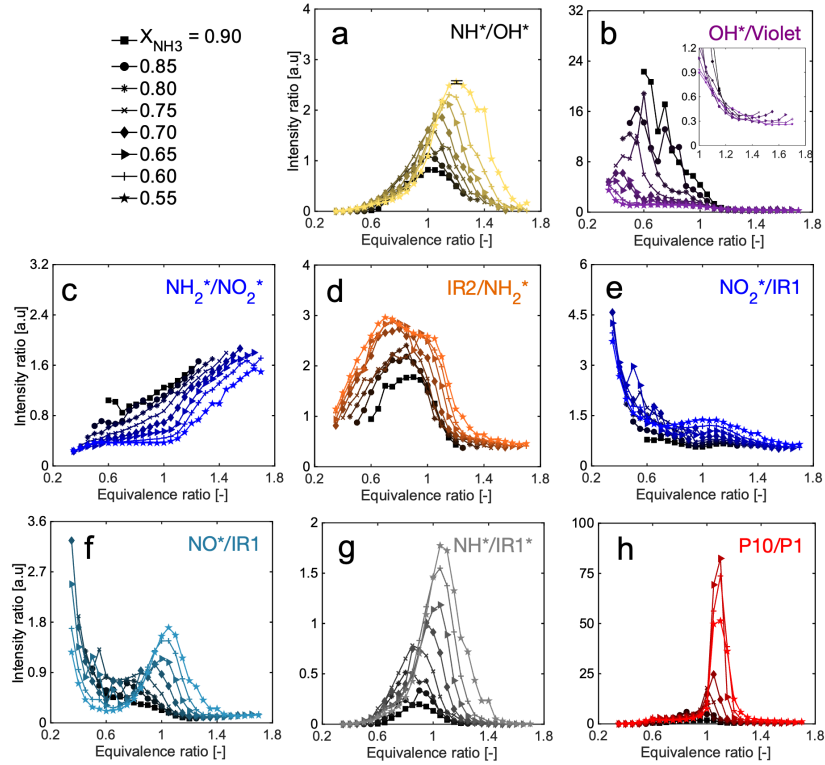


Fig. 5: Chemiluminescence intensity ratios as a function of equivalence ratio for different NH_3 fuel fractions and a constant Reynolds number of $\text{Re} = 6000$.

In summary, some ratios (e.g., NH^*/OH^* , $\text{NH}_2^*/\text{NO}_2^*$ or $\text{NH}^*/\text{IR1}$) have some merit that could qualify them as useful surrogates of equivalence ratio and/or NH_3 fuel fraction in specific and well controlled applications. However, there is no ratio that can be used to infer equivalence ratio and/or NH_3 fuel fraction accurately across the whole range of possible operating conditions. This is different from NH_3/CH_4 fuel blends for which the CN^*/OH^* and NH^*/CH^* ratios were identified as very promising surrogates of equivalence ratio and NH_3 fuel fraction, respectively, for both laminar [15] and turbulent swirl flames [16]. The absence of truly useful chemiluminescence ratios implies that more advanced ways of uncovering the intimate relationship between NH_3/H_2 flames and their chemiluminescence are needed, and this is the topic of the upcoming Sec. 5.

4.3. Exhaust emissions

It is also interesting to assess if chemiluminescence can be used to predict the exhaust emission quantitatively [43]. Out of the 252 data points, only 193 cases were utilized for emission measurements, excluding those that exhibited less stability. Figure 7 shows the measured 15% O_2 -corrected dry NO , NO_2 and N_2O exhaust concentration as a function of equivalence ratio for different NH_3 fuel fractions at a constant Reynolds number of $\text{Re} = 6000$. The observed trends in NO emissions can be correlated to the NH_3/H_2 kinetics where the Fuel NO_x route dominates the NO_x formation [44]. To gain a comprehensive understanding of the combustion kinetics associated with ammonia/hydrogen mixtures, it is essential to examine the mechanisms governing the formation and reburn of NO . These processes are shown in Fig. 8. The main NH_3 oxidation pathway is through the interaction with OH radicals, resulting in the production of NH_2 radicals [45]. This process, specifically the reaction $\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$, has been demonstrated to function as a heat release marker for NH_3/H_2 flames [13], as shown in Fig. 3. Subsequently, the O and OH radicals play a crucial role in the production of NH via the conversion of NH_2 to NH . Then, the NH radicals interact again with OH , resulting in the conversion of NH to HNO , as proved in [37, 46, 47]. As shown in Fig. 4, the peak of chemiluminescence intensity derived from NH^* and OH^* occurs between $\phi = 0.85$ and $\phi = 1$, as observed for NO^* , indicating that the highest production of HNO occurs within this range. Indeed, HNO results as the main source of NO production in NH_3/H_2 mixtures, particularly through its interaction with residual molecular oxygen (O_2). Consequently, significant NO production occurs near stoichiometric conditions, specifically when $\phi \simeq 0.9$. Conversely, under rich conditions, where molecular oxygen has been largely converted and depleted, NO production from HNO conversion diminishes. The introduction of an increased quantity of hydrogen into the mixture does not result in NO emission under rich conditions, particularly when the ϕ exceeds 1.15. This is consistent with prior studies such as [48]. The observed increase and subsequent decrease in NO trend can be attributed to the increase and decrease of OH , O , H , and HNO radicals. In the rich conditions, NH_2 , which is the most important NO -Reburn component [44], become abundant to convert NO to N_2 . As demonstrated, comparison with Fig. 4 shows

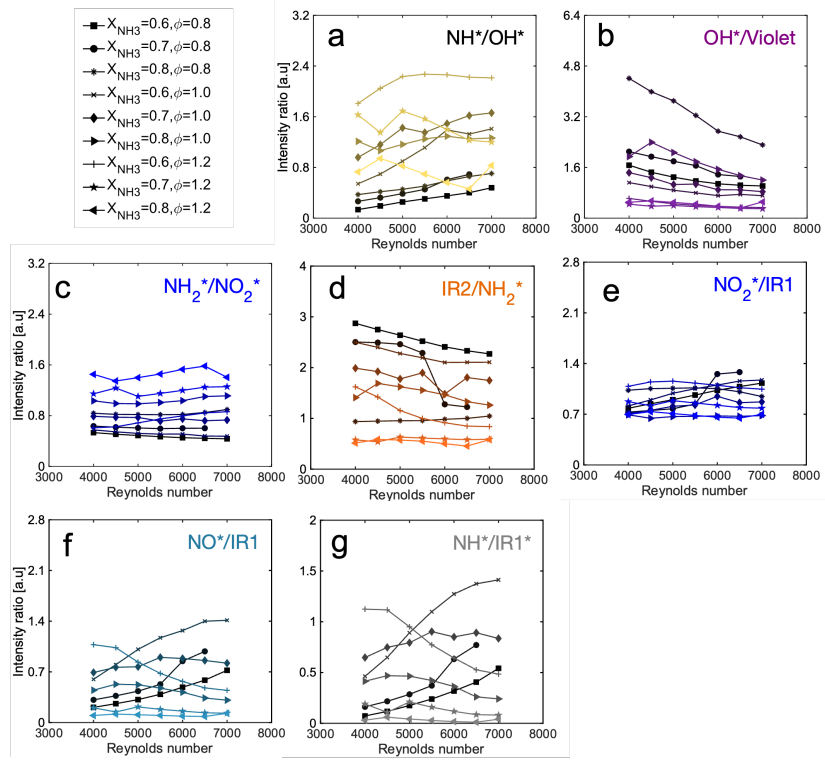


Fig. 6: Chemiluminescence intensity ratios as a function of Reynolds number for different NH_3 fuel fractions and equivalence ratios.

that trends of NO as a function of the equivalence ratio resemble that of NO^* , OH^* and NH^* . This suggests that NO emissions may be recovered by suitably post processing the available chemiluminescence information. In addition, Fig. 7 also shows the

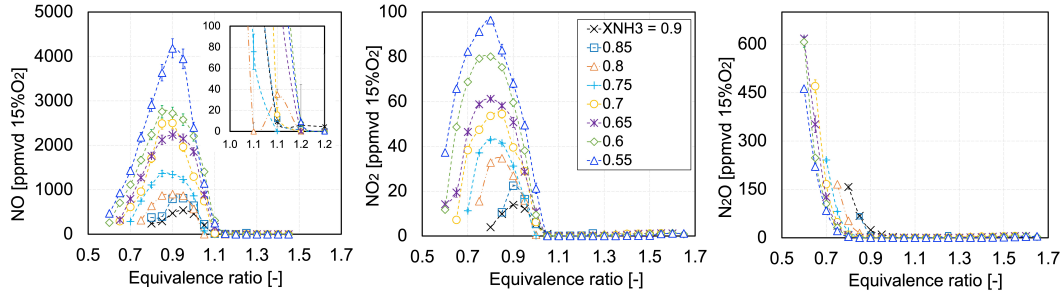


Fig. 7: Measured 15% O_2 -dry NO, NO_2 and N_2O exhaust concentration as a function of the equivalence ratio for different NH_3 fuel fractions at a constant Reynolds number of $\text{Re} = 6000$.

results of NO_2 and N_2O emissions gathered during the experimental campaign. NO_2 formation arises from oxidation of NO when excessive O_2 is available, specifically through $\text{NO} + \text{O}_2 \rightarrow \text{NO}_2 + \text{O}$ and $\text{NO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}$ reactions, and contribute minimally to total NO_x formation, in particular when $\phi \leq 1.1$, with a maximum near $\phi \simeq 0.85$. N_2O is formed only under very lean conditions or relatively high equivalence ratio when the ammonia fraction is high, where there are insufficient H/O radicals to inhibit conversion to NO, or the temperature is low enough to decompose N_2O to N_2 and O_2 .

5. Gaussian Process Regression (GPR)

Figure 9 shows the predictions of the GPR algorithm for equivalence ratio, NH_3 fuel fraction and NO, N_2O , NO_2 emissions as a function of their true values for the training and validation data points. To perform the GPR, only radicals that exhibited a clear correlation by chemiluminescence analysis (see Figs. 4,5) were used, specifically NH^* , Violet*, NO_2^* , and NH_2^* . The chemiluminescence intensity of the four radicals were normalized by OH^* to yield a ratio of chemiluminescence intensities, i.e., a quantity that is no longer a function of the flame surface area within the probe volume. Additionally, the emission data and the

suggests that the model is well-calibrated and the data for these parameters is robust and comprehensive. However, the error bars for NO and NO₂ are comparatively larger, reflecting the increased uncertainty and stochastic nature of these emissions, highlighting the need for more extensive data collection and potentially more advanced modeling techniques to improve prediction accuracy. Despite these larger uncertainties, the use of probabilistic modeling provides valuable insights into the range of possible emission outcomes, which is critical for emission measurement in ammonia combustion. The performance of the GPR algorithm massively outperforms that possible with one or more intensity ratios. To the best of the authors' knowledge, this is the first demonstration of combined quantitative measurements of equivalence ratio, NH₃ fuel fraction and NO, N₂O, NO₂ emissions in turbulent NH₃/H₂ flames using chemiluminescence. This lays strong foundation for the development of optical sensors for the monitoring and control of practical NH₃/H₂ flames.

6. Conclusions

The chemiluminescence signature of turbulent NH₃-H₂-air swirl flames was investigated in the UV, visible and IR ranges. By gathering a comprehensive experimental database consisting of 252 operating conditions, spanning a wide range of equivalence ratio ($0.35 \leq \phi \leq 1.70$), NH₃ fuel fraction ($0.55 \leq X_{NH_3} \leq 0.90$) and Reynolds number ($4000 \leq Re \leq 7000$), this study addressed a significant gap in the existing literature regarding the characteristics of chemiluminescence in turbulent NH₃-H₂ flames. A detailed summary of the main findings is provided as follows:

- Key findings include the identification of dominant excited radicals (e.g., NO*, OH*, NH*, NO₂*, and NH₂*) and their associated spectral ranges, which align with prior studies of laminar flames. The study also demonstrated that while various chemiluminescence intensity ratios were examined, none proved effective as direct surrogates for equivalence ratio or NH₃ fuel fraction.
- The concentration of NO, NO₂ and N₂O in the exhaust gases was measured in the 193 highly stable cases, collecting a wide-ranging and useful database for information on emission for these mixtures. NO resulted as main responsible for emissions, particularly when equivalence ratio is slightly lean, with a peak at $\phi \simeq 0.90$. Increasing the fraction of H₂ in the fuel blend increases NO emissions. When $\phi \geq 1.15$, NH₃/H₂ flames do not emit any NO. NO₂ contributes minimally to the emission of NO_x, especially when $\phi \simeq 0.85$. Lean NH₃/H₂ combustion have to be avoided due to the high N₂O formation.
- A pivotal contribution of this work is the application of a machine learning-based method, namely Gaussian Process Regression (GPR), to the gathered chemiluminescence data. The GPR methodology allowed for the prediction of the equivalence ratio, the NH₃ fuel fraction and the NO, NO₂, N₂O emissions of the NH₃/H₂ flames using only the NH*/OH*, Violet/OH* and NH₂*/OH* chemiluminescence intensity ratios. Excellent predictions are achieved by GPR algorithm in terms of equivalence ratio (± 0.05) and NH₃ fuel fraction (± 0.02). Regarding emissions, GPR achieved satisfactory results: NO (± 300 ppm), N₂O (± 50 ppm) and NO₂ (± 10 ppm).

This work underscores the potential of machine learning-based methods, in particular the Gaussian Process Regression (GPR), combined with chemiluminescence data derived from a wide experimental database, for the development of optical, non-intrusive sensors for real-time monitoring and control of NH₃/H₂ turbulent flames. The extensive experimental database provides a solid basis for future development in flame diagnostics and NO_x emissions mitigation strategies.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary material

Supplementary material are available.

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