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## EXPERIMENTAL AND NUMERICAL INVESTIGATION OF NH<sub>3</sub>/H<sub>2</sub>/N<sub>2</sub> COMBUSTION IN A PREMIXED/STRATIFIED SWIRL BURNER

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### 1 ABSTRACT

2 *Interest in using renewably produced, partially cracked*  
3 *ammonia in gas turbines is gaining traction, but challenges*  
4 *relating to emissions of NO<sub>x</sub> and unburned ammonia remain. The*  
5 *present work progresses existing research on using hydrogen*  
6 *stratification to reduce NO<sub>x</sub> from ammonia/hydrogen flames by*  
7 *experimentally and numerically investigating the effects of also*  
8 *injecting nitrogen from the cracking process. It additionally*  
9 *assesses the NO<sub>x</sub> reduction capability of a recently developed*  
10 *novel swirl burner by adding hydrogen to the stratified flow to*  
11 *maintain the diffusive equivalence ratio at two high NO*  
12 *production conditions, slightly lean and stoichiometric.*

13 *At slightly globally rich conditions, maintaining the*  
14 *diffusive equivalence ratio at 0.9 resulted in an order of*  
15 *magnitude reduction in NO emissions with only a 33% increase*  
16 *in unburned NH<sub>3</sub>, compared to a fully premixed flame with the*  
17 *same fuel and air flow rates. This stratified configuration was*  
18 *found to increase consumption of NO by NH<sub>2</sub>, likely due to flame*  
19 *morphology effects, while NO production from OH and HNO*  
20 *pathways was reduced. The reduced OH intensity was posited as*  
21 *the cause for increased NH<sub>3</sub> emission. A strong emissions*  
22 *sensitivity to diffusive equivalence ratio was found, as the case*  
23 *with a stoichiometric diffusive equivalence ratio did not show*  
24 *such marked improvements over its corresponding premixed*  
25 *condition. Both stratified and premixed flames were found to be*  
26 *stable, however stratification has potential to trigger*  
27 *instabilities at different frequencies to premixed.*

28  
29 **Keywords:** Ammonia, hydrogen, combustion, emissions,  
30 stratification, partial premixing.

31  
32  
33

### 34 NOMENCLATURE

35	Φ <sub>D</sub>	Diffusive Equivalence Ratio
36	Φ <sub>G</sub>	Global Equivalence Ratio
37	CFD	Computational Fluid Dynamics
38	CRN	Chemical Reactor Network
39	S <sub>G</sub>	Swirl number
40	d	Diameter
41	RANS	Reynolds-Averaged Navier-Stokes
42	FGM	Flamelet Generated Manifold
43	PDF	Probability Density Function
44	TFSC	Turbulent Flame Speed Closure
45	PSR	Perfectly Stirred Reactor
46	PFR	Plug Flow Reactor
47	CRZ	Central Recirculation Zone
48	ERZ	External Recirculation Zone
49	ROP	Rate of Production
50	ROC	Rate of Consumption

### 51 1. INTRODUCTION

52  
53 Renewably produced ammonia is considered a promising  
54 carbon-free energy vector due to its relative ease and low cost of  
55 storage and transportation compared to pure hydrogen [1].  
56 Although these advantages are even greater if pure ammonia is  
57 used directly as a fuel, there are combustion challenges relating  
58 to its low reactivity and NO<sub>x</sub> emissions [2,3].

59 Blending ammonia with other fuels to increase reactivity has  
60 been studied extensively. Mixing ammonia with methane or  
61 hydrogen has shown favourable improvements in burning  
62 velocity [4,5] and flammability limits [6]. Combustion with  
63 methane as part of the fuel will always result in carbon dioxide  
64 emissions, so mixing with hydrogen is the better option for  
65 decarbonisation. Furthermore, as ammonia has significant  
66 hydrogen content of ~18% on a mass basis [7], an

1 ammonia/hydrogen fuel blend can be achieved by partially  
2 cracking the ammonia immediately prior to combustion [8]. This  
3 has the added benefit of reducing cost by having to store only  
4 one fuel.

5 Numerous studies have also investigated NO<sub>x</sub> mitigation  
6 strategies from ammonia/hydrogen fuel blends. Mashruk et al.  
7 demonstrated the NO<sub>x</sub> emission dependence on ratio of ammonia  
8 to hydrogen [9], and the strong unimodal relationship between  
9 global equivalence ratio ( $\Phi_G$ ) and NO emissions, with a peak  
10 near  $\Phi_G = 0.9$  [6]. These studies noted that negligible NO<sub>x</sub>  
11 emissions could be achieved at  $\Phi_G = 1.2-1.3$  due to NO  
12 consumption by NH<sub>2</sub> but resulted in significant unburned NH<sub>3</sub>  
13 emissions due to a decrease in the availability of H, O and OH  
14 radicals. They also showed significant N<sub>2</sub>O emissions at lean  
15 conditions ( $\Phi_G < 0.8$ ) due to a reduction in flame temperature  
16 inhibiting N<sub>2</sub>O consumption by free H atoms and shorter flames  
17 reducing residence time for the third-body reaction to act in  
18 [10,11,12]. N<sub>2</sub>O is an important exhaust gas to monitor as it has  
19 a global warming potential roughly 250 times larger than carbon  
20 dioxide, meaning a flame with no CO<sub>2</sub> emissions but around  
21 240ppm N<sub>2</sub>O would have a similar global warming effect to a  
22 methane-air flame, as calculated in [13].

23 Recently, partially premixed ammonia/hydrogen  
24 combustion has received considerable attention to further reduce  
25 NO emissions. An NH<sub>3</sub>/H<sub>2</sub> partially premixed concept was  
26 initially proposed and examined by Pugh et al. [14] at rich  
27 conditions. A diffusive flow of either NH<sub>3</sub> or H<sub>2</sub> was injected  
28 through a central lance with the main aim of creating local fuel-  
29 rich regions in the middle of the reaction zone. This resulted in a  
30 reduction in NO emissions but significant unburned NH<sub>3</sub>  
31 emissions were recorded. This study also examined the effect of  
32 elevated inlet pressures and temperatures more relevant to gas  
33 turbine conditions and reported an increase in NO emissions,  
34 particularly at rich conditions. As this is a complex  
35 nonmonotonic relationship depending on multiple variables, any  
36 kinetic mechanism selected for predicting emissions from  
37 pressurised stratified flames would require careful testing and  
38 validation. Franco et al. [15] proposed an alternative  
39 configuration for NH<sub>3</sub>/H<sub>2</sub> flames, using two co-axial tubes,  
40 injecting fuel axially through the inner tube and air tangentially  
41 through the outer tube via a bluff body. However, the results  
42 presented by Franco et al. [15] did not deliver details of unburned  
43 ammonia, thus requiring further investigations. Mashruk et al.  
44 [16] recently presented a novel stratified combustion system that  
45 can operate in both premixed and stratified modes using  
46 ammonia/hydrogen blends. They observed that an increase in  
47 hydrogen stratification resulted in a reduction of NO and NO<sub>2</sub>  
48 emissions, but increased N<sub>2</sub>O because of the reduced fuel in the  
49 premixed flow. It should be noted that the above works used only  
50 blends of ammonia, hydrogen and air, neglecting the nitrogen  
51 produced alongside the hydrogen in the cracking process.

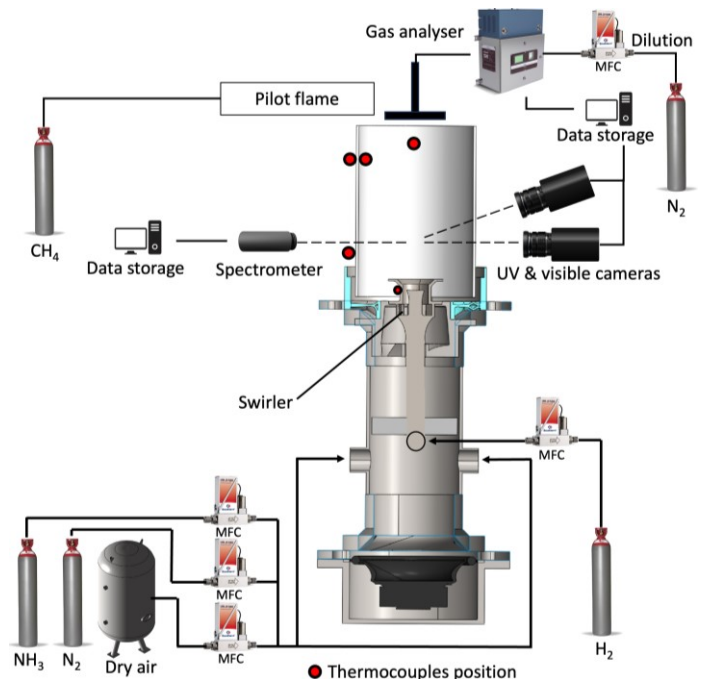
52 The current work builds upon previous investigations by  
53 studying the influence of stratification in NH<sub>3</sub>/H<sub>2</sub>/N<sub>2</sub> flames  
54 utilising the same burner described by Mashruk et al. [16] at  
55 Cardiff University. Initially the premixed flow was maintained  
56 as a 20%<sub>(vol.)</sub> cracked ammonia blend and extra diffusive

57 hydrogen was added to the stratified flow to preserve two set  
58 diffusive equivalence ratios ( $\Phi_D$ ), whilst varying the global  
59 equivalence ratio ( $\Phi_G$ ). Additionally, a numerical study using the  
60 CFD-CRN approach enabled a rate of production analysis to be  
61 carried out on the emissions results.

## 62 2. MATERIALS AND METHODS

63 This study assessed the NO<sub>x</sub> reduction capability of a  
64 recently commissioned burner system operating on a base blend  
65 of 20%<sub>(vol.)</sub> cracked ammonia ((66.7/25/8.3%<sub>(vol.)</sub> NH<sub>3</sub>/H<sub>2</sub>/N<sub>2</sub>).  
66 Extra diffusive H<sub>2</sub> was injected into the stratified flow with the  
67 aim of promoting NO<sub>x</sub> production, to aid in identifying  
68 mechanisms for NO<sub>x</sub> reduction. In Case 1 Stratified, the extra  
69 diffusive H<sub>2</sub> flow rate was set to maintain the central diffusion  
70 flame at a slightly lean equivalence ratio ( $\Phi_D = 0.9$ ), known to  
71 produce peak NO emissions. For Case 1 Premixed, the same  
72 extra H<sub>2</sub> was instead added to the premixed flow, to offer a direct  
73 comparison. The global equivalence ratio was then varied  $0.8 <$   
74  $\Phi_G < 1.12$ . Addition of extra diffusive H<sub>2</sub> slightly varied the fuel  
75 blend, but this change was mirrored in the premixed  
76 configuration so comparisons could be drawn. This process was  
77 repeated in Case 2, but with the central diffusion flame  
78 maintained at stoichiometry ( $\Phi_D = 1.0$ ) to increase flame  
79 temperature. As Case 2 had a richer diffusive flame, the global  
80 equivalence ratio could be increased further, allowing  $0.8 <$   
81  $\Phi_G < 1.2$  to be tested. As mentioned previously, operating at  
82 conditions leaner than  $\Phi_G = 0.8$  produces prohibitively high N<sub>2</sub>O  
83 emissions and so was not investigated here. All experiments  
84 were conducted at a constant thermal power of 10kW.

### 85 2.1 Swirl Combustor



86  
87 **FIGURE 1: SCHEMATIC OF THE EXPERIMENTAL SETUP (NOT TO SCALE).**

1 Experiments were conducted using an optically accessible  
 2 radial-tangential swirl combustor ( $S_g = 1.05$ ) shown in Figure 1  
 3 at atmospheric conditions (1.1 bar, and 288K).

4 Fuel and air were supplied using Bronkhorst mass flow  
 5 controllers ( $\pm 0.5\%$  between 15-95% of maximum flow). Figure  
 6 2 shows a diagram of the combustor architecture and flow paths.  
 7 When operating in fully premixed mode, all  $H_2$  was injected at  
 8 the base of the swirler, mixing with  $NH_3$ ,  $N_2$  and air before  
 9 flowing through the injector nozzle ( $d = 31.5\text{mm}$ ), using a central  
 10 injection lance ( $d = 22.5\text{mm}$ ) as a bluff body. In stratified mode,  
 11 the central injection lance was unblocked to allow some  $NH_3$ ,  $N_2$   
 12 and air through. Additionally, a portion of the  $H_2$  was injected  
 13 from the end of the central injection lance, ensuring the diffusion  
 14 flame was maintained at either  $\Phi_D = 0.9$  or 1.0 to promote  $NO_x$   
 15 production. The global equivalence ratio  $\Phi_G$  was calculated  
 16 relative to the stoichiometric air-fuel ratio (AFR) as ( $\Phi_G = \text{total}$   
 17  $AFR_{\text{stoichiometric}} / \text{total } AFR_{\text{actual}}$ ), including both premixed and  
 18 diffusive flows shown in Figure 2. The diffusive equivalence  
 19 ratio  $\Phi_D$  was calculated in the same manner but only considering  
 20 the flow through the central injector.

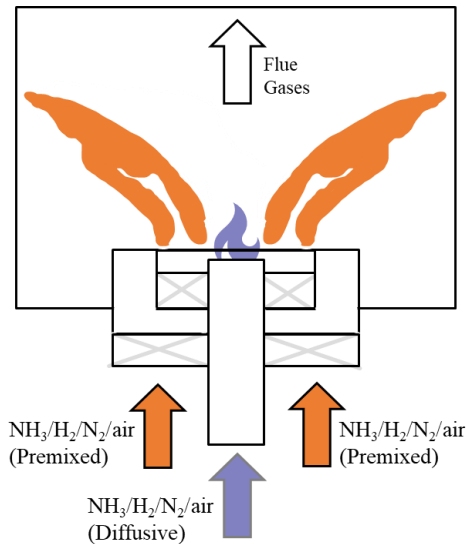


FIGURE 2: SIMPLIFIED DIAGRAM OF COMBUSTOR ARCHITECTURE.

21 To facilitate optical access for flame monitoring,  
 22 chemiluminescence imaging and spectrometry, the flame was  
 23 confined within a quartz glass tube ( $d = 156\text{mm}$ ). The flame was  
 24 monitored from a distance of 5m using a Logitech Brio camera.

## 2.2 Exhaust Gas Measurements

27  $NO$ ,  $NO_2$ ,  $N_2O$ ,  $NH_3$ ,  $O_2$  and  $H_2O$  were measured  
 28 simultaneously using an Emerson CT5100 quantum cascade  
 29 laser system. The cross-shaped sample probe with equidistant  
 30 holes for homogenous sample collection was situated 25mm  
 31 above the quartz tube outlet. Measured oxygen content was  
 32 negligible at stoichiometric conditions, indicating no outside air  
 33 was entrained into the sampling probe. The samples were carried  
 34 to the gas analyser via a heated line, with measurements

35 performed at 463K. For each condition, 120 samples were  
 36 captured with a sampling rate of 1Hz ( $\pm 1\%$  repeatability, 0.999  
 37 linearity), averaged, and normalised to dry 15%  $O_2$  following  
 38 equation 14 in [17]. Ongoing discussion surrounds this emission  
 39 normalisation method [18], due to elevated water content in the  
 40 exhaust of hydrogen-based fuels inflating dry ppmv values.  
 41 However, as this paper focuses solely on cracked ammonia as a  
 42 fuel, and no direct comparisons were drawn with carbon-based  
 43 fuel, this method was deemed acceptable. For conditions where  
 44 raw readings were above the analysers range,  $N_2$  dilution was  
 45 used ( $\pm 10\%$  repeatability), as explained in detail in [11].

## 2.3 Chemiluminescence Measurements

48  $OH^*$  (309nm;  $A^2\Sigma-X^2\Pi$  system),  $NH^*$  (336nm  $A^3\Pi-X^2\Sigma$   
 49 system) and  $NH_2^*$  (630nm; single peak of  $NH_2$   $\alpha$  band) images  
 50 were captured simultaneously by multiple LaVision cameras  
 51 each with a Sony ICX285AL sensor and Hamamatsu HB105831  
 52 intensifier and appropriate Edmund Optics bandpass filters as in  
 53 [11]. The cameras recorded at a sampling frequency of 10Hz for  
 54 a period of 20 seconds and the captured images were background  
 55 corrected, 3x3 median filtered and averaged in Davis v10. The  
 56 averaged chemiluminescence images then went through an Abel  
 57 Deconvolution script in Matlab [19]. In this study, a positive  
 58 correlation between ground state and excited radicals is assumed,  
 59 as in [14,20].

60 An Avaspec-ULS4096CL spectrometer was used to capture  
 61 broadband chemiluminescence intensity for a wide range of  
 62 wavelengths, from 200-1100nm. It featured a 100 $\mu\text{m}$  slit and a  
 63 300 lines/mm grating, resulting in a full width half maximum  
 64 resolution of 4.6nm. The spectrometer specified a 4096-pixel  
 65 CMOS detector measuring 7 x 200 $\mu\text{m}$ , set to an exposure time  
 66 of 1 second and averaged over 120 scans to improve the signal  
 67 to noise ratio. Via a 600 $\mu\text{m}$  fibre optic cable, it was connected to  
 68 a collimating lens for UV and visible light, mounted 30mm  
 69 above the burner outlet and 240mm away from the central axis.

## 2.4 Pressure and Temperature Measurements

72 A water-cooled Kistler 211B6 pressure transducer mounted  
 73 in the combustion chamber near the burner exit was used to  
 74 measure combustor dynamics. Pressure fluctuations were  
 75 measured at a sampling rate of 25kHz for a period of 20 seconds  
 76 and then Fourier Transformed using a Matlab script for analysis.

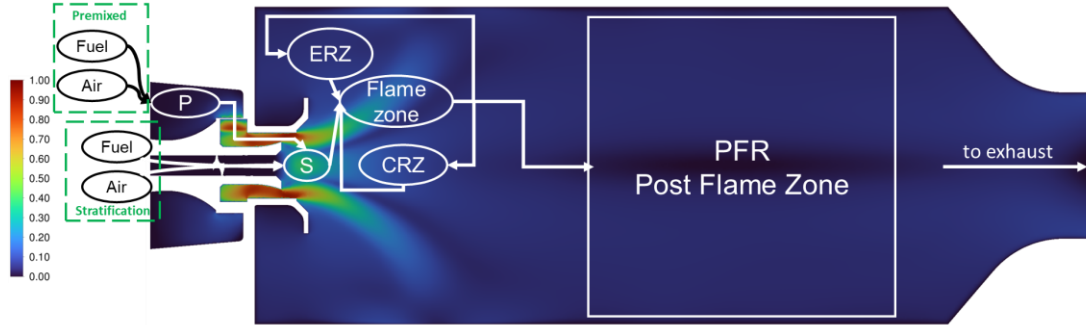
77 The red dots in Figure 1 denote positions of R and K type  
 78 thermocouples which had sampling rates of 1Hz and were  
 79 averaged over a two-minute period for each operating condition.

## 2.5 CFD-CRN approach

82 The combination of Computational Fluid Dynamics (CFD)  
 83 and Chemical Reactor Networks (CRNs) allows for the precise  
 84 configuration of CRNs by discretising volumes accurately. This  
 85 method is commonly used in analysing complex combustion  
 86 processes like those in gas turbines [21] with relatively low  
 87 computational cost and short processing times.

88 In this research, the CFD-CRN approach was applied to  
 89 simulate and analyse the ammonia/hydrogen/nitrogen  
 90 combustion. First, CFD was used to simulate a single test case,





**FIGURE 3:** NORMALISED VELOCITY FIELD PREDICTED BY CFD SIMULATION. VOLUME DISCRETISATION AND ZONE DIVISION FOR CRN ANALYSIS.

1 obtaining temperature and velocity fields being crucial for  
 2 defining different zones in the experimental setup. CRN  
 3 numerical simulations of the flame were carried out using  
 4 CHEMKIN-PRO. The CFD simulation was set up in ANSYS  
 5 Fluent 2R2 using the Reynolds-Averaged Navier-Stokes  
 6 (RANS) approach, to simulate one of the test points in the  
 7 experimental campaign. A previous study [22] demonstrates that  
 8 surrogate models can accurately predict  $\text{NO}_x$  emissions,  
 9 temperature, and velocity fields. In this work, the burner's  
 10 geometry is modelled using a three-dimensional (3D)  
 11 computational domain, comprising a total of 6M polyhedral  
 12 cells. The Realizable  $k-\epsilon$  model with an enhanced wall function  
 13 was the selected turbulence model. The Partially Premixed  
 14 Combustion Model was implemented with the Flamelet  
 15 Generated Manifold (FGM) approach [23]. The flamelets were  
 16 carried out in Ansys Fluent, while the turbulence-chemistry  
 17 interaction involved pre-integrating the look-up table with a  $\beta$ -  
 18 PDF. The chemical kinetics from Otomo et al. [24] for the  
 19 oxidation of ammonia-hydrogen flames, comprising 33 species  
 20 and 213 reactions, was chosen for finite chemistry calculation.  
 21 Zimont's Turbulent Flame Speed Closure (TFSC) [25] modelled  
 22 the source term for the progress variable, defined as  $c = Y_c/Y_{eq}$ ,  
 23 where  $Y_c = Y_{\text{NO}} + Y_{\text{N}_2} + Y_{\text{H}_2\text{O}} - Y_{\text{H}_2}$ , and  $Y_{eq}$  is its  
 24 equilibrium value. The laminar flame speeds included in the  
 25 FGM combustion model were generated natively within Ansys  
 26 Fluent after the boundary conditions were set and 1-D flamelets  
 27 calculated. These laminar flame speeds were verified in  
 28 CHEMKIN-PRO using the axisymmetric opposed-flow  
 29 diffusion flame model by varying the equivalence ratio to  
 30 account for the wide ranging degree of premixing present in a  
 31 stratified flame. Figure 3 displays the axial velocity field with  
 32 zone subdivisions characterising the Chemical Reactor Network

33 (CRN). Four inlets of air,  $\text{NH}_3$ ,  $\text{H}_2$  and  $\text{N}_2$  were used to feed two  
 34 Perfectly Stirred Reactors (PSRs) considering Premixed (P) and  
 35 Stratified (S) sections, respectively. Additionally, a PSR for the  
 36 Flame zone and other two PSRs for Central Recirculation Zone  
 37 (CRZ) and External Recirculation Zone (ERZ) were included.  
 38 One Plug Flow Reactor (PFR) represented the flow zone where  
 39 the velocity was completely axial. To validate temperature trends  
 40 within the PSRs and PFR reactors in the CRN, a thermal analysis  
 41 was carried out; Figure 4 shows the temperature field derived  
 42 from CFD analysis. To determine the role of various reactions in  
 43 changing NO emissions with stratification, absolute rate of  
 44 production (ROP) values were calculated within the flame zone.  
 45 The rate of consumption (ROC) is presented as a negative ROP,  
 46 consistent with other studies [12]. Estimations of necessary heat  
 47 loss were obtained from thermocouple measurements, located in  
 48 appropriate positions in the burner.

### 3. RESULTS AND DISCUSSION

#### 3.1 Effect of Stratification on Emissions

54 In Case 1 Stratified, extra diffusive  $\text{H}_2$  was injected into the  
 55 stratified flow to maintain  $\Phi_D = 0.9$  to promote NO production.  
 56 It was compared to Case 1 Premixed, where the extra diffusive  
 57  $\text{H}_2$  was injected into the premixed flow.

58 The order of magnitude reduction in NO emissions seen in  
 59 Figure 5 from Case 1 Stratified at  $\Phi_G = 1.05$  can be explained by  
 60 two main mechanisms, a reduction in NH and OH production  
 61 and an increase in NO consumption by  $\text{NH}_2$ . HNO is an  
 62 intermediary radical which can be formed from NH and OH  
 63 radicals via the reaction shown in Equation 1.



66

67

68 Figure 6 demonstrates the reduction in NO production for  
 69 Case 1 Stratified via HNO radicals, as well as from OH radicals  
 70 directly via Equation 2. Again, assuming a positive correlation  
 71 between ground state and excited radicals, these numerical  
 results were validated by the chemiluminescence images shown



**FIGURE 4:** NORMALISED TEMPERATURE DISTRIBUTION PREDICTED BY CFD SIMULATION.

1 in Figure 7. OH\* intensity was found to be similar, but over a  
 2 smaller flame volume, supporting lower NO production from  
 3 routes consuming OH and HNO. Although OH\* intensity can be  
 4 directly correlated with changes in temperature, Figure 8 shows  
 5 only small differences between the two configurations in the post  
 6 flame zone.

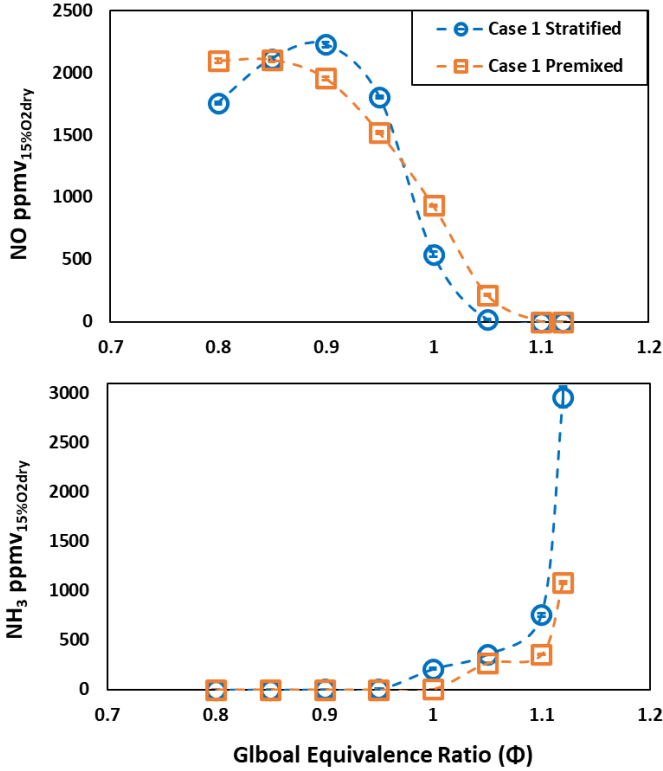


FIGURE 5: MEASURED EMISSIONS FROM CASE 1 WITH CHANGING GLOBAL EQUIVALENCE RATIO. NO (TOP) AND NH<sub>3</sub> (BOTTOM). (BEST-FIT LINES FOR CLARITY RATHER THAN MODELLED DATA).

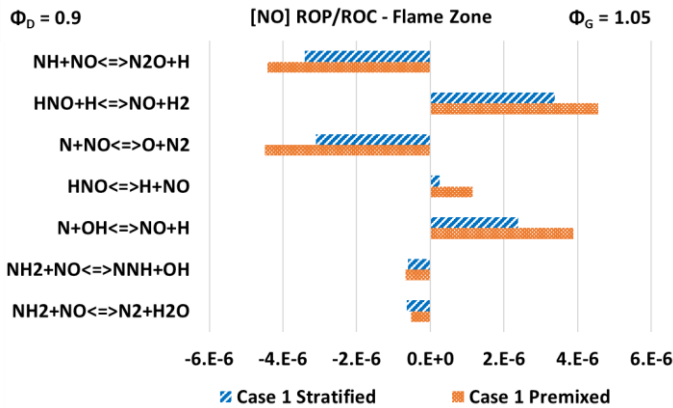


FIGURE 6: FLAME ZONE ABSOLUTE ROP/ROC [UNIT - MOLE/CM<sup>3</sup>-SEC] FOR THE MOST SIGNIFICANT NO REACTIONS AT Φ<sub>G</sub> = 1.05 FOR CASE 1 STRATIFIED (BLUE) AND PREMIXED (ORANGE)

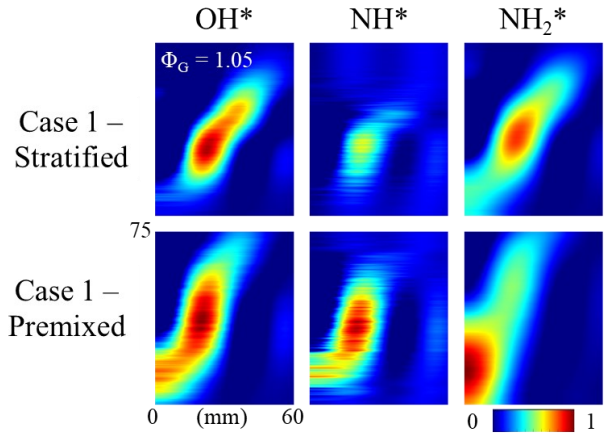


FIGURE 7: ABEL TRANSFORMED CHEMILUMINESCENCE IMAGES (OH\*, NH\* AND NH<sub>2</sub>\*) OF CASE 1 STRATIFIED (TOP) AND PREMIXED (BOTTOM) AT Φ<sub>G</sub> = 1.05. EACH SPECIES NORMALISED TO ITS CASE 1 Φ<sub>G</sub> = 1.05 MAXIMUM.

7 NH\* intensity was significantly lower in Case 1 Stratified,  
 8 again supporting lower NO production from routes consuming  
 9 HNO. Compared to Case 1 Premixed, the stratified configuration  
 10 showed less NO consumption by NH via the reaction shown in  
 11 Equation 3, which would also suggest a reduction in N<sub>2</sub>O  
 12 emissions. Consistent with previous studies [9,12] most  
 13 conditions produced negligible N<sub>2</sub>O emissions due to the  
 14 relatively high equivalence ratios examined here, and so N<sub>2</sub>O  
 15 was not plotted for brevity. However, at the leanest global  
 16 equivalence ratio investigated (Φ<sub>G</sub> = 0.8), single digit ppmv  
 17 (15% O<sub>2</sub> dry) N<sub>2</sub>O values were measured for both Case 1  
 18 configurations, and the Stratified N<sub>2</sub>O value was lower, further  
 19 indicating the accuracy of the numerical investigation. NO<sub>2</sub>  
 20 emissions followed the same general trend as NO and so were  
 21 not plotted for brevity. The peak of 70ppmv (15% O<sub>2</sub> dry) NO<sub>2</sub>  
 22 was found at the leanest conditions measured, with Case 1  
 23 Stratified slightly lower and both configurations reaching  
 24 negligible readings by Φ<sub>G</sub> = 1.0.

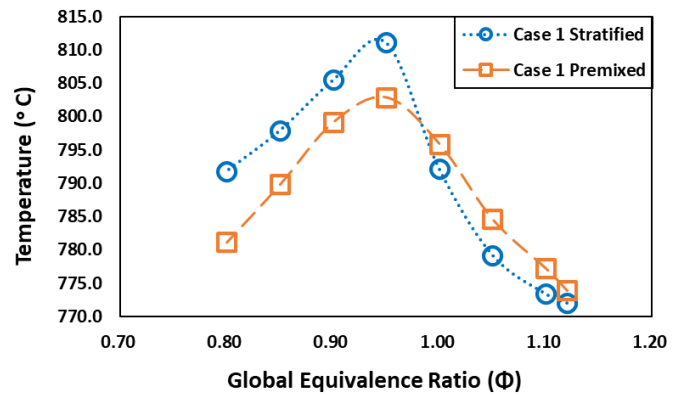
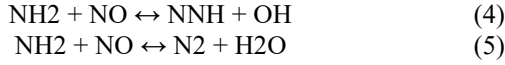


FIGURE 8: TEMPERATURE READINGS FROM A THERMOCOUPLE LOCATED IN THE CENTRE OF THE QUARTZ CONFINEMENT 50MM UPSTREAM OF THE OUTLET FOR CASE 1

1 The other mechanism by which Case 1 Stratified had lower  
 2 NO emissions than Case 1 Premixed above stoichiometry was an  
 3 increase in NO consumption by NH<sub>2</sub>, from the reactions in  
 4 Equations 4 and 5.



6 These reactions do not immediately appear significant in  
 7 Figure 6 until their contribution to the total NO consumption is  
 8 considered. For Case 1, the contribution of these reactions was  
 9 35% larger in the stratified flame than in the premixed flame.  
 10 Figure 7 shows Case 1 Stratified had slightly lower NH<sub>2</sub>\*  
 11 intensity, centred farther away from the burner nozzle than Case  
 12 1 Premixed. This suggests less NH<sub>2</sub> was produced in the locally  
 13 lean ( $\Phi_D = 0.9$ ) area near the central injector and was instead  
 14 produced further downstream where the local equivalence ratio  
 15 was more rich. This more spatially dispersed NH<sub>2</sub> would then  
 16 have a longer residence time to consume NO produced in the  
 17 area near the central injector and be available to consume NO in  
 18 the ERZ.

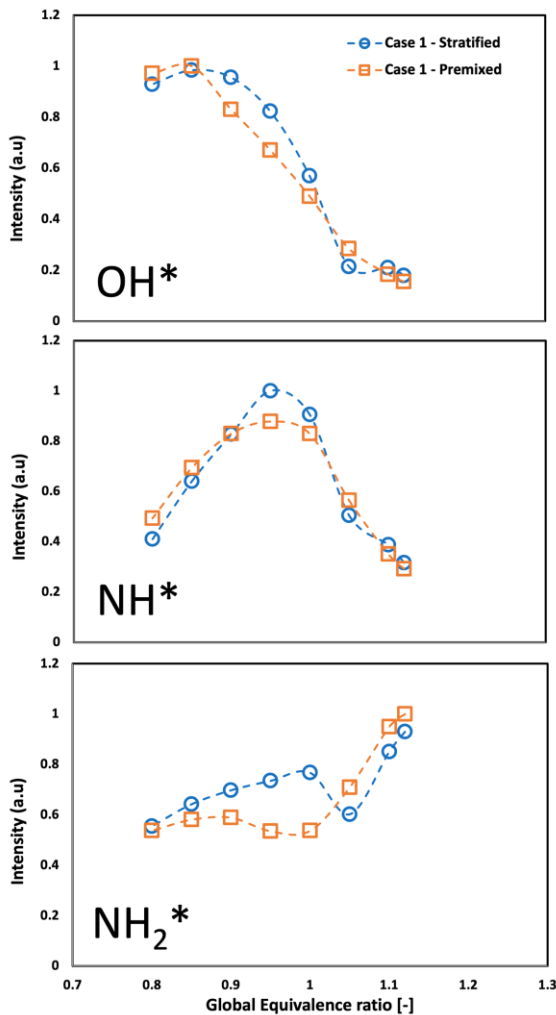


FIGURE 9: NORMALISED OPTICAL CHEMILUMINESCENCE SPECTROMETRY RESULTS FOR OH\*, NH\* AND NH<sub>2</sub>\*

20 Also shown in Figure 6, the thermal NO reactions of  
 21 Equations 2 and 6 were slightly less significant in the stratified  
 22 configuration than premixed for Case 1 at  $\Phi_G = 1.05$ . This small  
 23 reduction in significance of thermal NO reactions is reflected in  
 24 the small reduction in temperature for the stratified configuration  
 25 at rich conditions shown in Figure 8.



29 Unburned NH<sub>3</sub> emissions have previously been shown [26]  
 30 to increase between  $0.8 < \Phi_G < 1.2$  in fully premixed NH<sub>3</sub>/H<sub>2</sub>  
 31 flames due to reduced availability of OH radicals. This can  
 32 explain the increase in NH<sub>3</sub> emissions shown in Figure 5 for Case  
 33 1 Stratified. Figure 7 does demonstrate a reduction in OH\*  
 34 intensity compared to Case 1 Premixed, but it is more clearly  
 35 shown by the normalised chemiluminescence spectra intensity in  
 36 Figure 9 at  $\Phi_G = 1.05$ .

37 The approximately 15% increase in NO emissions from  
 38 Case 1 Stratified shown in Figure 5 at slightly lean conditions  
 39 can be attributed to the change in NH and OH production,  
 40 consistent with when  $\Phi_G = 1.05$ . However, the role of NH<sub>2</sub> in  
 41 consuming NO was diminished, as expected from the lower  
 42 NH<sub>2</sub>\* intensity at lean conditions shown in Figure 9. There was  
 43 a smaller difference in NO emissions between the two  
 44 configurations at lean conditions, which is reflected in Figure 10.  
 45 However, some differences can still be seen. For example, both  
 46 HNO and OH consumption to form NO were increased for Case  
 47 1 Stratified. Chemiluminescence data in Figures 9 and 11  
 48 support these numerical results by showing higher OH\* intensity  
 49 at  $\Phi_G = 0.9$ . Figure 10 also shows the reduced significance of  
 50 NH<sub>2</sub> in the NO consuming Equations 4 and 5, as there was less  
 51 NH<sub>2</sub> available to be consumed in these reactions at globally lean  
 52 conditions, compared to the globally rich conditions.

53

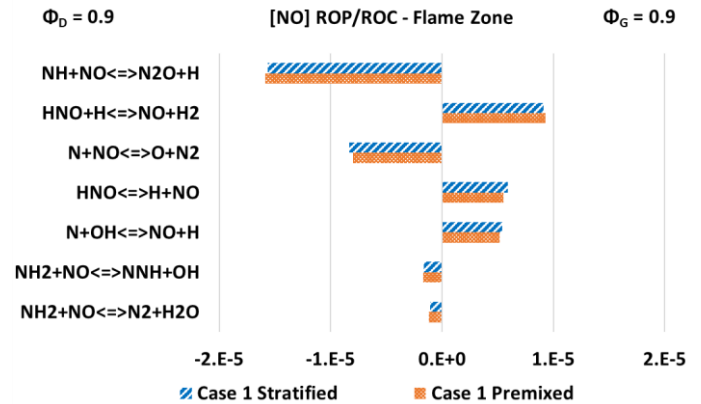
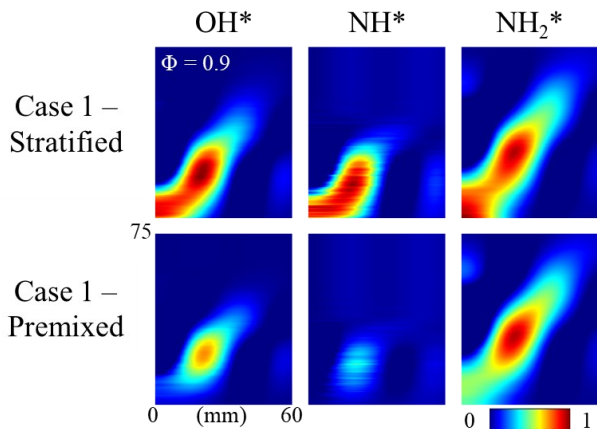


FIGURE 10: FLAME ZONE ABSOLUTE ROP/ROC [UNIT – MOLE/CM<sup>3</sup>·SEC] FOR THE MOST SIGNIFICANT NO REACTIONS AT  $\Phi_G = 0.9$  FOR CASE 1 STRATIFIED (BLUE) AND PREMIXED (ORANGE)

54

55



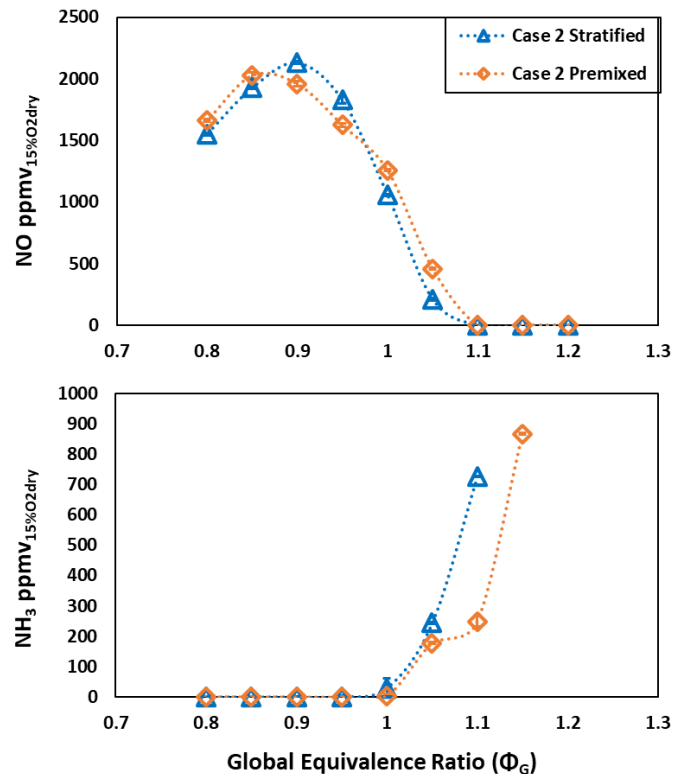
**FIGURE 11:** ABEL TRANSFORMED CHEMILUMINESCENCE IMAGES ( $\text{OH}^*$ ,  $\text{NH}^*$  AND  $\text{NH}_2^*$ ) OF CASE 1 STRATIFIED (TOP) AND PREMIXED (BOTTOM) AT  $\Phi_G = 0.9$ . EACH SPECIES NORMALISED TO ITS CASE 1  $\Phi_G = 0.9$  MAXIMUM

1 Studies have shown that heat loss from the flame to the  
 2 confinement walls can have a significant influence on emissions  
 3 from ammonia flames, with wall quenching reducing NO  
 4 emissions, but increasing  $\text{N}_2\text{O}$  and  $\text{NH}_3$  emissions [27]. This is  
 5 not the case in this study, demonstrated by two main reasons.  
 6 First, Figures 7 and 11 show that although stratification did  
 7 change the flame morphology, neither configuration caused the  
 8 flame to impinge on the quartz glass confinement. The right-side  
 9 edge of each chemiluminescence image is 60mm from the  
 10 centreline of the flame, and the quartz tube is 18mm beyond that.  
 11 The emissions data provides the second reason. Okafor et al. [27]  
 12 reported  $\text{N}_2\text{O}$  and  $\text{NH}_3$  emissions of 580ppmv and 4457ppmv at  
 13  $\Phi_G = 0.8$ . Although this was from a pure ammonia flame and so  
 14 not directly comparable to the current study, the fundamentals of  
 15 ammonia combustion do apply. That is, emissions of unburned  
 16 fuel at lean equivalence ratios represents a reduced combustion  
 17 efficiency from excessive heat loss from the flame. That is not  
 18 the case in the present study, proven by the negligible emissions  
 19 of  $\text{NH}_3$  at all conditions below stoichiometry, and the negligible  
 20 or single digit ppmv emissions of  $\text{N}_2\text{O}$  at all conditions.

21 Both configurations in Case 1 reached negligible NOx  
 22 emissions at a global equivalence ratio of 1.1, which is leaner  
 23 than for  $\text{NH}_3/\text{H}_2$  flames reported previously [9]. This is likely  
 24 due to the  $\text{N}_2$  present in the cracked ammonia fuel included in  
 25 this study reducing reactivity and combustion efficiency. The  
 26 combined emissions profile of Case 1 Stratified is particularly  
 27 interesting at  $\Phi_G = 1.05$ . Here, relatively low NO and  $\text{NH}_3$   
 28 emissions of 20 and 358 ppmv (15%  $\text{O}_2$  dry), respectively were  
 29 found. This was an order of magnitude reduction in NO  
 30 emissions with only a 33% increase in  $\text{NH}_3$  emissions compared  
 31 to the fully premixed configuration with the same total flow  
 32 rates. In summary, this reduction in NO was a result of a  
 33 reduction in NO production from OH and NH radicals, paired  
 34 with an increase in NO consumption by  $\text{NH}_2$ . Lesser availability  
 35 of OH radicals also resulted in an increase in unburned  $\text{NH}_3$   
 36 emissions.

### 3.2. Effect of Varying Diffusive Equivalence Ratio

37 To investigate the effect of different central diffusion  
 38 equivalence ratios,  $\Phi_D$  was increased from 0.9 in Case 1, to 1.0  
 39 in Case 2. As in the previous section, the extra diffusive  $\text{H}_2$   
 40 injected centrally in the stratified configuration was then injected  
 41 into the premixed flow to provide baseline emissions for this fuel  
 42 blend. As Case 1 had slightly different total flowrates to Case 2,  
 43 the stratified configurations from each Case cannot be compared  
 44 directly. It is however useful to compare the stratified  
 45 configurations' relative difference from their respective  
 46 premixed configurations.



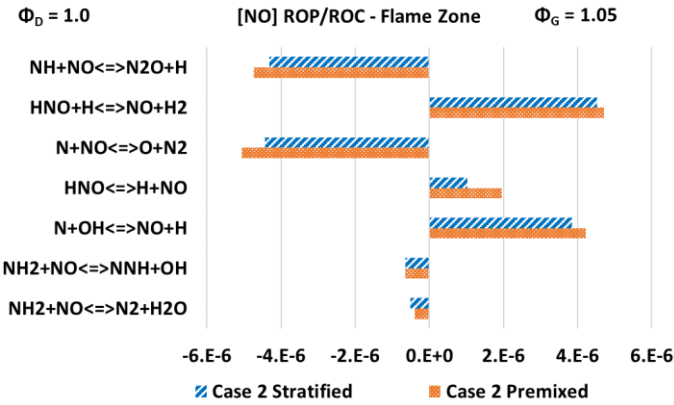
**FIGURE 12:** MEASURED EMISSIONS FROM CASE 2 WITH CHANGING GLOBAL EQUIVALENCE RATIO. NO (TOP) AND  $\text{NH}_3$  (BOTTOM). OUT OF RANGE  $\text{NH}_3$  AT RICH CONDITIONS NOT PLOTTED. (BEST-FIT LINES FOR CLARITY RATHER THAN MODELLED DATA).

48 Figure 12 shows that for Case 2, stratification with the  
 49 diffusive flame maintained at a more rich equivalence ratio of  
 50  $\Phi_D = 1.0$  was less effective in reducing NO emissions than the  
 51  $\Phi_D = 0.9$  in Case 1. At  $\Phi_G = 1.05$ , Case 2 Stratified had NO  
 52 emissions roughly half that of the Case 2 Premixed, but 37%  
 53 higher unburned  $\text{NH}_3$ , a poorer trade-off than found in Case 1.  
 54 This was a significant difference from a relatively small change  
 55 in flow rates, so numerical simulations were performed to clarify  
 56 the mechanisms responsible, which were then compared with  
 57 chemiluminescent data again assuming a positive correlation  
 58 between the ground state and excited radicals. Figure 13 shows  
 59 the differences in ROP/ROC between Case 2 Stratified and  
 60 Premixed configurations was the same as for Case 1 in Figure 6,



1 but with smaller differences. This was expected as the  
 2 differences between NO emissions was smaller.

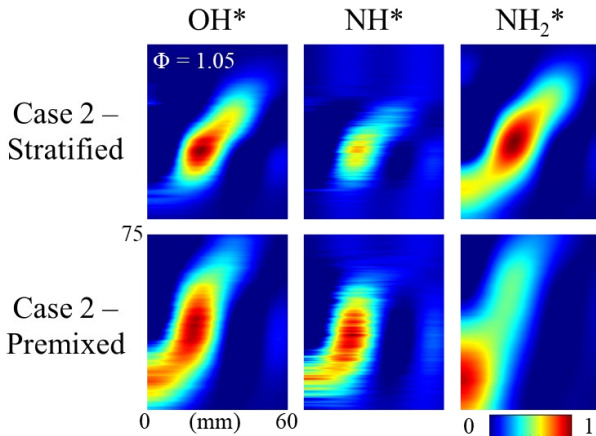
3



**FIGURE 13:** FLAME ZONE ABSOLUTE ROP/ROC [UNIT – MOLE/CM<sup>3</sup>-SEC] FOR THE MOST SIGNIFICANT NO REACTIONS AT  $\Phi_G = 1.05$  FOR CASE 2 STRATIFIED (BLUE) AND PREMIXED (ORANGE)

4

5 Figure 13 shows a smaller relative difference in the ROP  
 6 from reactions which consume HNO to form NO for Case 2  
 7 configurations. An explanation for this difference could be due  
 8 to the stoichiometric diffusive flame having a higher local flame  
 9 temperature near the central injector, increasing the availability  
 10 of free H atoms to react with HNO. As NH and OH combine to  
 11 form HNO via the reaction in Equation 1, a smaller difference in  
 12 OH\* and NH\* could be expected between the Case 2  
 13 configurations when compared to the Case 1 configurations. This  
 14 is demonstrated in Figure 14, where the NH\* in particular has a  
 15 similar intensity across the two configurations.

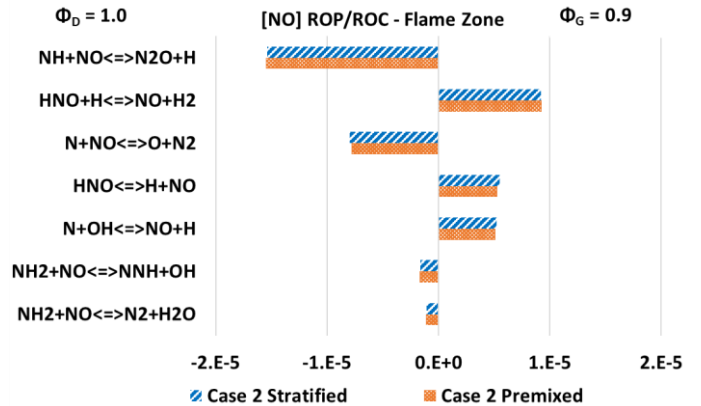


**FIGURE 14:** ABEL TRANSFORMED CHEMILUMINESCENCE IMAGES (OH\*, NH\* AND NH<sub>2</sub>\*) OF CASE 2 STRATIFIED (TOP) AND PREMIXED (BOTTOM) AT  $\Phi_G = 1.05$ . EACH SPECIES NORMALISED TO ITS CASE 2  $\Phi_G = 1.05$  MAXIMUM.

16 The other major difference shown in Figure 13 is the  
 17 smaller De-NOxing impact of the NH<sub>2</sub> radicals in Equations 4  
 18 and 5. In Case 1, the contribution of these reactions in the  
 19 stratified configuration was 35% larger than in the premixed  
 20 configuration, but only 22% larger in Case 2. The difference in  
 21 consumption of NH and NO from Equation 3 was similar for  
 22 both Cases. This reduction in NH<sub>2</sub> significance could relate to  
 23 the ratio of NO produced in the diffusive flame versus total NO  
 24 produced. The peak NO production was found at  $\Phi_G = 0.9$ ,  
 25 suggesting that Case 1 Stratified ( $\Phi_D = 0.9$ ) would produce more  
 26 NO in the diffusive flame than Case 2 Stratified ( $\Phi_G = 1.0$ ).  
 27 Compared to their respective premixed configurations, they  
 28 should produce the same total emissions due to their total fuel  
 29 and air flow rates being the same. However, Case 1 producing a  
 30 larger percentage of that total NO in the region near the central  
 31 injector would allow that NO more residence time to be  
 32 consumed by the NH<sub>2</sub>.

33 Figure 12 also shows a smaller increase in NO emissions at  
 34 the lean conditions for Case 2 Stratified than was found for Case  
 35 1 Stratified. This was reflected in the ROP/ROC plot shown in  
 36 Figure 15, where the only variation of significance was again in  
 37 the HNO decomposition reaction. As in Section 3.1, NO<sub>2</sub>  
 38 followed the same trend as NO. In Case 2, NO<sub>2</sub> peaked at a  
 39 slightly lower value of 64ppmv (15% O<sub>2</sub> dry) at  $\Phi_G = 0.8$  and  
 40 both configurations produced negligible readings at  $\Phi_G = 1.0$ .  
 41 N<sub>2</sub>O emissions were negligible at all equivalence ratios tested  
 42 and so neither are plotted here.

43



**FIGURE 15:** FLAME ZONE ABSOLUTE ROP/ROC [UNIT – MOLE/CM<sup>3</sup>-SEC] FOR THE MOST SIGNIFICANT NO REACTIONS AT  $\Phi_G = 0.9$  FOR CASE 2 STRATIFIED (BLUE) AND PREMIXED (ORANGE)

44

45 To summarise, the stoichiometric central diffusion flame in  
 46 Case 2 had a smaller effect on reducing NO emissions than the  
 47 slightly lean one presented in Case 1. This is likely related to the  
 48 stoichiometric diffusive flame having a locally higher  
 49 temperature, increasing the availability of free H atoms to react  
 50 with HNO and ultimately produce NO.

51

52

53

### 3.3. Effect of Stratification on Flame Stability

All tested configurations and conditions provided a stable flame, with no indication of lean or rich blowoff owing to all fuel blends being near stoichiometric. The dynamic pressure fluctuations within the quartz tube flame confinement were measured for all test conditions. However, as the same trends were observed for both Cases, only Case 1, which provided the best emissions performance is presented here.

Figure 16 shows the stratified configuration generally had lower RMS pressure fluctuations than the premixed configuration. The stratified case did not seem to possess the same sensitivity to equivalence ratio as the premixed and was comparatively constant at most test conditions.

It has been suggested that  $\text{NH}_2^*$  can be used as a heat release marker in ammonia-based flames [20]. Figures 7 and 14 showed that stratification had a strong effect on flame morphology, with the  $\text{NH}_2^*$  production being centred further downstream than in premixed configurations. This relocated centre of heat release could have changed the time delay and hence phase difference between the heat release fluctuations and pressure fluctuations to be out of phase, reducing the thermoacoustic instability in line with the Rayleigh Criterion [28]. The introduction of equivalence ratio fluctuations from stratification could also have affected the phase difference.

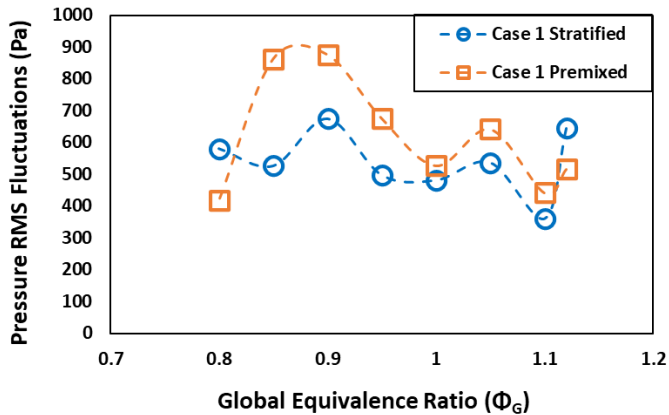


FIGURE 16: ROOT MEAN SQUARE FLUCTUATIONS IN COMBUSTOR PRESSURE WITH CHANGING GLOBAL EQUIVALENCE RATIO FOR CASE 1. (BEST-FIT LINES FOR CLARITY RATHER THAN MODELLED DATA).

Figure 17 shows the Fourier transformed pressure signal for the Case 1 test point with the best emissions performance ( $\Phi_G = 1.05$ ) above 50 Hz. Both configurations produced relatively high amplitude broadband combustion noise below 50 Hz of a similar magnitude, likely related to the injector geometry. There were however some significant differences at higher frequencies, so only those are presented and discussed here.

Both configurations experienced a significant pressure fluctuation at 95Hz and 251Hz, but stratification halved the amplitude when compared to the premixed configuration. Interestingly, the stratified configuration produced a peak at

around 430Hz which is not present in the premixed data. This newly excited instability could have been triggered by equivalence ratio fluctuations that a stratified flame experiences, as a premixed flame only experiences velocity fluctuations. These instabilities are too low frequency to be associated with the natural frequency of the combustor, which was calculated to be the broadband signature around 630Hz present in both configurations.

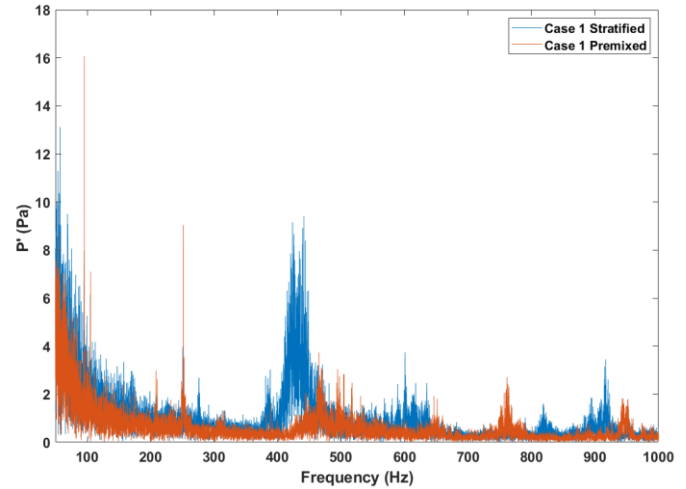


FIGURE 17: SPECTRAL COMPARISON OF CASE 1 STRATIFIED AND PREMIXED AT  $\Phi_G = 1.05$  ABOVE 50 HERTZ

### 4. CONCLUSIONS

The effect of supplying varying amounts of extra diffusive  $\text{H}_2$  to the stratified flow of a 20% cracked ammonia flame was investigated using a turbulent swirl burner, at a constant thermal power of 10kW. Chemiluminescence data and numerical simulations were used to interpret changing emissions trends.

At stoichiometric and rich equivalence ratios, stratified configurations increased consumption of NO by  $\text{NH}_2$ , and reduced NO production from OH and HNO reaction pathways. The reduced OH intensity also resulted in an increase in unburned  $\text{NH}_3$  emissions, which was offset by a significantly larger reduction in NO emissions. At slightly lean equivalence ratios, an increase in NO emissions was found, also due to changes in OH and NH production paired with diminished  $\text{NH}_2$  intensity consuming less NO. Negligible  $\text{N}_2\text{O}$  was measured at all conditions as expected.

Emissions showed a strong sensitivity to the equivalence ratio of the stratified flow, related to diffusive flame temperature and NO –  $\text{NH}_2$  residence times. Assuming an equal weighting for NO and unburned  $\text{NH}_3$  emissions, the case where the diffusive flame had a slightly lean equivalence ratio showed better combined emissions performance.

Both examined configurations exhibited stable combustion. Whilst stratification generally reduced the amplitude of pressure fluctuations within the combustion chamber, it did also trigger new instabilities at different frequencies to the premixed flame which need to be properly assessed in further analyses.

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10 of open access, the author has applied a CC BY public copyright  
11 licence to any Author Accepted Manuscript version arising.

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