Can Split Cycle Engine Architecture Optimise Ammonia Combustion?

Dr. Angad Panesar, Ms. Elisa Wylie (PhD Candidate), Dr. Steven Begg, Dr. Guillaume De Sercey

Advanced Engineering Centre
University of Brighton

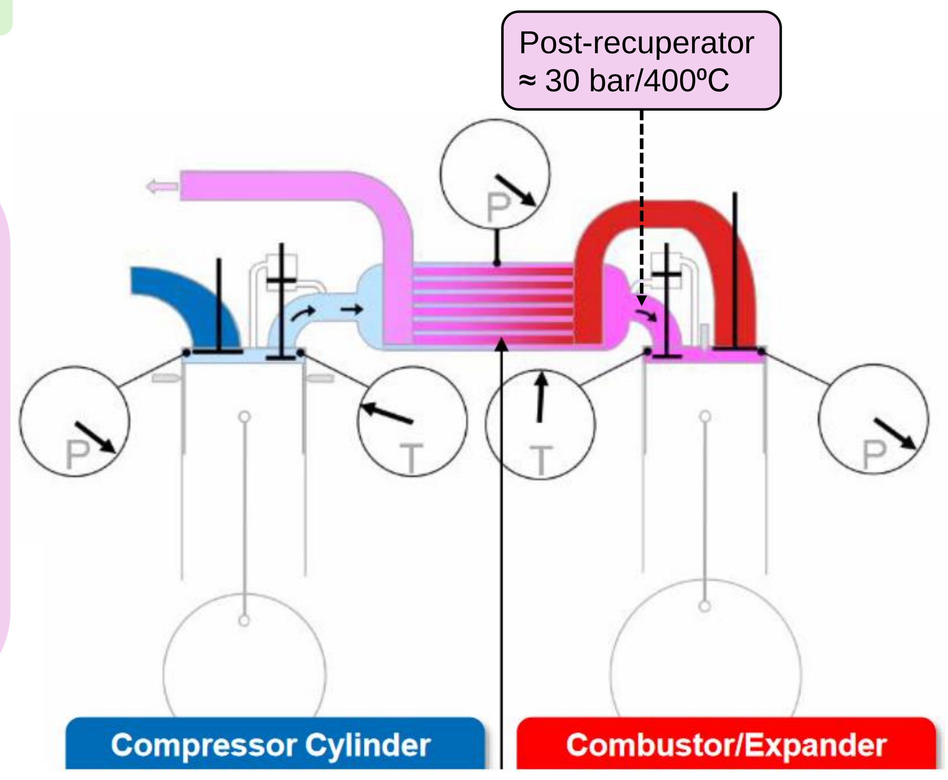
MariNH3 Clean, green ammonia engines for maritime

Scope of Research Study and Objective

Identify and quantify the feasibility of unique benefits for gaseous NH_3 homogeneous combustion in a split cycle engine architecture

Rational in Approach - Why NH_3? Why Split Cycle?

- NH_3 is carbon free with high H_2 density (17.8% wt.), infrastructure is established with production of ≈200 Mt/year [3], liq. NH_3 stores H_2 at higher densities than liq. H_2 (121 vs. 70.8 kg-H_2/m³ [3])
- NH_3 has a high autoignition temperature with narrow flammability range (13.3 - 17.1% lower flammability limit, LFL, to 25 - 39.4% upper flammability limit, UFL [1]), relatively low flame speed (0.15 m/s), is dangerous to health at > 300 ppm [3] and the nitrogen content may exacerbate NOx formation. Hence, combustion focused solution is crucial, maintaining an operating window that enables ignition, but minimises peak temperatures.
- Recuperated Split Cycle Engine (RSCE), post-recuperator temperature and pressures are ≈ 30 bar/400ºC, and NH_3 reaches bubble point at 77ºC [4]. Therefore, NH_3 could be stored as liq. (maximise energy density) and port-injected post-recuperator, where conditions enable vaporisation and energetic mixing, supporting development of homogeneous conditions.



Methods and Chemistry

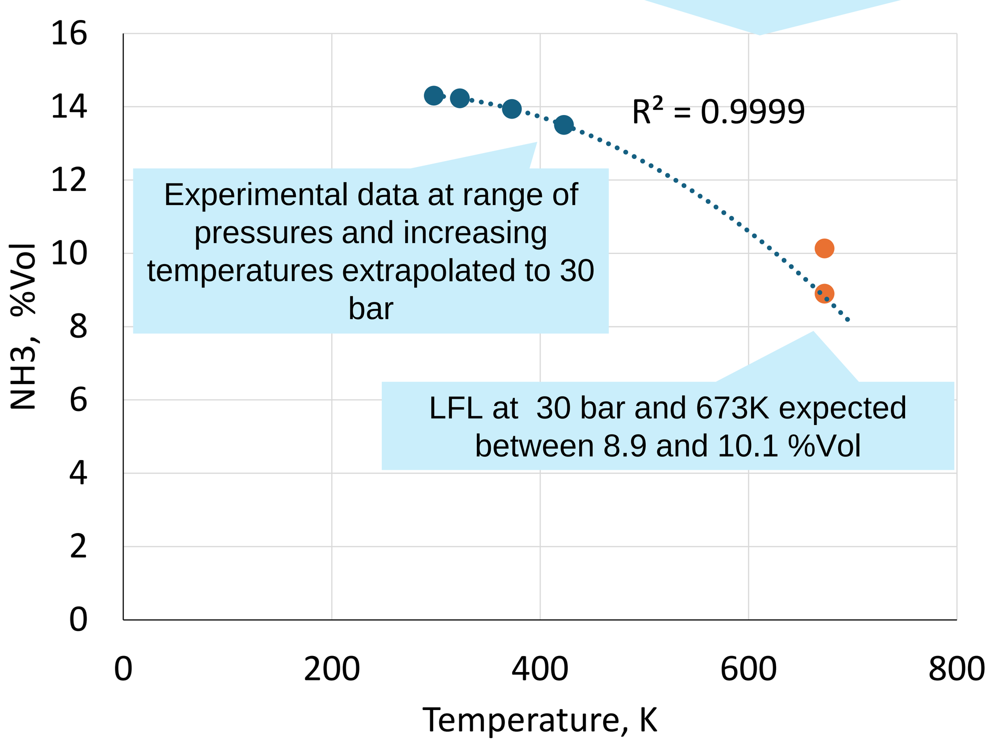
- Stage 1: Results are compared for combustion of CH_4 and $H_2$20% in a single cylinder spark ignition research engine (SCRE) and NH_3 in a digital twin of the SCRE and expander of RSCE (Chemkin-Pro Spark Ignition Engine Model - CSIE).
- Stage 2: Various NH_3 parameter studies were run in the CSIE model of the RSCE, including manifold temperature/pressure, intake valve closing (IVC) time and burn efficiency (BE). Each fuel was run at the leanest condition before combustion stability was compromised, where combustion efficiency was deteriorating in the SCRE, leading to increased unburnt fuel exhaust emissions and potential misfire (CH_4 ϕ=0.7374, $H_2$20% and NH_3 ϕ=0.64).

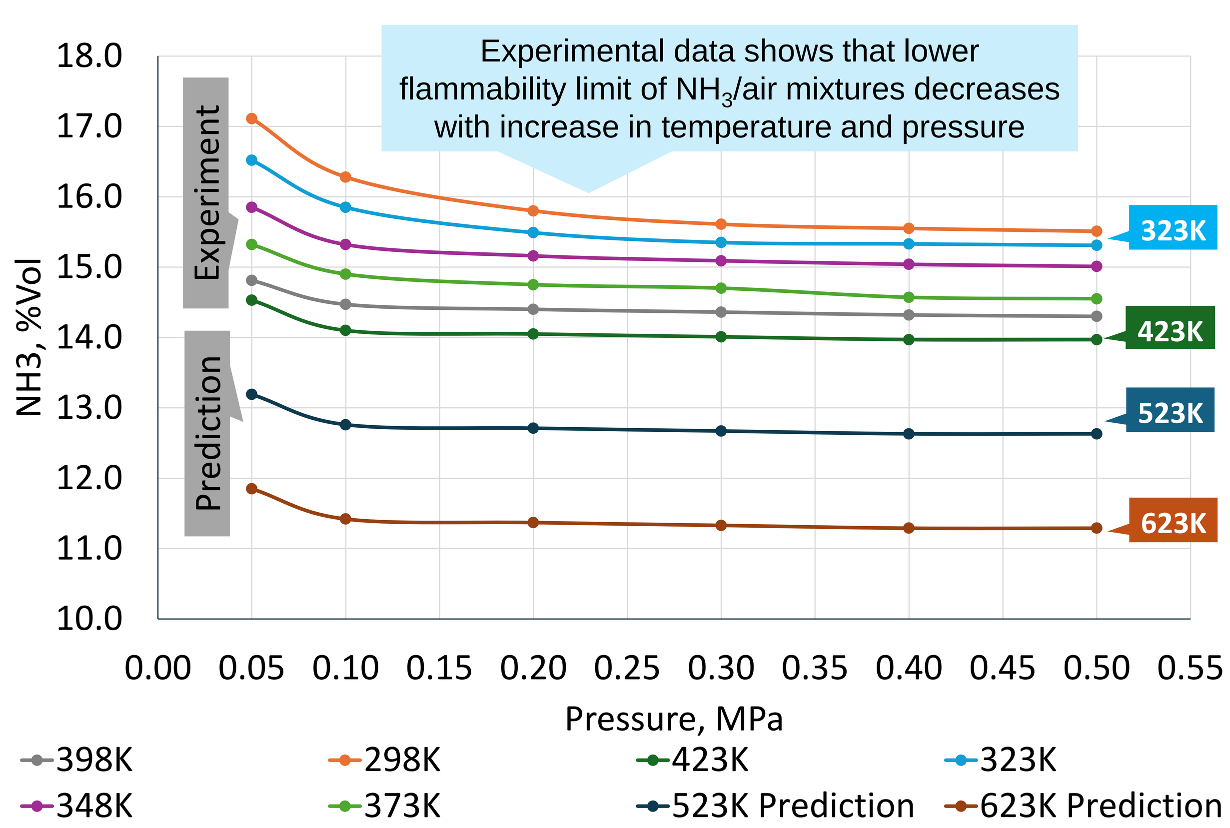
Chemkin Spark Ignition Engine Model, CSIE	
IVC (CA°)	-145
EVO (CA°)	143
Engine speed (rpm)	900
Engine compression ratio	12.6
Bore/Stroke (mm)	131/158
Swept volume (Litres)	2.13
Con- rod length (mm)	267.5
Con rod to Crank ratio	3.39
Woschni coefficients	C11 = 2.28, C12 = 0.308, C2 = 0.324
Dimensionless heat transfer coefficients	a = 0.035, b = 0.8, c = 0.33 [36]
Gas-Phase Kinetics and thermodynamics	GRI-Mech 3.0

Combustion of NH_3 at ϕ=0.64 can be represented by:

$$NH_3 + \frac{93}{80}\left(O_2 + \frac{94}{25}N_2\right) \rightarrow \frac{7}{500}NH_3 + \frac{69}{10000}NO_x + \frac{1479}{1000}H_2O + \frac{243}{50}N_2 + \frac{8353}{20000}O_2$$

Flammability limits of NH_3 widen with increase in temperature, varying linearly with temperature and logarithmically with pressure[1]. Extrapolation of recent experimental results [1] indicates a LFL of 12%Vol for NH_3/air mixtures at greater than 350 ºC, supported by previous experimental work that indicated 11.2%Vol for LFL at greater than 400 ºC [2], equating to an equivalence ratio of ≈ϕ0.45. The estimated %Vol NH_3 in this study is above its LFL in the tested conditions (14.6% vol at 400 ºC and ϕ=0.64). This means that it is theoretically possible to run at leaner mixes in the RSCE manifold conditions. However, NH_3 has an autoignition temperature of 854 ºC (without a catalyst), hence, whilst a flame could be sustained at this ϕ, spark is required for ignition at TDC conditions for both the RSCE and SCRE (400 ºC/40 bar and 451 ºC/45 bar respectively).





At concentrations near the LFL and at standard conditions consumption of NH_3 can follow the path shown by:

$$(1)\ H + O_2 \leftrightarrow O + OH$$

$$(2)\ NH_3 + OH \leftrightarrow NH_2 + H_2O \quad (3)\ 2OH \leftrightarrow O + H_2O \quad (4)\ NH_2 + OH \leftrightarrow NH + H_2O$$

$$(5)\ NH_2 + NO \leftrightarrow NNH + OH \quad (6)\ NH_2 + NO \leftrightarrow N_2 + H_2O$$

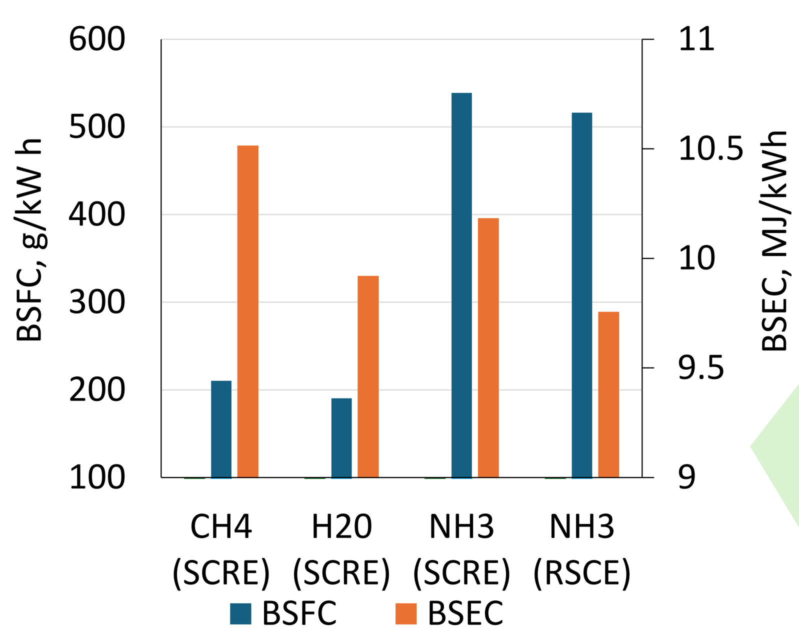
Where reactions (1) and (5) both increase flame temperatures, whilst (6) is the main inhibitor of temperature increase [1]. As pressure increases, (3) is replaced with (4), whist (7) competes with (1) and (8) for H species:

$$(7)\ H + O_2(+M) \leftrightarrow HO_2(+M)$$

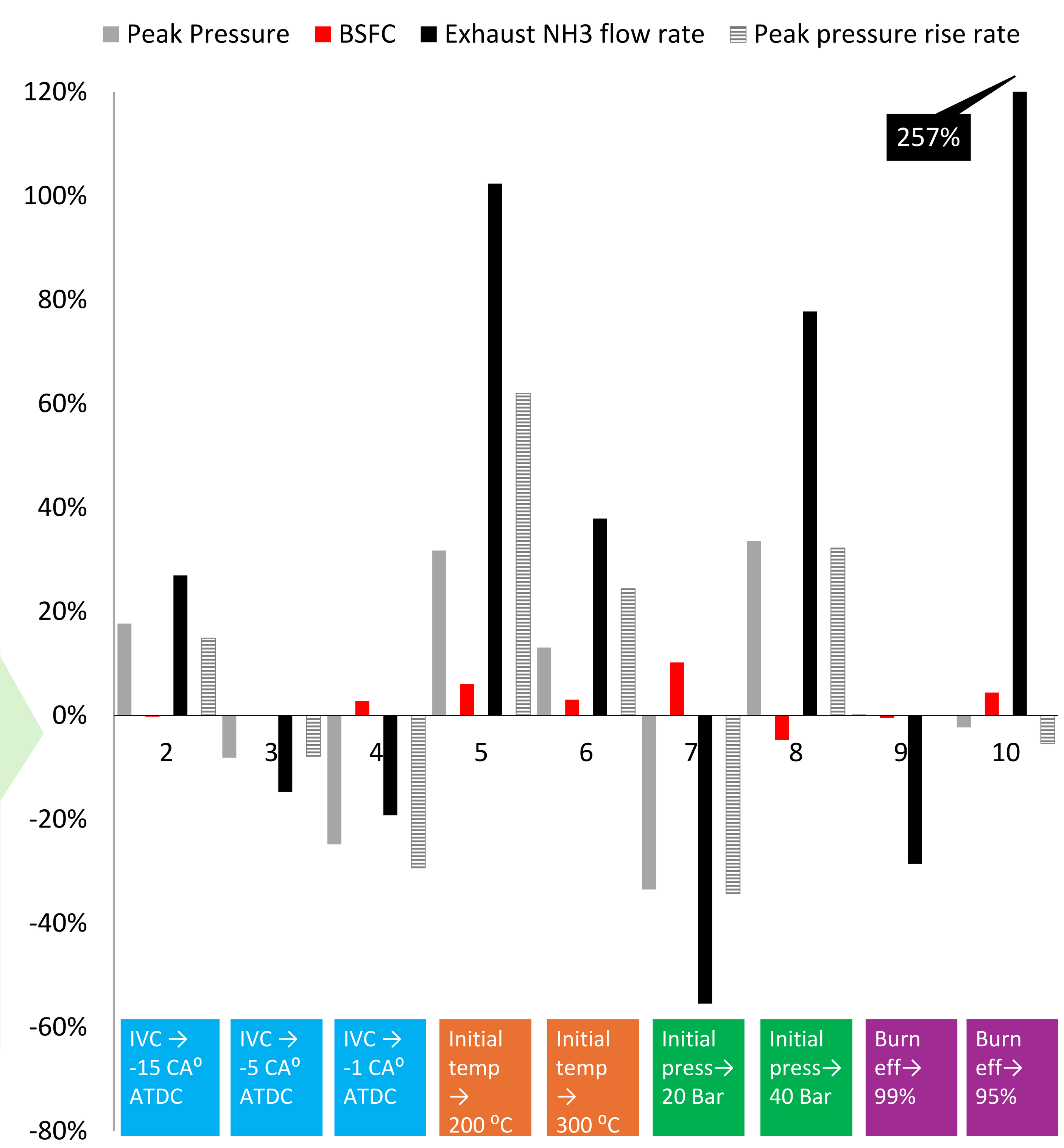
$$(8)\ N_2O + H \leftrightarrow N_2 + OH$$

Therefore, cool combustion which inhibits formation of NOx, can be supported by lean mixtures at high initial temperatures and pressures.

Headline Findings and Results



- Compared to CH_4 and H20% in the SCRE, NH_3 underperforms in BSFC (g/kWh) in both the SCRE and RSCE, *BUT* outperforms for BSEC (MJ/kWh) in the RSCE configuration. Hence, whilst there is a penalty in mass to power conversion, due to the reduction in gravimetric energy density, there are gains for fuel energy to power conversion efficiency. This is reflected in the 1.5% point increase in BTE for NH_3 combustion in the RSCE architecture.
- Furthermore, whilst both the SCRE and RSCE require spark to support ignition, the resulting cool combustion maintained peak cylinder temperatures below 2100 K, resulting in minimal NOx emission (g/kWh) approaching even stringent heavy duty Euro VII limits. Next steps will examine NOx emissions with combustion efficiencies from engines.



Baseline for comparison: NH_3 in the RSCE at IVC -10 CAº, 30 bar and 400 ºC manifold conditions. Key metrics included peak pressure, peak pressure rise rate (PPRR), BSFC and exhaust NH_3 flow rate (ENE).

- *Firstly,* advancing IVC (-10 to -15 CAº) increases PPRE and ENE, with no gain in performance (constant BSFC), whilst delaying IVC (-5 to -1 CAº) reduces PPRR and ENE, but is also detrimental to performance (increased BSFC). Trade-off occurs at IVC -5 CAº offering reduction in PPRR and ENE without compromising BSFC.
- *Secondly,* reductions in initial temperature increased air and fuel density and, therefore, brake power (30 to 40 kW/cylinder from 400 to 200 ºC) which increased BSFC, ENE and PPRR. Increase in PPRR was due to an increase in fuel density (at increased air density and constant ϕ) increasing the magnitude of the combustion event. Increase in ENE and associated increase in BSFC was due to the constant BE (98.6%, as observed for this equivalence ratio in the SCRE) causing an increase in unburnt NH_3 with flow rate, and a resultant reduction in fuel to power conversion efficiency.
- *Thirdly*, reduction in initial pressure was beneficial to PPRR and ENE, but detrimental to performance (increase in BSFC). Increase in initial pressure had the reverse effect, because increasing initial pressure benefits volumetric efficiency, which, at constant lambda, results in an increase in fuel density with an associated increase in ENE at constant BE.

Initial Conclusions and Ongoing Investigations

- NH_3 fuelling is feasible with the post-recuperator injection strategy, with gains in performance (BTE) and emissions (NOx) in the RSCE architecture.
- Optimum conditions were: ϕ=0.64 NH_3, with -5 CAº IVC, 40 bar and 400ºC manifold temperature and pressure, in combination with spark ignition.
- Further studies, H2 fumigation 5-10%, compared to optimum NH3, benefit due to inc. blend calorific value and trade off inc. NOx.

University of Nottingham UK | CHINA | MALAYSIA
UKRI Science and Technology Facilities Council
University of Birmingham
University of Brighton
Cardiff University Prifysgol Caerdydd

This work was supported by the Engineering and Physical Sciences Research Council, grant number EP/W016656/1

Funded by UKRI Engineering and Physical Sciences Research Council

References

[1] W. Fu et al. *Energy & Fuels,* 2024.
[2] G. Harris et al. *Icheme symposium series*, 1977, vol. 49, pp. 29-36.
[3] M. Aziz et al. *Energies,* vol. 13, no. 12, p. 3062, 2020.
[4] X. Zhang et al. *Frontiers in Energy Research,* vol. 9, p. 741704, 2021.
[5] R. Patil et al. *Flow, Turbulence and Combustion,* pp. 1-22, 2024.