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TRACEABLE AMMONIA QUANTIFICATION AND METROLOGICAL UNCERTAINTY EVALUATION IN A SHOCK TUBE

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Abstract:
This work emphasizes on the development of an ultra-rapid spectrally resolved tunable diode laser absorption spectroscopy (TDLAS)-based spectrometer with a scan frequency of 40 kHz for dynamic NH_3 quantification in a shock tube. Thanks to the high laser scan frequency, the NH_3 mole fraction at various stages during the dynamic process can be quantified. Besides, considering lacking metrology in shock tubes for dynamic studies, we comprehensively evaluated the uncertainty sources and budgets of thermodynamic parameters and species concentration based on *Guide to the expression of uncertainty in measurements* (GUM). The established metrological uncertainty evaluation method for shock tube experiments can be beneficial to provide traceable and high-quality data, which is vital for dynamic studies as well as chemical kinetic modelling.

Keywords: Ammonia; TDLAS; Shock tube; Uncertainty budget

1 INTRODUCTION

Ammonia is a promising zero-carbon fuel which has a comparable specific mass density to conventional fossil fuels. Compared to hydrogen, it has a 70% relatively higher specific volume density and higher boiling point, making it much easier to be liquefied and therefore significantly reducing the cost of storage and transportation. The volumetric hydrogen content of ammonia is also 70% relatively higher than hydrogen which means that ammonia is not only a good zero-carbon fuel but also a promising hydrogen carrier. A much narrower flammability limit of ammonia compared to hydrogen increases its safety property for daily usage. The "green" ammonia synthesized by "Power-to-X" technologies ensures life-cycle carbon neutrality of using ammonia and guides to the eventual "ammonia economy" [1].

When considering ammonia as a fuel to be applied on a large scale, fundamental thermodynamic studies are required. The shock tube is one of the typical facilities that can create a quasi-instantaneously and homogeneously high-temperature and pressure environment. It is commonly used for high-temperature chemistry validation where the thermal conversion process in shock tubes can be simulated using a zero-dimensional model. To get speciation data from shock tubes, diagnostic methods are required such as laser diagnostics, mass spectrometry, or gas chromatography. Among them, tunable laser diode laser absorption spectroscopy (TDLAS) is an *in-situ*, line-of-sight, and non-invasive measurement method with high time resolution and selectivity [2]. By coupling TDLAS to shock tubes, it is able to get highly accurate time-resolved speciation data within the time scales of only several hundred microseconds to several milliseconds.

Up to now, there are limited studies on speciation measurements of ammonia and ammonia fuel blends using TDLAS in shock tubes. Alturaifi et al. [3-5] conducted several experiments by coupling TDLAS to the shock tube for NH_3, N_2O and H_2O measurements during ammonia pyrolysis and oxidation. He and Zheng et al. [6-9] used TDLAS to measure NH_3, NO, CO, CO_2, H_2O and temperature during ammonia and ammonia fuel blends oxidation. At PTB (National Metrology Institute of Germany), we measured the time-resolved NO profiles for pure NH_3 and NH_3/H_2 fuel blends. Recently, we selected a new NH_3 absorption line and coupled it to the shock tube for NH_3 quantification [10-13].

The importance of quantifying ammonia in shock tube experiments is not only because it is the reactant, but also due to its sticky property, as well as the interest in evaluating unconsumed ammonia emissions. From the literature studies and our

previous works, there are still two concerns that are worthwhile for further investigations. Firstly, the NH_3 absorption cross-sections measurements in shock tubes were all based on the assumption that an unchanged NH_3 mole fraction before incident shock wave (T_1, P_1), to immediately after reflected shock wave (T_5, P_5). This assumption was obtained relying on the simulation results while has not been experimentally validated to our best knowledge. In our previous work, we already observed around 20% NH_3 decomposition at the first spectra (at 200 µs) after (T_5, P_5) at a temperature of 1933 K, therefore the cross-section measurements were limited to 1800 K. This reminds us of the importance of prerequisites for absorption cross-section measurements which merits more investigations. Secondly, there is still lacking metrological uncertainty evaluation methodology for speciation data measured in shock tubes by TDLAS although it has been used for several decades, which is particularly important in providing reliable experimental data.

Consequently, we upgraded our previous spectrometer by enhancing the scan frequency from previously 10 kHz to 40 kHz, and the corresponding data acquisition rate from 20 MS/s to 80 MS/s. The purpose is on the one hand to capture enough spectra at different stages during the dynamic process in shock tubes, especially regarding the ultra-short time duration of around 100 µs after the incident shock wave (T_2, P_2). On the other hand, we want to shorten the measurement time of the first spectra after the reflected shock wave (T_5, P_5) to minimize the potential pyrolysis of NH_3 at high temperatures. Based on the ultra-rapid TDLAS spectrometer, we quantified and compared the NH_3 mole fractions before the incident shock wave (T_1, P_1), after the incident shock wave (T_2, P_2) and immediately after the reflected shock wave (T_5, P_5) (within 25 µs). Also, we conducted comprehensive uncertainty evaluations on thermodynamic parameters and speciation mole fractions following the rules of *Guide to the expression of uncertainty in measurement* (GUM) [14].

2 METHODOLOGY

For TDLAS, the intensity of a monochromatic continuously tunable laser source transmitted through a gaseous sample is given by the Beer-Lambert law [15]:

$$I(\upsilon) = E(t) + I_0(\upsilon) \cdot T(t) \cdot exp[-\alpha(\upsilon)] \quad (1)$$

with the background emission $E(t)$ at time t, initial laser intensity $I_0(\upsilon)$, the spectrally broadband transmission losses $T(t)$, and the absorbance $\alpha(\upsilon)$.

The absorbance spectrum $\alpha(\upsilon)$ can be computed using the following equation:

$$\alpha(\nu) = -p \ln\left(\frac{I(\nu)-E(t)}{I_0(\nu)\cdot T(t)}\right) = \frac{S(T)\cdot p\cdot L\cdot g(\upsilon-\upsilon_0)\cdot x}{k_B\cdot T} \quad (2)$$

where $S(T)$ is the absorption line strength at gas temperature T, $g(\upsilon-\upsilon_0)$ is the area normalized (integrated area=1) line shape function (centered at the wavenumber υ_0), k_B is the Boltzmann constant, p is the total pressure, x is the NH_3 mole fraction, and L is the optical path length.

By integrating the absorbance spectrum, the NH_3 mole fraction can be obtained by the following equation without the necessity to solve the line shape function.

$$A=\int \alpha(\nu)=\frac{S(T)_{\mathrm{sum}}\cdot p\cdot L\cdot x}{k_B\cdot T} \quad (3)$$

3 EXPERIMENTAL SETUP

The schematic of the experimental setup is shown in Figure 1. The shock tube at PTB consists of a 3.5-meter driver section and a 4.5-meter driven section. The inner surface was electropolished with a diameter of 70 mm. A manometer (627F, MKS Instruments, PTB International System of Units (SI)-traceable) was installed on the top of the driven section near the diaphragm section to record the initial filling pressure. Five pressure sensors (Kistler model 603C) combined with charge amplifiers (Kistler model 5018A) were utilized for pressure measurements and shock velocity calculation.

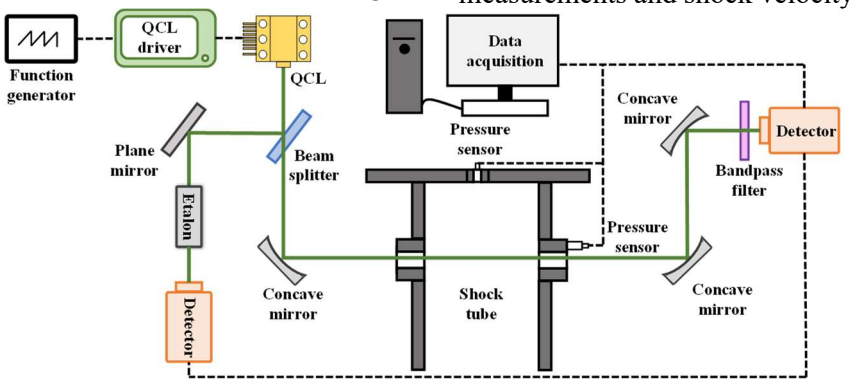

Figure 1. Schematic of the experimental setup

For laser diagnostics, two opposite CaF_2 windows were installed at the same plane as the fourth pressure sensor. The mid-infrared NH_3 laser centered at 1084.6 cm^{-1} is a continuous-wave distributed-feedback quantum cascade laser (CW-DFB-QCL, Alpes Lasers). The wavelength can be

tuned from 1083 to 1089 cm^{-1} by varying the current and/or temperature using a QCL driver (ITC4005QCL, Thorlabs). The laser current was modulated by a triangle-shaped ramp at a scan frequency up to 40 kHz supplied by a function generator (33500B, KEYSIGHT). From Figure 1, the laser beam was divided into two sub beams by a beam splitter (BSW711, Thorlabs). One was used to determine the dynamic laser tuning using a Germanium etalon (length 76.244 mm, traceable to PTB's length standard) before starting the measurements. The results of the etalon measurement were used to convert the x-axis of the measured spectra from the time to the wavenumbers domain. The other laser beam went through the optical windows with a path length of 7 cm via two concave mirrors (CM508-200-M01, focal length: 200 mm, Thorlabs) and was focused onto a photodetector (PVI-4TE-10, VIGO) by a concave mirror (CM508-050-M01, focal length: 50 mm, Thorlabs). A narrow bandpass filter (FB9000-500, Thorlabs) was placed in front of the detector to discriminate the signal against the background emission *E(t)* in Equation (1), e.g., thermal emission from the shock-heated gases. To match the ultra-rapid scan frequency, we upgraded the acquisition system with a new DAQ card (16-bit 80 MS/s, M2p.5943-x4, Spectrum Instrumentation).

The NH_3/Ar mixtures were prepared in a 50 L stainless steel tank using high quanlity pure NH_3 and pure Ar (HiQ 5.0, Linde). A manometer (627F, MKS Instruments, PTB SI-traceable) was installed on the top of the mixing tank to monitor the mixture pressure. Before preparing the mixtures, this tank was vacuumed overnight to a pressure below 1×10^{-7} mbar (TTR 91N, Leybold). When starting to prepare the mixture, a small amount of target gas first flushes the pipes twice to clean up residual gas. The mixtures were stirred by a magnetic stirrer (cyclone 300 ac, Büchiglasuster) for at least two hours to ensure homogeneity.

Table 1 shows the average mixture compositions and experimental conditions of three NH_3/Ar mixtures examined in this study. The ideal NH_3 mole fraction of Mixture 1, Mixture 2, and Mixture 3 is 0.5%, 1% and 1.5%, respectively. From Table 1, it can be found that the average NH_3 mole fraction is lower than the ideal value due to NH_3 adsorption effect, which will be discussed later.

Table 1. Average mixture compositions and experimental conditions

Mixture	x_{NH3}	x_{Ar}	P_1 /bar	T_1/K	P_2 /bar	T_2/K	P_5 /bar	T_5/K
1	0.0037	0.9963	0.0199-0.1177	295	0.2553-0.5543	603-1200	1.1502-1.7798	988-2394
2	0.0095	0.9905			0.2563-0.5492	597-1192	1.1589-1.7643	975-2374
3	0.0137	0.9863			0.2581-0.5880	620-1195	1.1711-1.8855	1027-2380

4 RESULTS AND DISCUSSIONS

a. Spectra

Figure 2 shows an exemplary pressure trace measured by the 4th pressure sensor and corresponding laser signal measured in a shock tube. The time zero is set as the arrival of the shock wave to the 5th pressure sensor. From Figure 2, two sharp pressure rises can be captured, indicating the arrival of the incident shock wave and reflected shock wave, respectively. The duration of the status (P_2, T_2) is quite short of around 100 µs. To get enough spectra at (P_2, T_2), the scan frequency was therefore enhanced to 40 kHz, namely 25 µs for a period. In this case, there are at least three complete spectra that can be captured. Besides, an ultra-rapid scan frequency was able to make the time duration of the first spectra at (P_5, T_5) as short as possible to reduce the possibility of pyrolysis at high temperature conditions.

Before starting the measurements, the etalon signal was firstly acquired to mark the relative laser wavelength. For each shot, the reference signal (I_0) and offset signal were recorded before filling the mixture. Then the transmitted signal (I_t) was automatically recorded trigged by the pressure signal. By using Equation (1-2) and transferring the time-domain to wavenumber-domain using etalon signal, the spectral absorbance at different stages can be calculated. Furthermore, the concentration can be quantified by integrating the absorbance spectra using Equation (3).

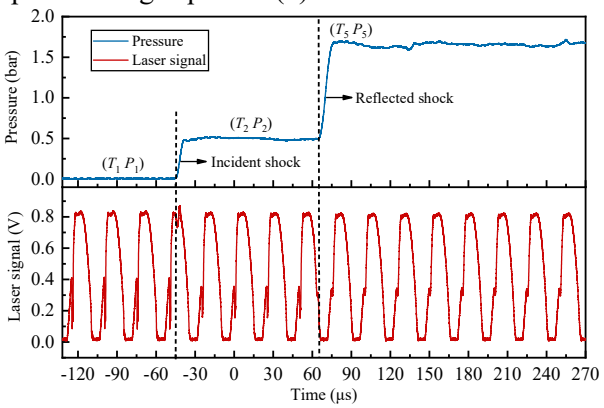

Figure 2. Exemplary pressure trace and laser signal

b. Metrological uncertainty evaluation

Although shock tube coupled with TDLAS have been widely applied for monitoring the dynamic speciation in the past decades, the uncertainty of the measurements is commonly analysed using the root sum squared method without a standard and metrological approach [3-5]. Given this, we conducted a comprehensive uncertainty evaluation using GUM Workbench® [14]. The coverage factor is given as 1.0 throughout the uncertainty evaluations in this study. For easier illustration, we took one case from Mixture 2 (P_1=0.0688 bar) as an example in the following steps.

Firstly, the heat capacity ratio of the mixture (γ) before incident shock wave is calculated by Equation (4),

$$\gamma = \frac{\sum C_{p_i} \cdot x_i}{\sum C_{v_i} \cdot x_i} \quad \text{(Eq.4)}$$

where x represents the mole fraction of the mixture composition; C_p and C_v represent the heat capacities at constant pressure and at constant volume, respectively.

The NH_3 mole fraction before incident shock wave ($x_{(P1,\ T1)}$) was calculated by Equation (3) including six relevant quantities. Specifically, k_B has a constant of 1.380649×10^{-23} J/K. The laser path length (L) is 7 cm, with an uncertainty of 1.1%. The absorption spectrum is averaged over 116 scans for the (P_1, T_1) period. The integral area of this averaged absorption spectrum ($A_{(P1,\ T1)}$) is 0.0984, with an uncertainty of 1.5% which includes the uncertainty of etalon measurements. The total line intensity ($S(T)_{(P1,\ T1)}$) of six transition lines at 295 K is 8.233×10^{-19} cm/mol, with an uncertainty of 10% from HITRAN [16]. The uncertainty of P_1 is 0.0001 bar according to the calibration certificate (PTB SI-traceable). The room temperature was controlled and measured at 295 K with an uncertainty of 0.5 K. As a result, $x_{(P1,\ T1)}$ is calculated to be 0.0101 with an uncertainty of 10.5%. Table 3 shows the uncertainty budgets of $x_{(P1,\ T1)}$. Clearly, the uncertainty of $S(T)_{(P1,\ T1)}$ accounts for a significantly greater contribution (96.6%) than other quantities, which indicates an efficient way to reduce the total uncertainty by reducing the uncertainty of the line intensity.

Other quantities for heat capacity calculation were obtained from the National Institute of Standards and Technology (NIST) database. Specifically, the C_p and C_v of NH_3 are 36.385 and 27.688 J/(mol·K), respectively, with an uncertainty of 0.25%. The C_p and C_v of Ar are 20.820 and 12.477 J/(mol·K), respectively, with an uncertainty of 0.15%. Overall, the heat capacity ratio γ of the mixture is 1.6608 with an uncertainty of 0.215%.

Secondly, the Mach number (M_a) of the shock front is another important parameter calculated by Equation (5),

$$M_a = \frac{u_s}{\sqrt{\frac{\gamma R}{\sum M_i x_i}_1}} \quad \text{(Eq.5)}$$

where u_s refers to the shock velocity; R is the gas constant; M is the molar mass.

The shock velocity has an uncertainty of 0.937 %. The gas constant R is defined as the Avogadro constant N_A (6.02214076×10^{23}) multiplied by k_B (8.31446261815324 J/(mol·K)). The molar mass of NH_3 and Ar were 17.0305 and 39.948 g/mol from NIST, respectively. Overall, the Mach number is 2.332 with an uncertainty of 0.943% where the uncertainty from shock velocity contributes 97.8%.

Thirdly, according to the gas dynamic equations based on one-dimensional shock wave coordinates, the pressures and temperatures (P_2, T_2, P_5, T_5) behind the incident and reflected shock waves can be calculated by Equation (6-9).

$$P_2 = P_1\left[1 + \frac{2\gamma}{\gamma+1}(M_a^2 - 1)\right] \quad \text{(Eq.6)}$$

$$T_2 = T_1\left[1 + \frac{2(\gamma-1)\gamma M_a^2+1}{(\gamma+1)^2 M_a^2}(M_a^2 - 1)\right] \quad \text{(Eq.7)}$$

$$P_5 = P_1\left[\frac{2\gamma M_a^2-(\gamma-1)}{\gamma+1}\right]\left[\frac{(3\gamma-1)M_a^2-2(\gamma-1)}{(\gamma-1)M_a^2+2}\right] \quad \text{(Eq.8)}$$

$$T_5 = T_1\frac{[2(\gamma-1)M_a^2+(3-\gamma)][(3\gamma-1)M_a^2-2(\gamma-1)]}{(\gamma+1)^2 M_a^2} \quad \text{(Eq.9)}$$

Based on the above analysis for the heat capacity ratio and Mach number, the uncertainties of P_2, T_2, P_5 and T_5 can be calculated to be 2.0%, 1.35%, 2.8% and 1.8%, respectively, as shown in Table 2. Combing the uncertainties of P_1 and T_1, it is evident that the uncertainties of thermodynamic parameters are increasing during the heating up process, of which the Mach number contributes the highest portion (over 90%) among all uncertainty sources.

Table 2. Uncertainty budgets of P_2, T_2, P_5 and T_5

Quantity		P_1	T_1	γ	Ma
Value		0.0688 bar	295 K	1.6608	2.332
Uncertainty (%)		0.15	0.17	0.215	0.9
P_2	Contribution (%)	0.6	-	0.1	99.3
	Value	**0.45 ± 0.008 bar (2.0%)**			
T_2	Contribution (%)	-	1.6	3.7	94.7
	Value	**735 ± 9.9 K (1.35%)**			
	Value	**1.636 ± 0.0458 bar (2.8%)**			
T_5	Contribution (%)	-	0.9	5.0	94.1

	Value	**1328 ± 23.9 K (1.8%)**

The NH_3 mole fraction at (P_2, T_2) and (P_5, T_5) can be calculated by Equation (3), the same method as for $x_{(P1, T1)}$. However, except for Boltzmann constant and path length, the values and uncertainties of the rest quantities have changed. As mentioned above, with an ultra-rapid scan frequency of 40 kHz, three complete spectra at (P_2, T_2) can be recorded and averaged. The area $A_{(P2, T2)}$ of the averaged absorbance is 0.0907 with an uncertainty of 1.5%. The line intensity at (P_2, T_2) is reduced to 3.098×10^{-19} cm/mol with an uncertainty of 10%. In a consequence, the NH_3 mole fraction at (P_2, T_2) is 0.0094 with an uncertainty of 10.5%.

To quantify the NH_3 mole fraction immediately after the reflected shock wave, we only used the first spectral absorbance to minimize the effect of possible pyrolysis with the growing time, especially for high temperature cases. With this ultra-rapid scan frequency, the largest time interval between the first scan and reflected shock wave is less than 25 μs, basically within 12.5 μs as only the first half period of the scan was considered. The line intensity at (P_5, T_5) is further reduced to 6.902×10^{-20} cm/mol with an uncertainty of 10%. As a result, the integrated absorbance $A_{(P5, T5)}$ is only about a half value compared to that at (P_1, T_1) or (P_2, T_2), leading to a larger uncertainty of 2%. Resultantly, the NH_3 mole fraction immediately after the reflected shock wave $x_{(P5, T5)}$ is 0.0099 with an uncertainty of 11%, which is 0.5% larger than that of $x_{(P1, T1)}$ and $x_{(P2, T2)}$ owing to a higher uncertainty in pressure, temperature, and integrated absorbance.

Table 3. Uncertainty budgets of NH_3 mole fraction at different stages

Quantity		k_B	L	$A_{(P1, T1)}$	$S(T)_{(P1, T1)}$	P_1	T_1
Value		1.380649×10^{-23} J/K	7 cm	0.0984	8.233×10^{-19} cm/mol	0.0688 bar	295 K
Uncertainty (%)		-	1.1	1.5	10	0.15	0.17
$x_{(P1, T1)}$	Contribution (%)	-	1.1	2.1	96.6	0.1	0.1
	Value	**0.0101 ± 0.0011 (10.5%)**					
Quantity		k_B	L	$A_{(P2, T2)}$	$S(T)_{(P2, T2)}$	P_2	T_2
Value		1.380649×10^{-23} J/K	7 cm	0.0907	3.098×10^{-19} cm/mol	0.45 bar	735 K
Uncertainty (%)		-	1.1	1.5	10	2.0	1.4
$x_{(P2, T2)}$	Contribution (%)	-	1.1	2.0	91.7	3.6	1.6
	Value	**0.0094 ± 0.0010 (10.5%)**					
Quantity		k_B	L	$A_{(P5, T5)}$	$S(T)_{(P5, T5)}$	P_5	T_5
Value		1.380649×10^{-23} J/K	7 cm	0.0427	6.902×10^{-20} cm/mol	1.636 bar	1328 K
Uncertainty (%)		-	1.1	2	10	2.8	1.8
$x_{(P5, T5)}$	Contribution (%)	-	1.0	3.4	86.3	6.6	2.7
	Value	**0.0099 ± 0.0011 (11%)**					

c. Ammonia quantification

The NH_3 mole fraction and corresponding uncertainties at (T_1, P_1), (T_2, P_2) and immediately after (T_5, P_5) of all cases for Mixture 1-3 are calculated by Equation (3), as shown in Figure 3. The dashed lines indicate the ideal mole fraction for mixture preparation. From Figure 3, when taking the measurement uncertainties into consideration, no evident NH_3 mole fraction variation can be observed, indicating no evident pyrolysis occurs during this dynamic process. Besides, it is concentration independent as three mixtures show consistent results. Note that this conclusion is only valid for the NH_3 mole fraction of the first spectra measured after the reflected shock wave, a time interval of less than 25 μs. As the time grows, the pyrolysis process will happen at such high T_5. Nevertheless, this study restricts the valid conditions of the assumption for cross-section measurements, especially for high temperatures. From Figure 3, another consistent phenomenon for three mixtures is that with the increase of P_1, the NH_3 mole fraction increases and then levels off when P_1 is larger than 0.06 bar. This result strongly indicates that at lower P_1, the relative NH_3 loss is larger. Especially for a low mole fraction mixture (e.g. Mixture 1), the largest relative NH_3 loss can be over 50% at the minimum P_1.

Note that before each experiment, we have used the same mixture as the experimental one to passivate the inner surface of the shock tube. Nonetheless, it is far from enough especially for low P_1 and low initial mole fraction mixtures. Some studies also used a specific higher concentration mixture as a compensation of NH_3 adsorption. However, this method also brings a risk that the NH_3 mole fraction after passivation is even higher than the target value. Up to now, there is still lacking golden standard passivation method for NH_3 studies in shock tubes. The difficulty is that the passivation process has a random nature, and highly depends on the initial pressure, mixture mole fraction, inner surface materials, passivation times, passivation time duration, vacuuming pumps and procedures. In

addition, the loss could also happen during the mixture preparation as NH_3 will also adsorb to the inner surface of the mixing tank, and it is quite difficult to monitor this process. Therefore, at least for low NH_3 mole fraction mixture and low P_1 conditions, it is strongly recommended to quantify the initial NH_3 mole fraction. A key quantity for thermodynamic parameters calculation, as well as an important input for modelling studies.

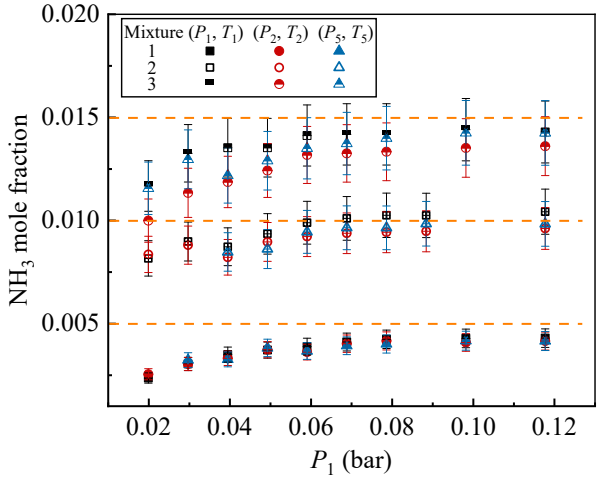

Figure 3. NH_3 mole fraction at (T_1, P_1), (T_2, P_2) and immediately after (T_5, P_5) of Mixture 1-3

5 SUMMARY

We developed an ultra-rapid TDLAS spectrometer (40 kHz scan frequency) and quantified the ammonia mole fraction before the incident shock wave (P_1, T_1), after the incident shock wave (P_2, T_2), and immediately after the reflected shock wave (P_5, T_5) (within 25 μs). No significant variation in NH_3 mole fraction was observed during the shock tube experiments, indicating no evident NH_3 pyrolysis during this dynamic process. This restricts the valid conditions for cross-section measurements. Additionally, we compared the NH_3 mole fraction at different P_1 values and found that NH_3 loss occurred, even with a passivation procedure, at lower P_1 (<0.06 bar in this study). For low NH_3 mole fraction mixtures, the largest relative NH_3 loss exceeded 50% at the minimum P_1 of 0.02 bar (ideally 0.5% NH_3 in the mixture). Therefore, it is strongly recommended to quantify the initial NH_3 mole fraction during shock tube experiments via an online *in situ* method, particularly for low NH_3 mole fraction mixtures and low P_1 conditions.

The uncertainties of thermodynamic parameters and the mole fraction of speciation measured by TDLAS in shock tubes have been metrologically evaluated. For the current study, the uncertainties of P_2, T_2, P_5 and T_5 are 2.0%, 1.35%, 2.8% and 1.8%, respectively. The uncertainties of NH_3 mole fraction at (P_1, T_1), (P_2, T_2), and immediately after (P_5, T_5) based on integrated absorbance are 10.5%, 10.5% and 11%, respectively. This methodology provides an insight into the uncertainty budgets of each quantity and can be generalized to other similar studies.

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