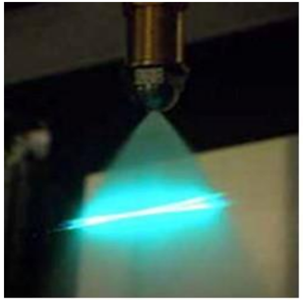
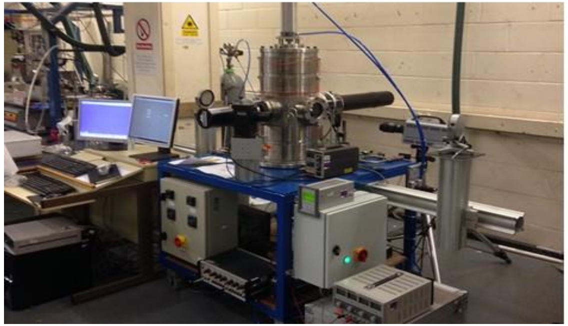
Implementation of chemical reaction networks for the study of ammonia combustors

Prof. Agustin Valera-Medina





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- INTRODUCTION
- CHALLENGES
- CENTRE OF EXCELLENCE ON AMMONIA TECHNOLOGIES (CEAT)
- DEVELOPMENTS
- CHEMICAL REACTION NETWORKS
- CONCLUSIONS

Introduction

Centre of Excellence on Ammonia Technologies
Canolfan Rhagoriaeth ar Dechnolegau Amonia

Exhibit 11: Distribution of global hydrogen resources and demand centers

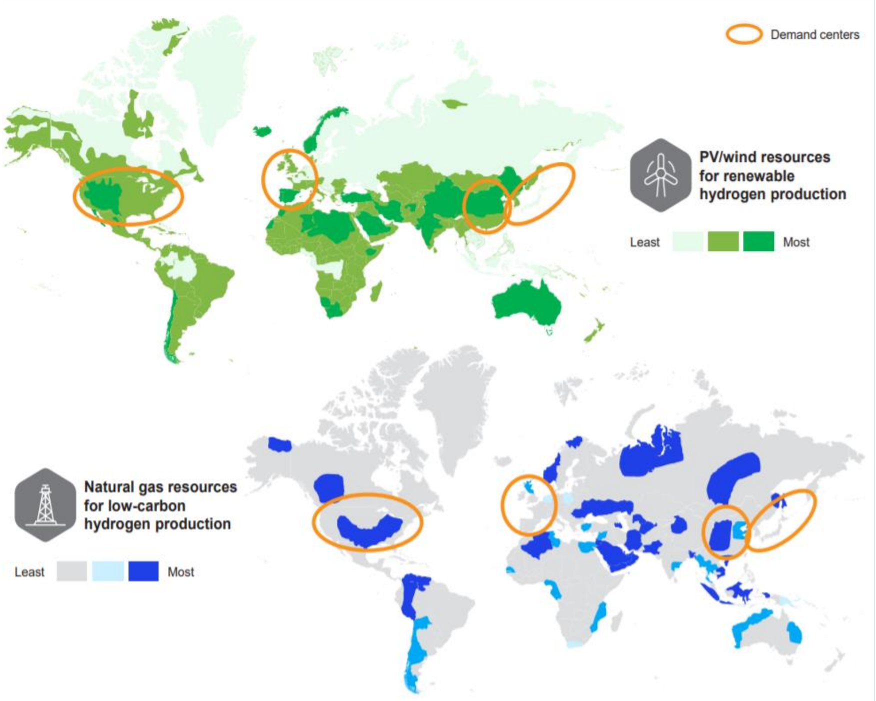
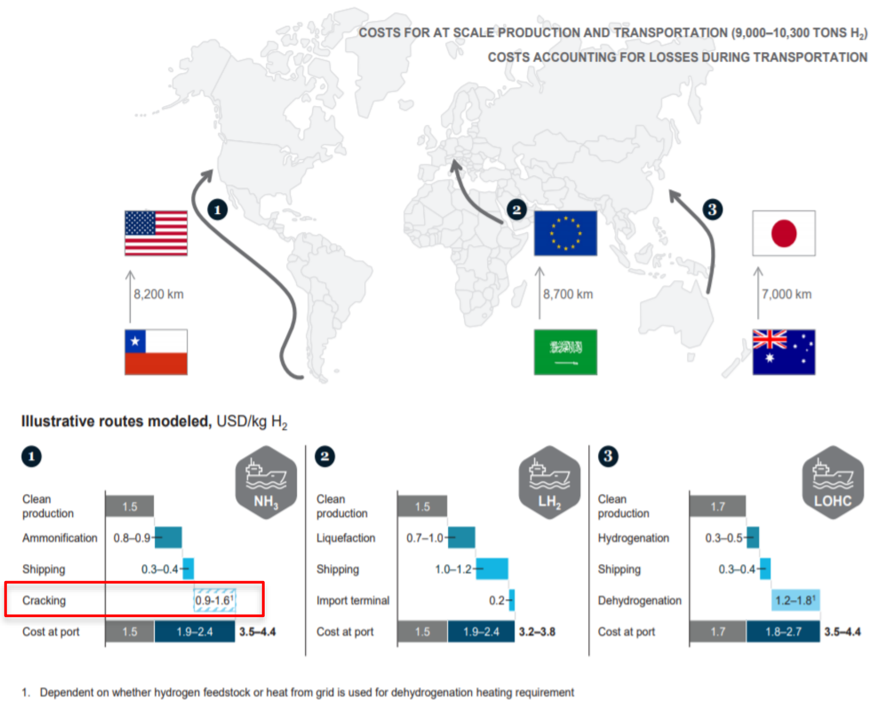


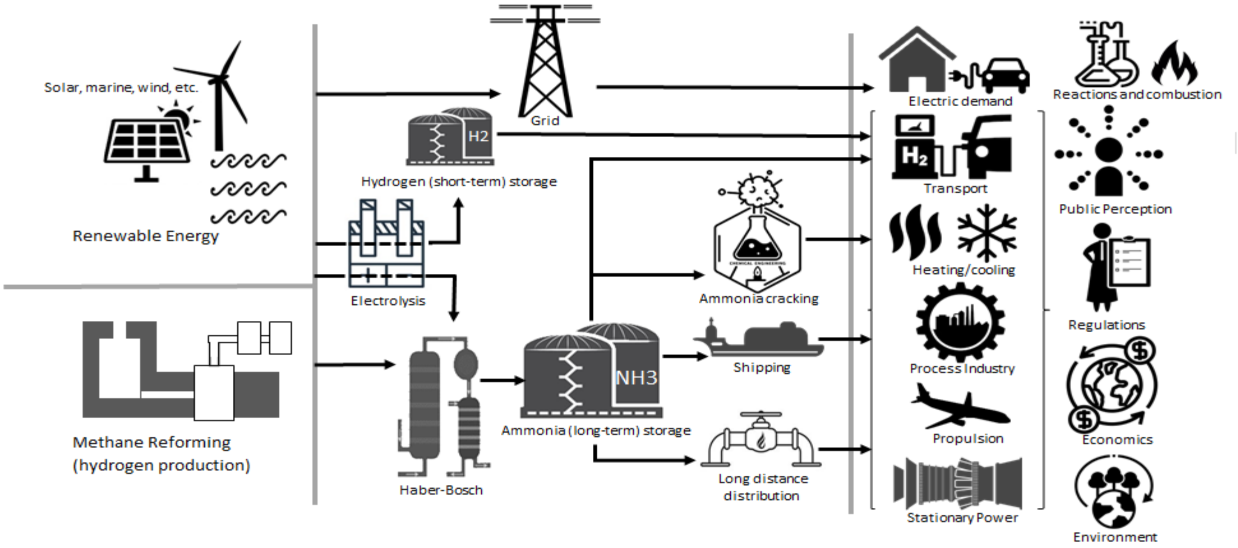
Exhibit 16: Landed costs of hydrogen at port for selected global transport routes



Hydrogen Distribution and comparison between vectors [Hydrogen Council 2021]

Introduction

- Although ammonia combustion is still seen as the lowest end of the use of ammonia for energy, cheaper distribution, higher hydrogen content and easier operation will change the position of NH3 in the energy arena.



Green Ammonia/Hydrogen Economy [Valera-Medina and Banares-Alcantara, 2020]

Challenges

However, the technology faces the following obstacles,

1.Ammonia Carbon-free synthesis (cost reduction, efficiency improvement)

2.Power generation at utility-scale from ammonia production (stable, low emissions)

3.Public acceptance through safe regulations and appropriate community engagement.

4.Economics – profitable scenarios (cannot be applied everywhere)

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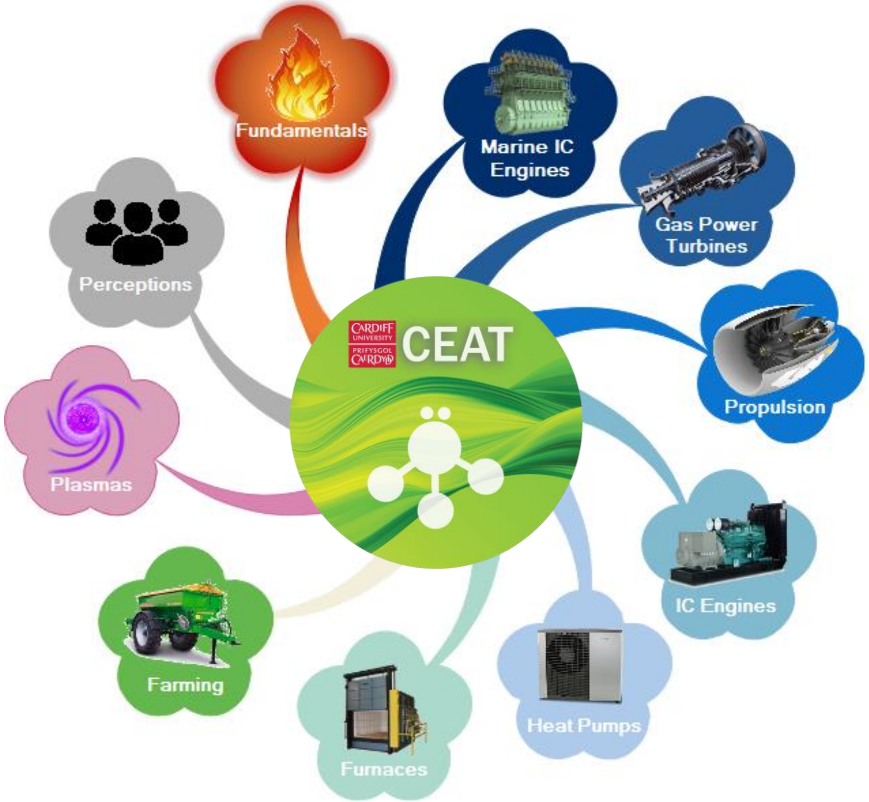


Current outcomes

- 1st International Demonstrator on Green Ammonia Energy
- Director of the Green Ammonia Working Group (UK)
- 2 Royal Society Policy Briefings
- Publication of 87 (+5 under 2nd review) papers, two books and 3 book chapters
- Editors in Chief of the new Journal on Ammonia Energy
- Lead of the 1st Symposium on Ammonia Energy
- Chair of the Combustion Section of the Ammonia Energy Association

Current funding profile

- Current projects are **£11.2m**

CEAT

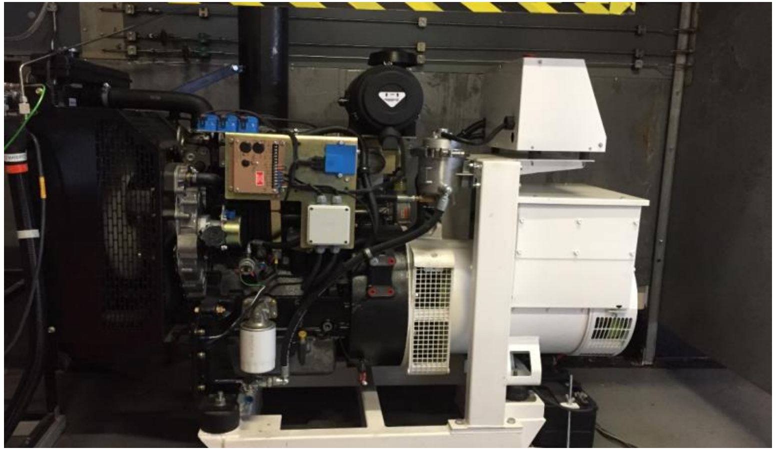
Vision

- Establish a physical facility for the Net Zero Innovation Institute with labs for CEAT/LCB/etc.
- CEAT, under the umbrella of NZII, will
  - Develop bespoke ammonia technologies for
    - Heat (boilers, furnaces)
    - Power (gas turbines, ICEs)
    - Transport (aerospace, terrestrial, heavy load)
    - Social sciences and Geopolitics
    - Biotechnology and physics
- Demonstrate NZ technologies at commercial scale at Aberthaw Green Park

Developments - ICEs

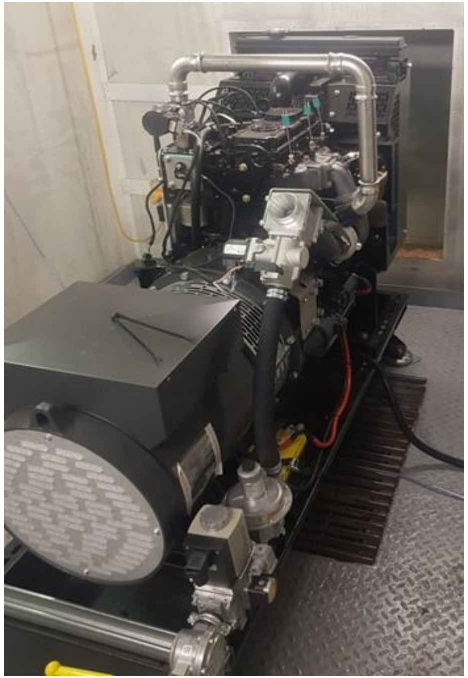
Internal combustion engine running on H2/NH3

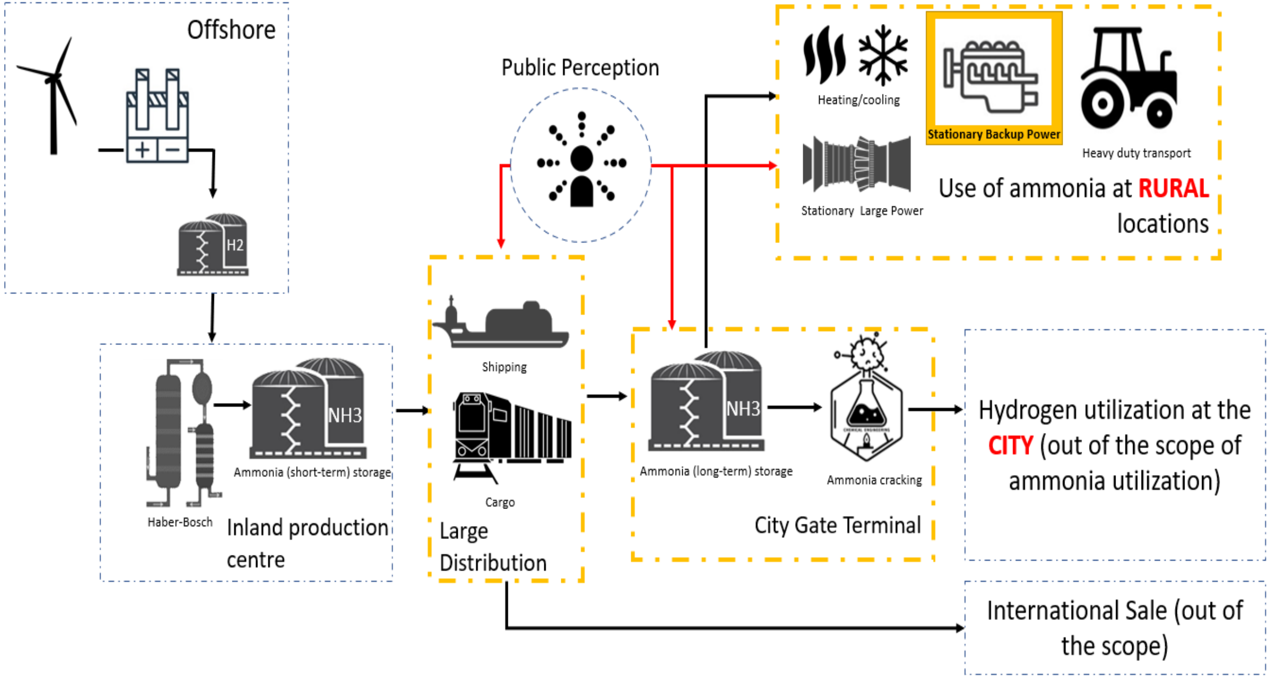
- Ammonia Demonstrator at RAL, Oxford. Cardiff developed the ammonia engine and container for the production of power and its transmission back to the grid.



Emissions (CO2 and NOx) using ICE-H2/NH3

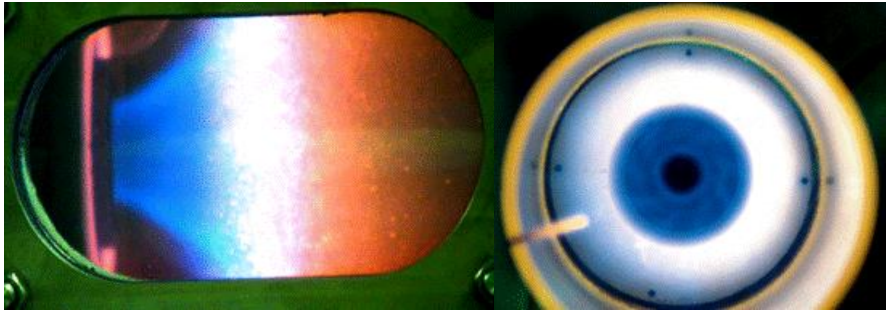
Developments - ICEs



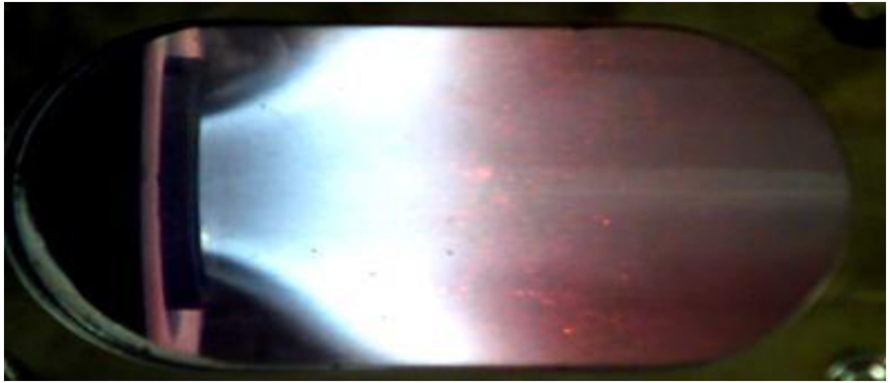


OceanREFuel Program to develop ammonia-based capabilities in the UK.

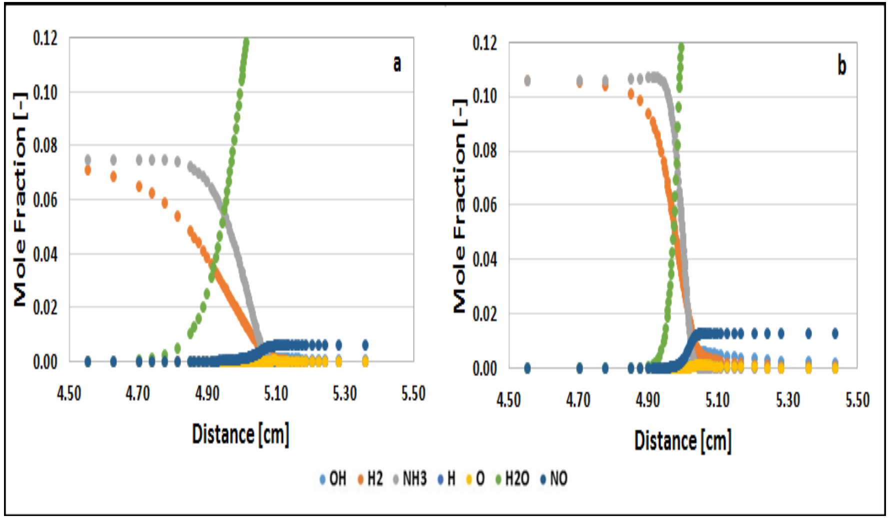
Developments – Micro Gas Turbines



66%$_{vol}$ NH_3 - 33%$_{vol}$ CH_4

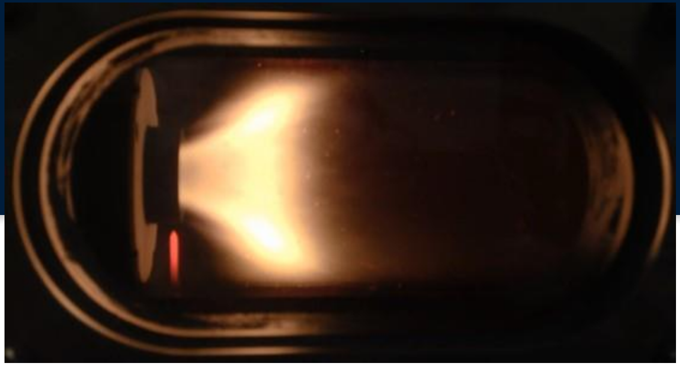


50%$_{vol}$ NH_3 - 50%$_{vol}$ H_2

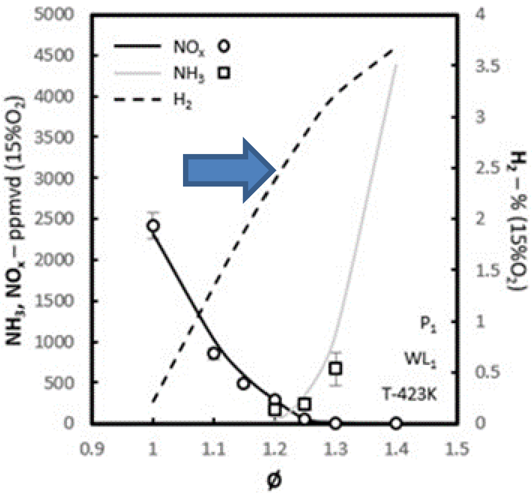


1-D Model for 50:50 ammonia/hydrogen reaction at a) Ø=0.52; b) Ø=0.80.

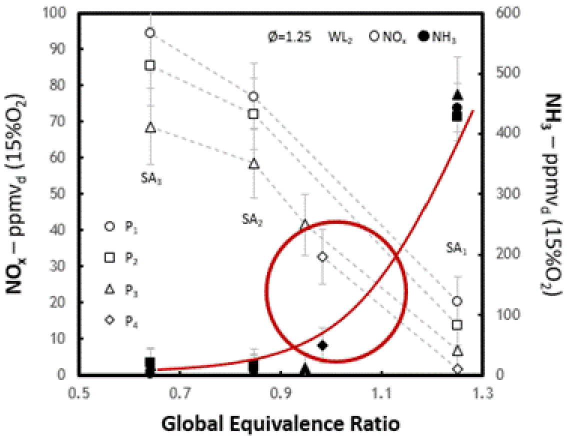
Developments – Micro Gas Turbines



$70\%_{vol}$ NH3 $30\%_{vol}$ H2. Cardiff University.

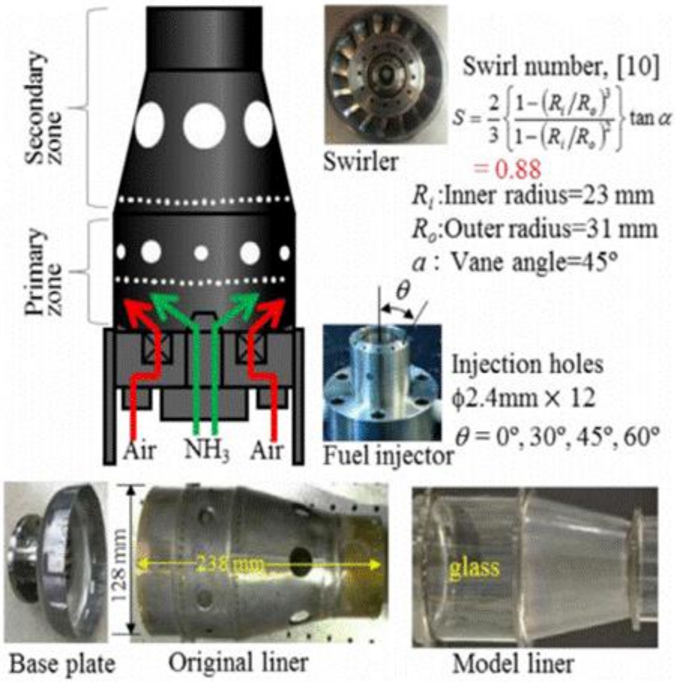


Clear reduction of NOx at high E.R. and high concentration of hydrogen



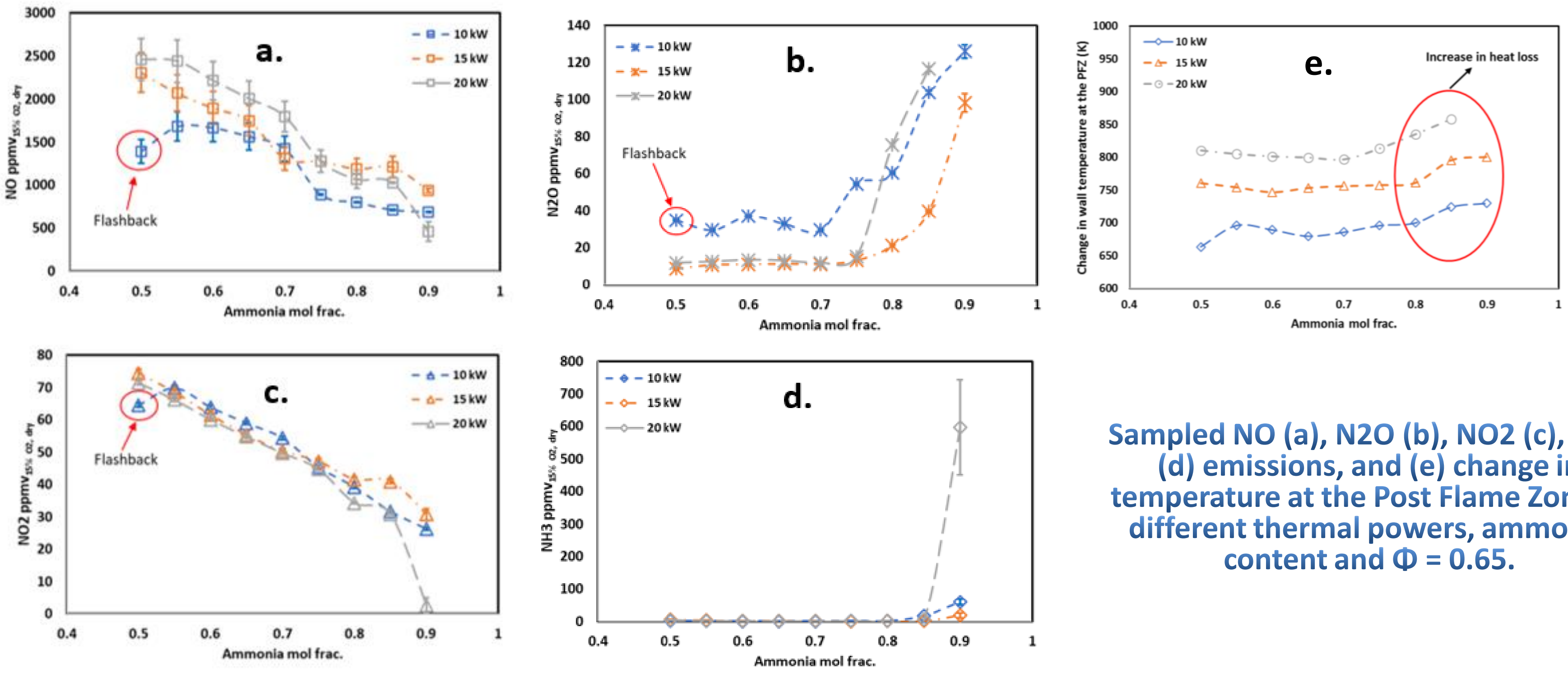
Fixed Primary Equivalence Ratio and Water Loading

Secondary Air (SA) addition with steam injection. Cardiff University [Pugh et al, 2018]



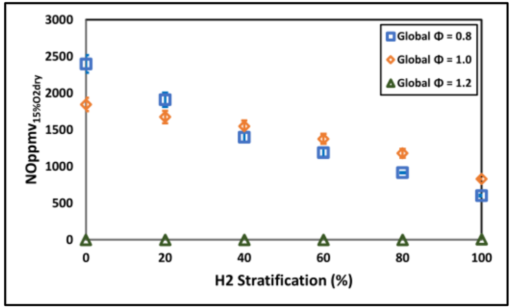
The MGT high-swirl combustor [Okafor et al, 2018]

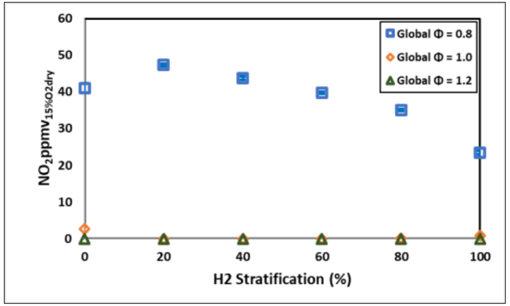
Developments – Micro Gas Turbines

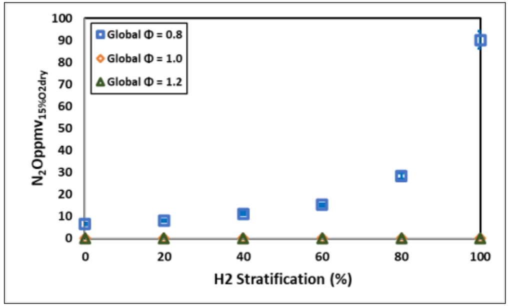


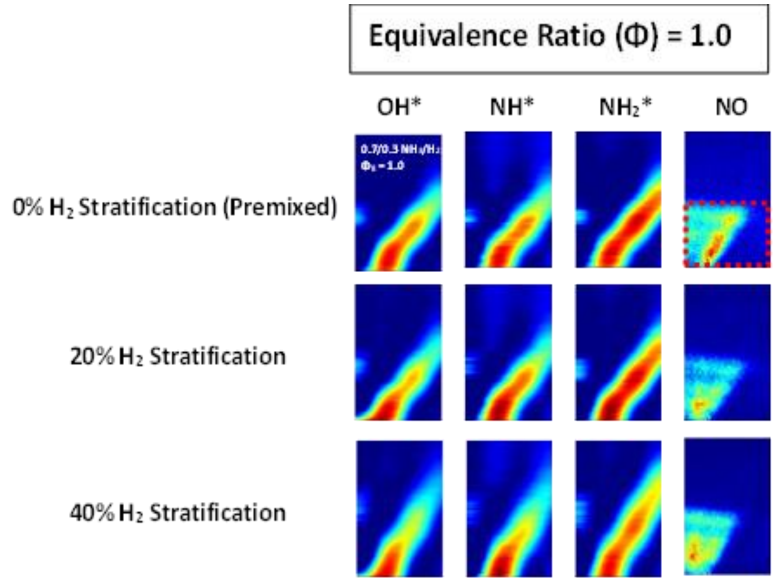
Sampled NO (a), N2O (b), NO2 (c), NH3 (d) emissions, and (e) change in temperature at the Post Flame Zone at different thermal powers, ammonia content and Φ = 0.65.

Developments – Micro Gas Turbines



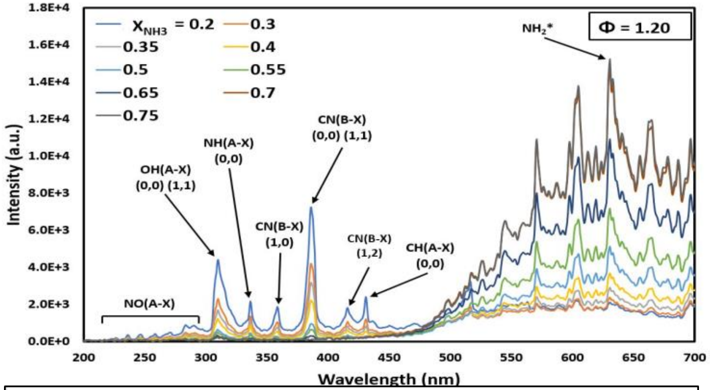


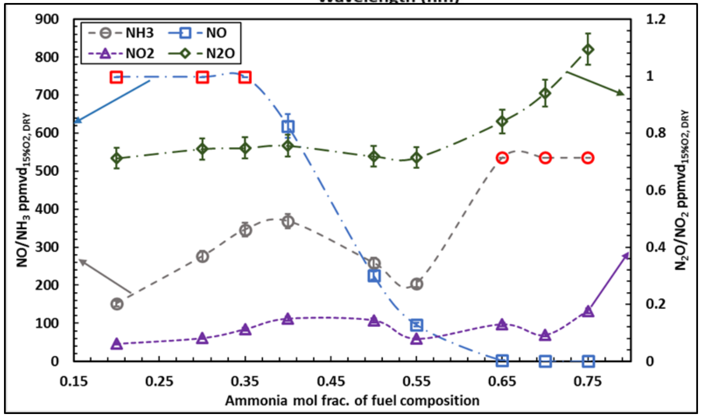


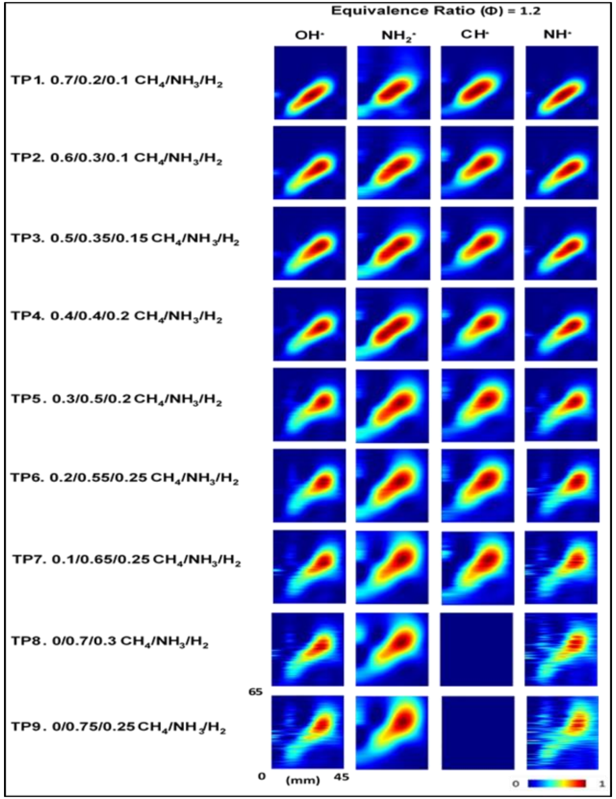


Stratification appears as a good potential for NOx mitigation whilst enabling good flame stability.

Developments – Micro Gas Turbines







Ternary Blends with stability. Ternary blends and their impacts. A 20/55/25% (vol%) CH4/NH3/H2 blend showed better reactivity, extinction strain rate (ESR), stability and low emissions compared to others at 1.2 equivalence ratio (Maskruk et al. 2022).

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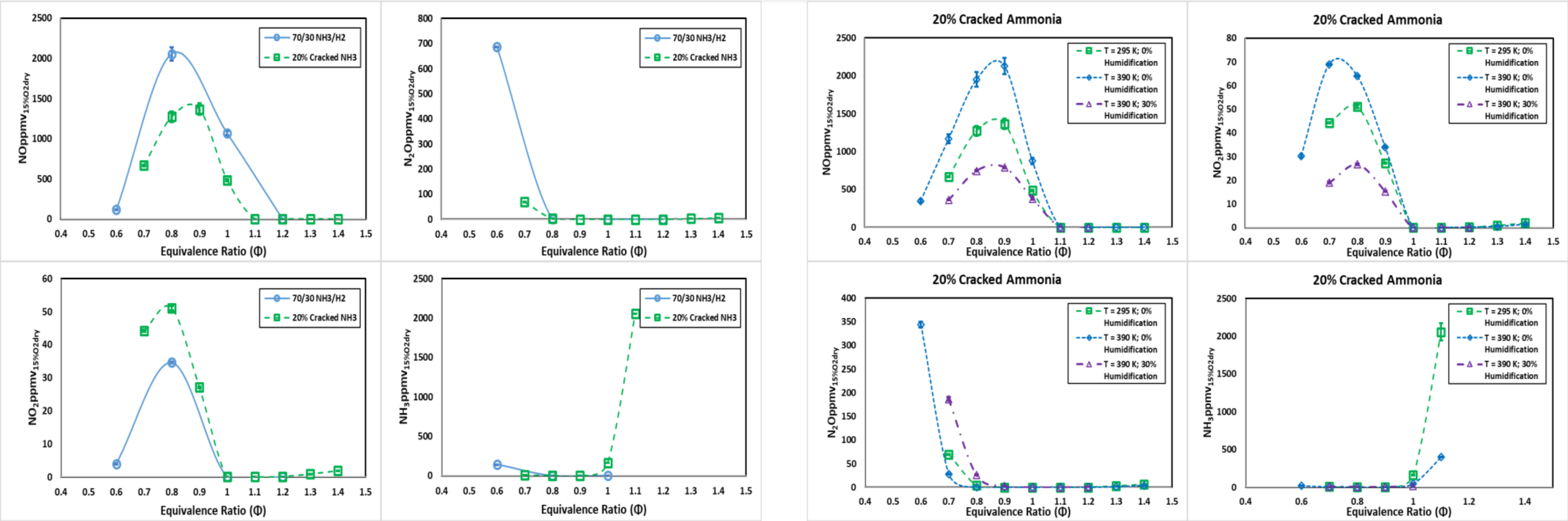
Developments – Micro Gas Turbines



Ammonia/Hydrogen vs Cracked Ammonia (20%) under atmospheric and higher temperature inlet conditions, with/without humidification.

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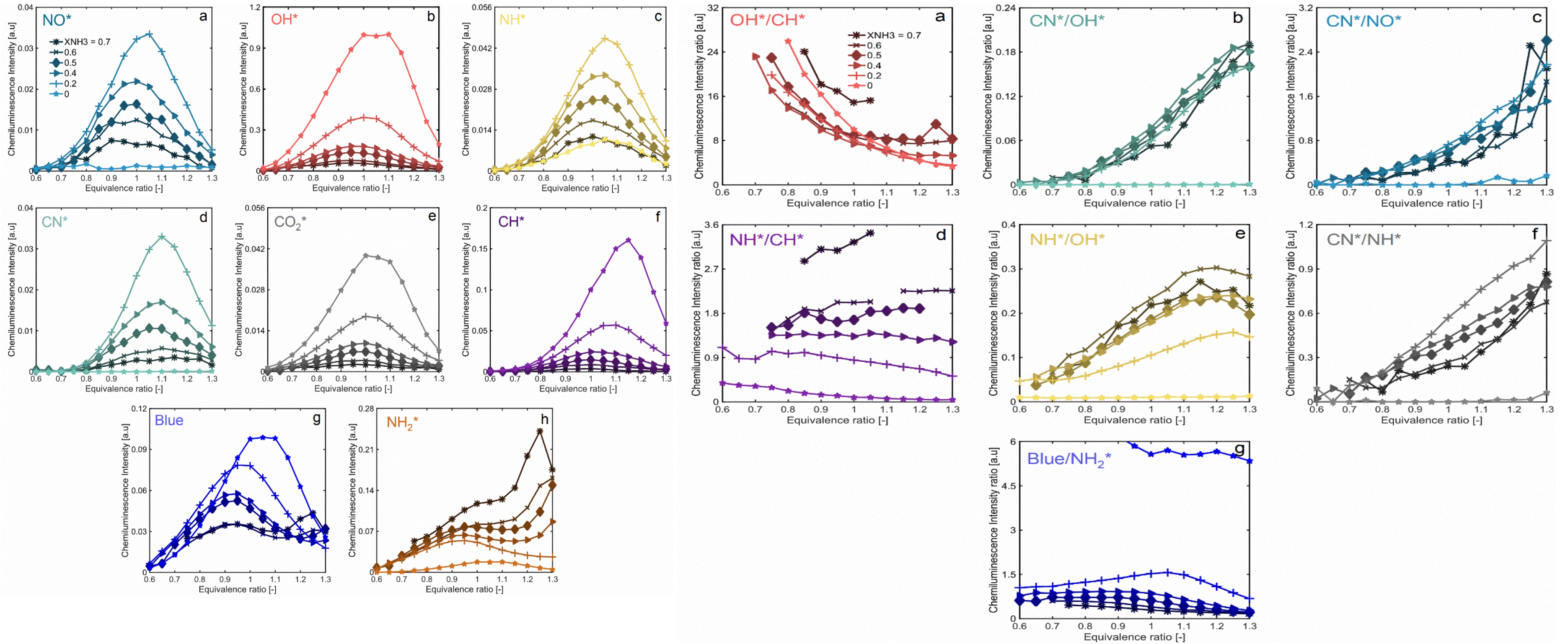
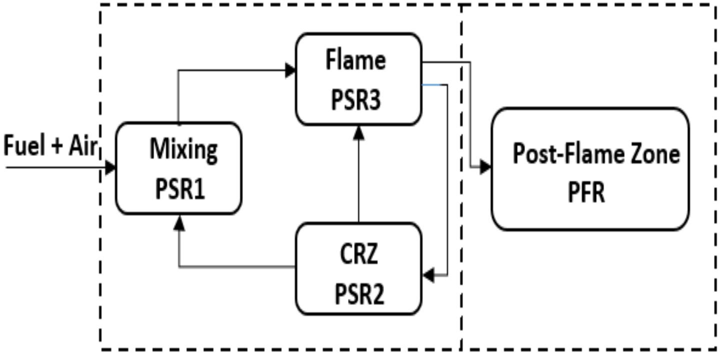
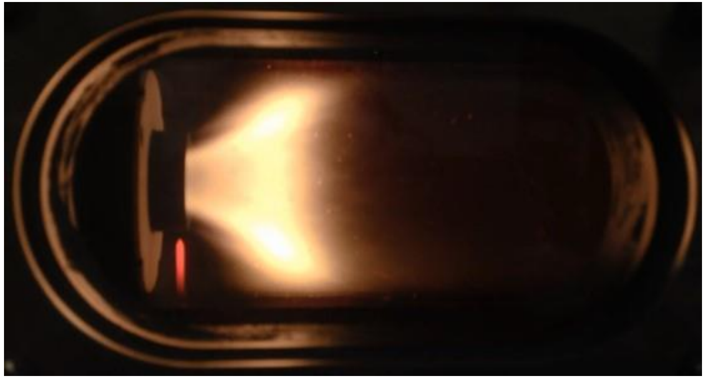
Developments – Micro Gas Turbines



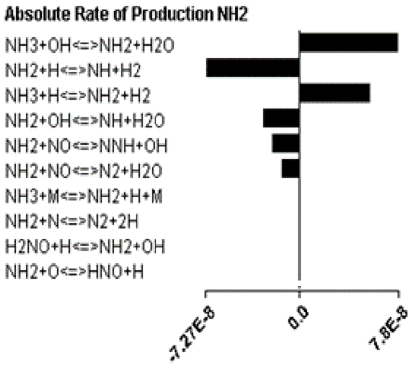
Spectral signals of various radicals and their correlation between each other [Mashruk S et al. 2022].

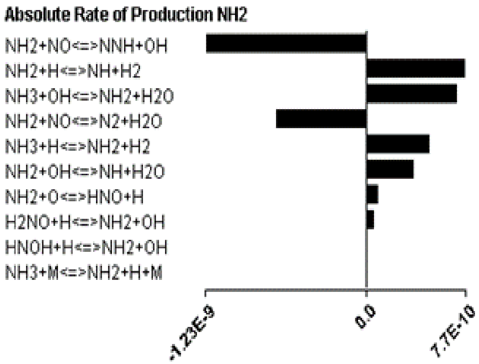
Developments – Micro Gas Turbines





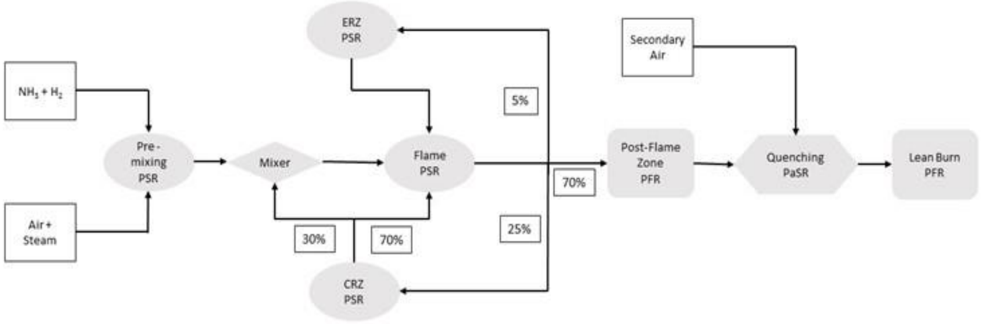
Reactions	*A*	*n*	*Ea*	*Ref.*
N+NO=N_2+O	2.10E+13	0	0	[26]
NO+H+M=HNO+M	1.50E+15	-0.4	0	[27]
HNO+H=NO+H_2	4.40E+11	0.7	650	[27]
N2O+H=NH+NO	6.70E+22	-2.16	37155	[28]
N2O+H=N_2+OH	5.00E+13	0.00E+00	1.52E+04	[29]

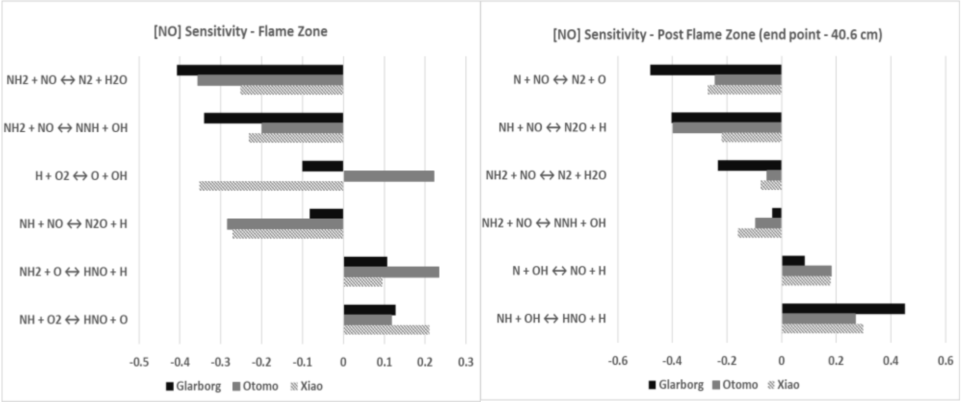


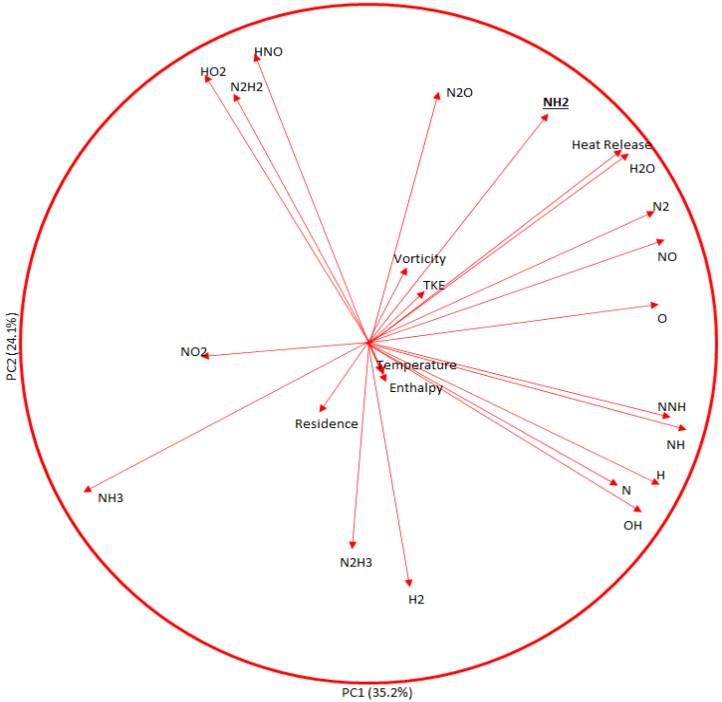


Correlation between experiments and numerical modelling adequate but not perfect.

Developments – Micro Gas Turbines

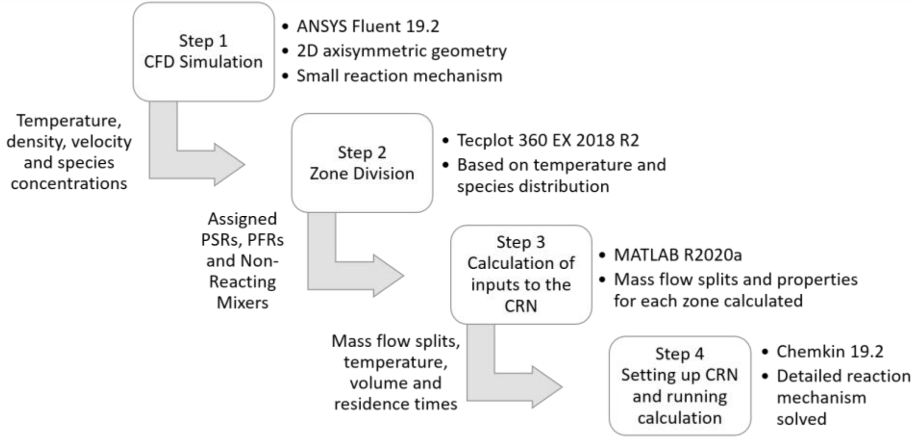


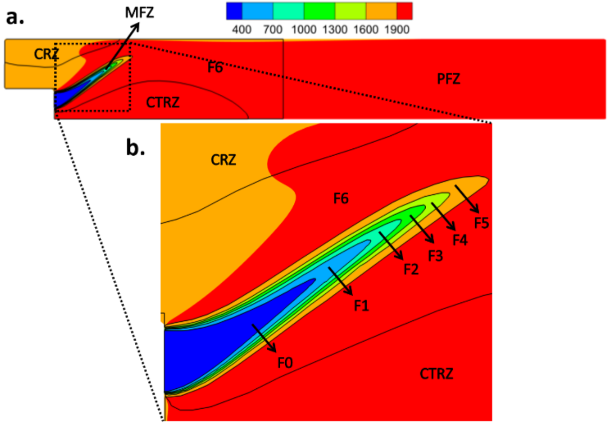


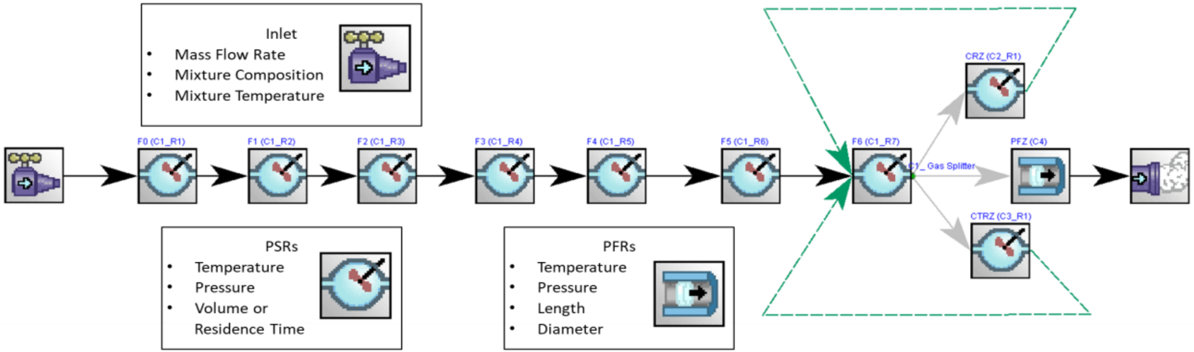


Bipolar multivariable analysis for NH2, with correlations between radicals and species.

Developments – Micro Gas Turbines

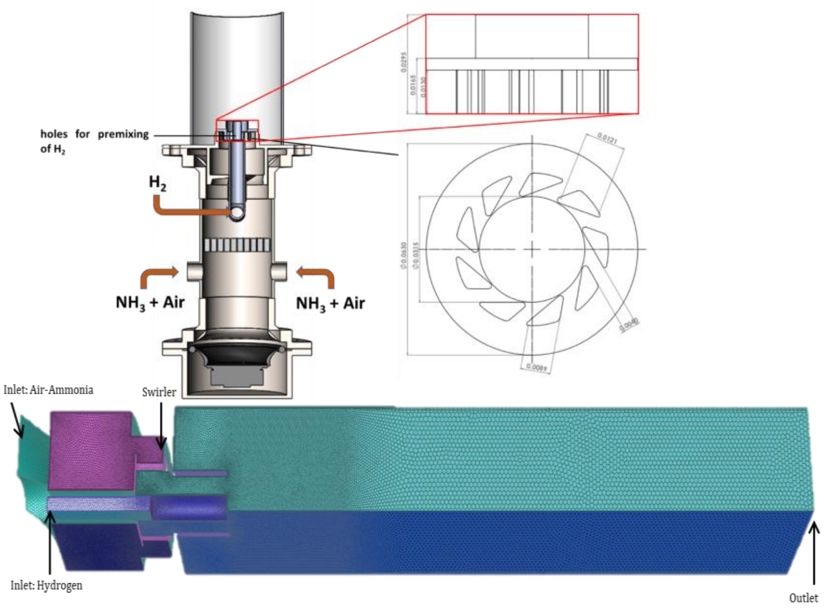


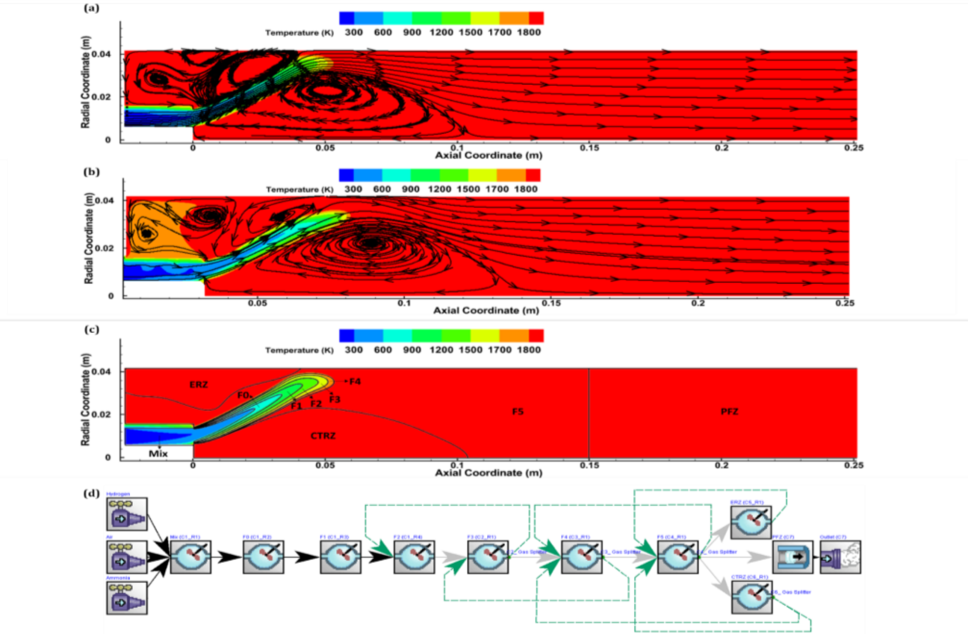




Reactor network code based on velocity clustering (top: cluster locations, middle: locations on fields, bottom: network)

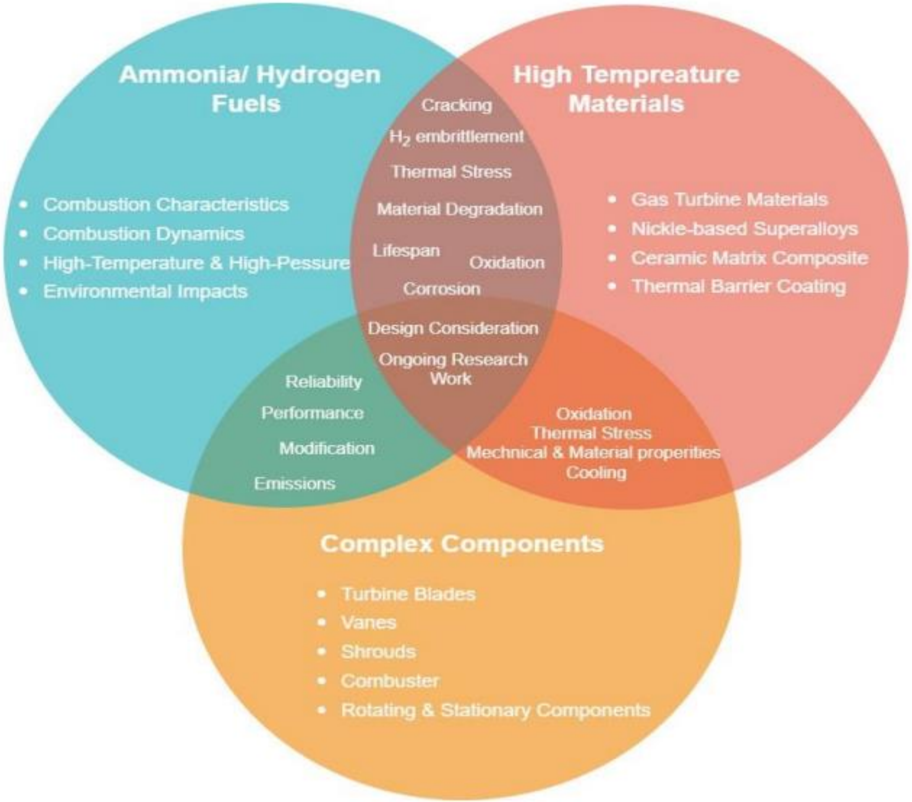
Developments – Micro Gas Turbines





Construction of CRN from CFD results for ϕ = 1.2. Temperature contour with imposed streamlines from 2D reacting flow CFD (a). Temperature contour with imposed streamlines from 3D reacting flow CFD (b). Division of zones for CRN based on temperature and velocity fields (c). Resulting CRN built in ANSYS Chemkin-Pro (d).

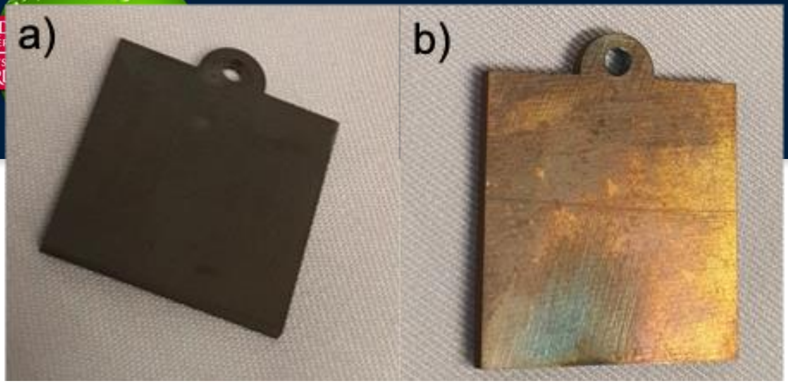
Developments – Gas Turbines

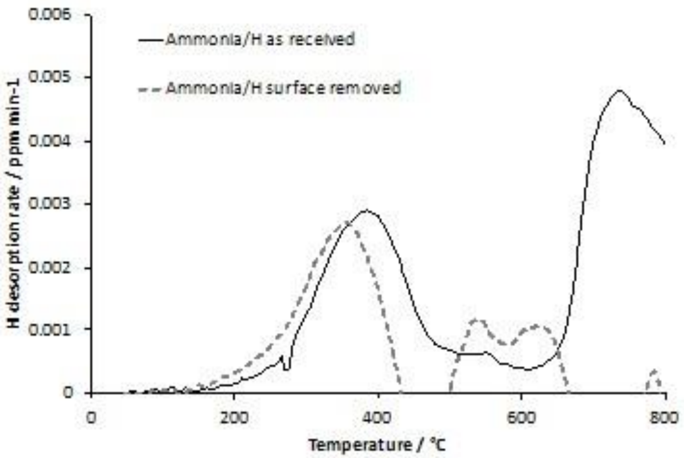


Complex Interactions with Gas Turbine materials

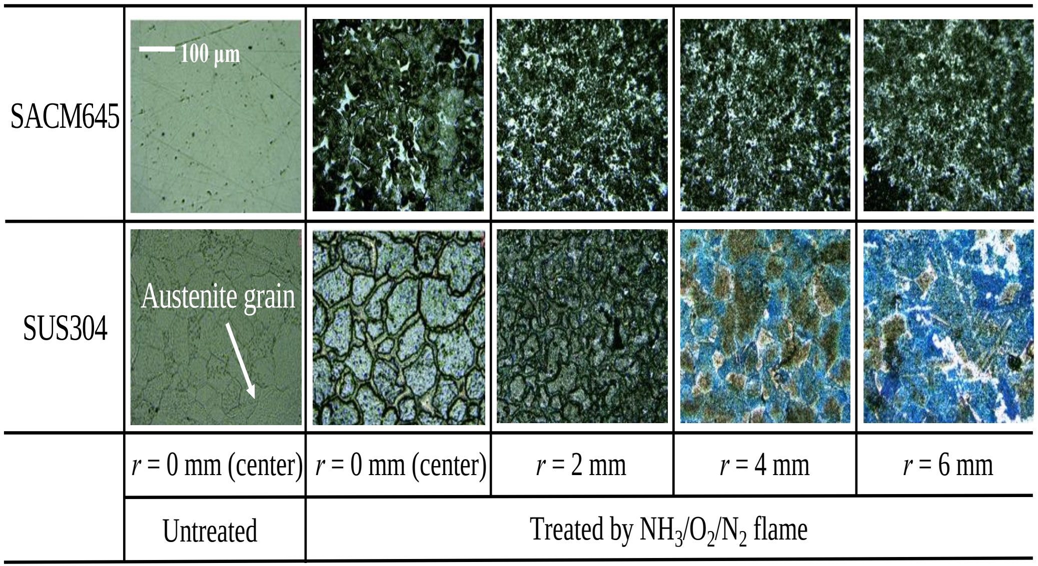
- Hydrogen Embrittlement
- Ammonia Nitration
- Acids
- Basic atmospheres
- Third Body reactions
- Heat Losses
- Radiation

Developments – Micro Gas Turbines





Samples exposed to ammonia/hydrogen and methane, respectively. Also, the peak at ~400oC denotes hydrogen permeation [Kovaleva M et al. 2022**].**



Optical micrographs of the SACM645 and SUS304 test plate surfaces after being exposed to the NH3/O2/N2 flame at 550 ºC for 5hr [Wang et al. 2023].

Developments – Micro Gas Turbines

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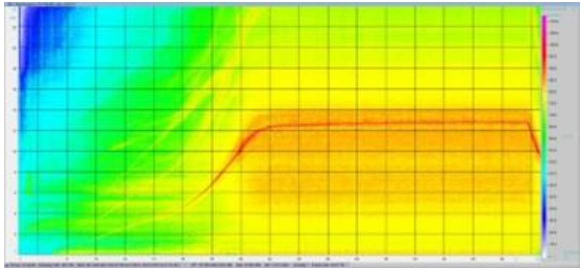
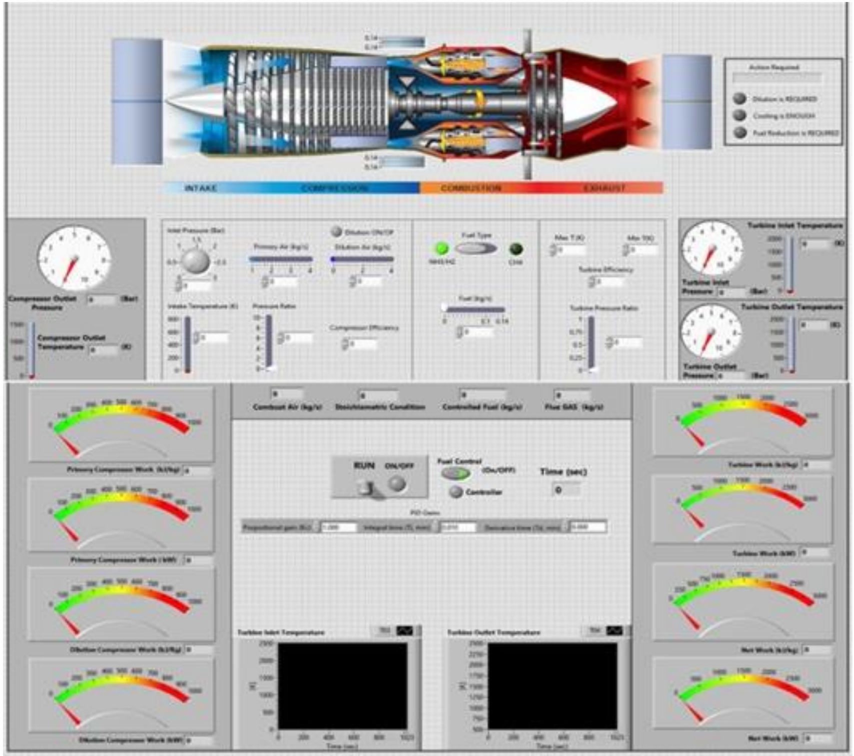
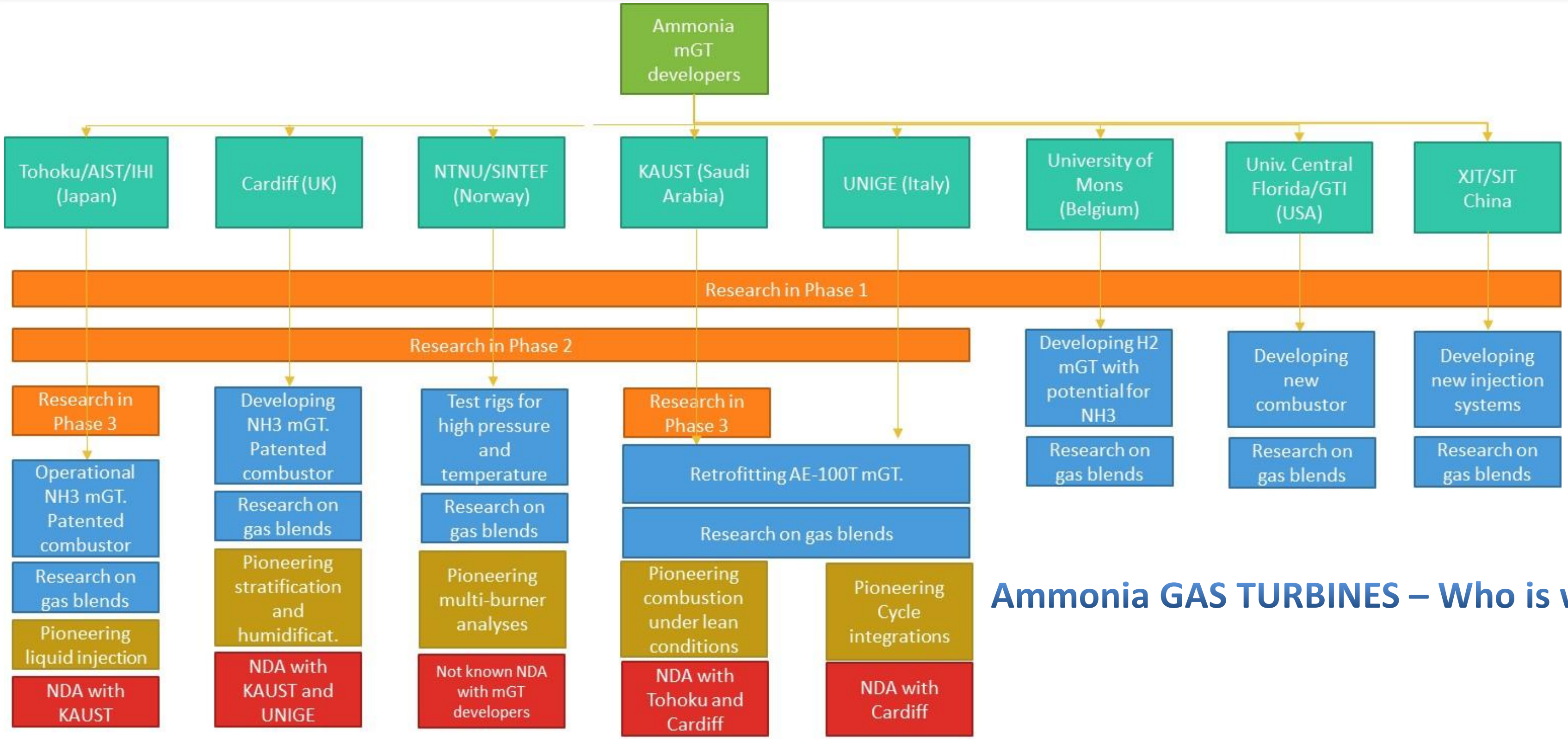




HELICOPTER AIR START UNIT (HASU)

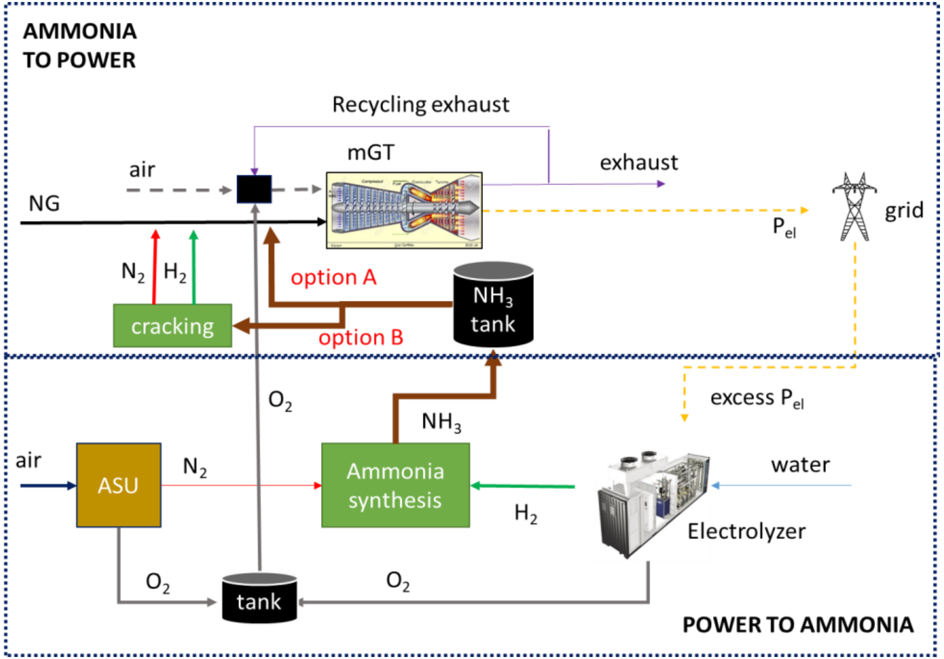
- Combustor will be replaced by new combustor
- Acoustic signature of the unit has been obtained
- A bespoke controlling systems is under development to enable stratified/humidified combustion

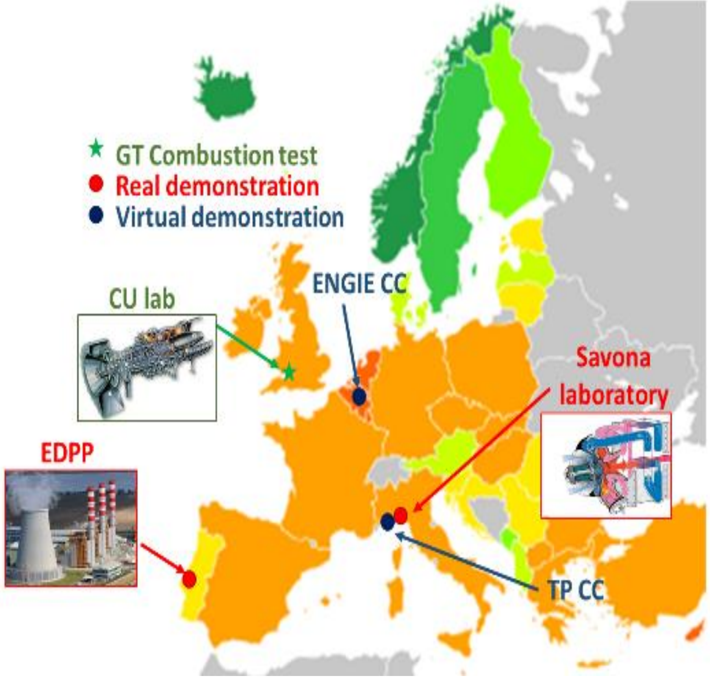
Developments – Micro Gas Turbines



Ammonia GAS TURBINES – Who is who

Developments – Gas Turbines

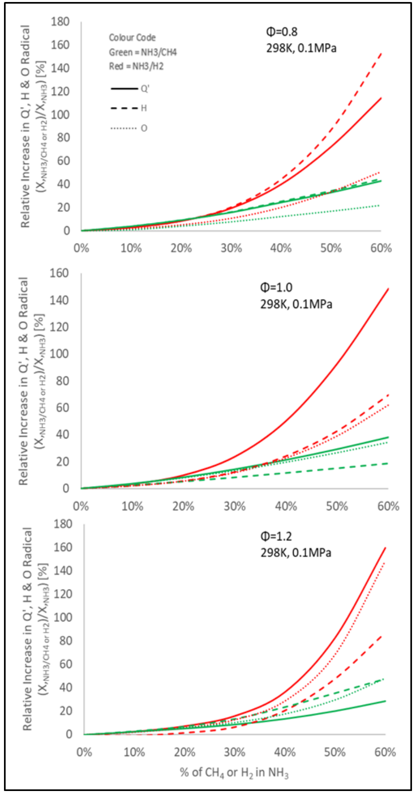


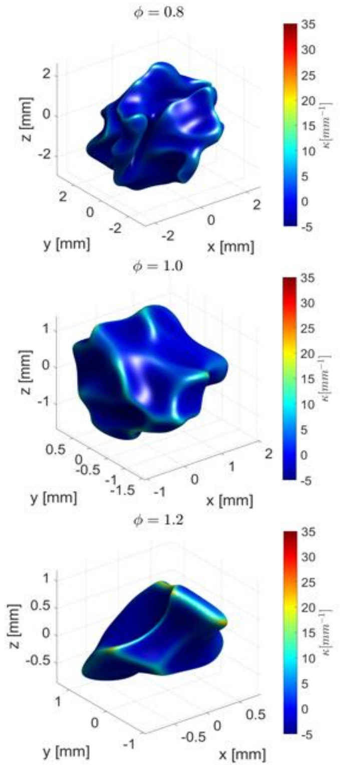


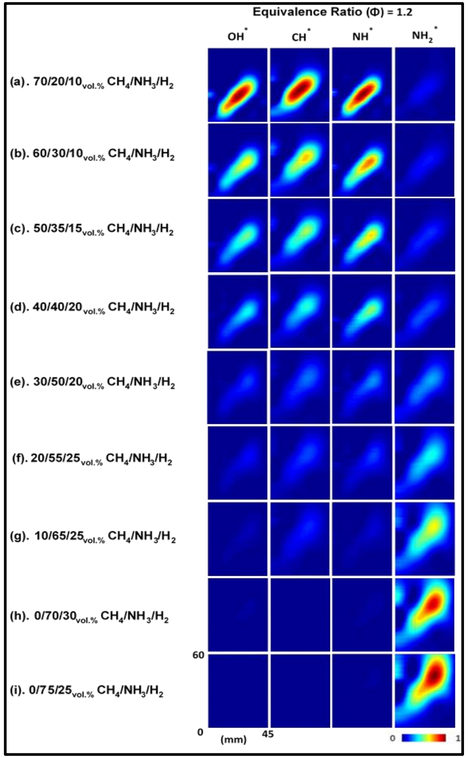
FLEXnCONFU – First large GT ammonia/hydrogen/NG demonstrator

This Project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement N. 884157

Developments – Gas Turbines







Initial Results

- **High NOx at low Equivalence Ratios**
- **Rich conditions boost the production of NH2***
- **Hydrodynamic and Thermodiffusive instabilities have a high impact on flame morphology**
- **Up to 20% NG/H2 replacement can be feasible without major retrofitting.**

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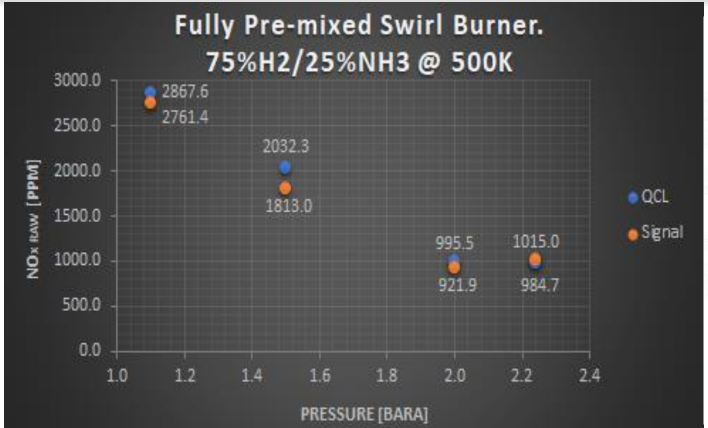
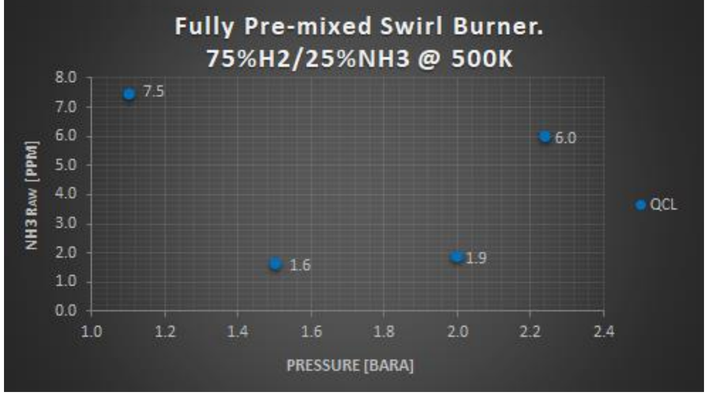
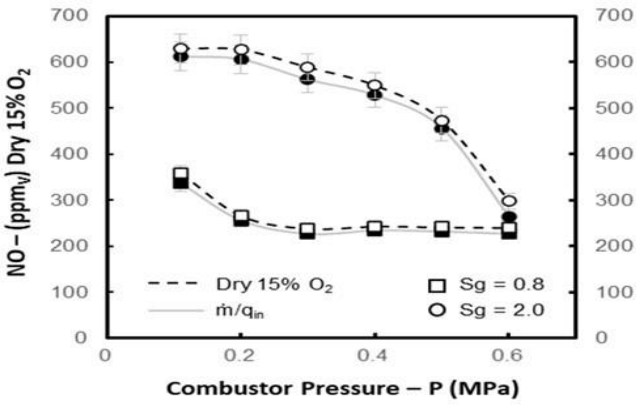
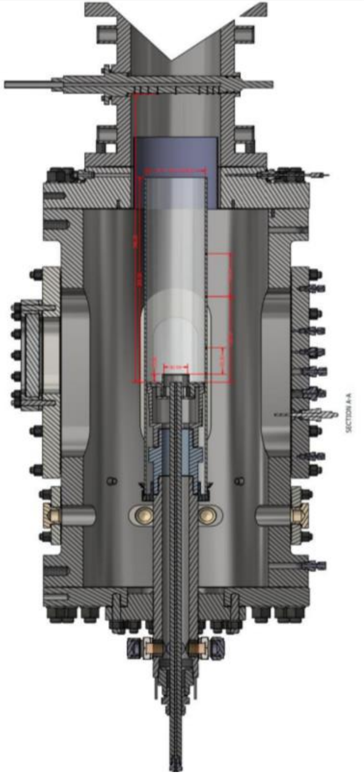
Developments – Gas Turbines









Notes: Equivalence ratio maintained
~0.29 and ~0.56
Power scaled with pressure
@12.5kW/1.1bar
Relative %heat loss from the flame reduces as power/pressure increases. This can be seen by increasing exhaust temperatures.

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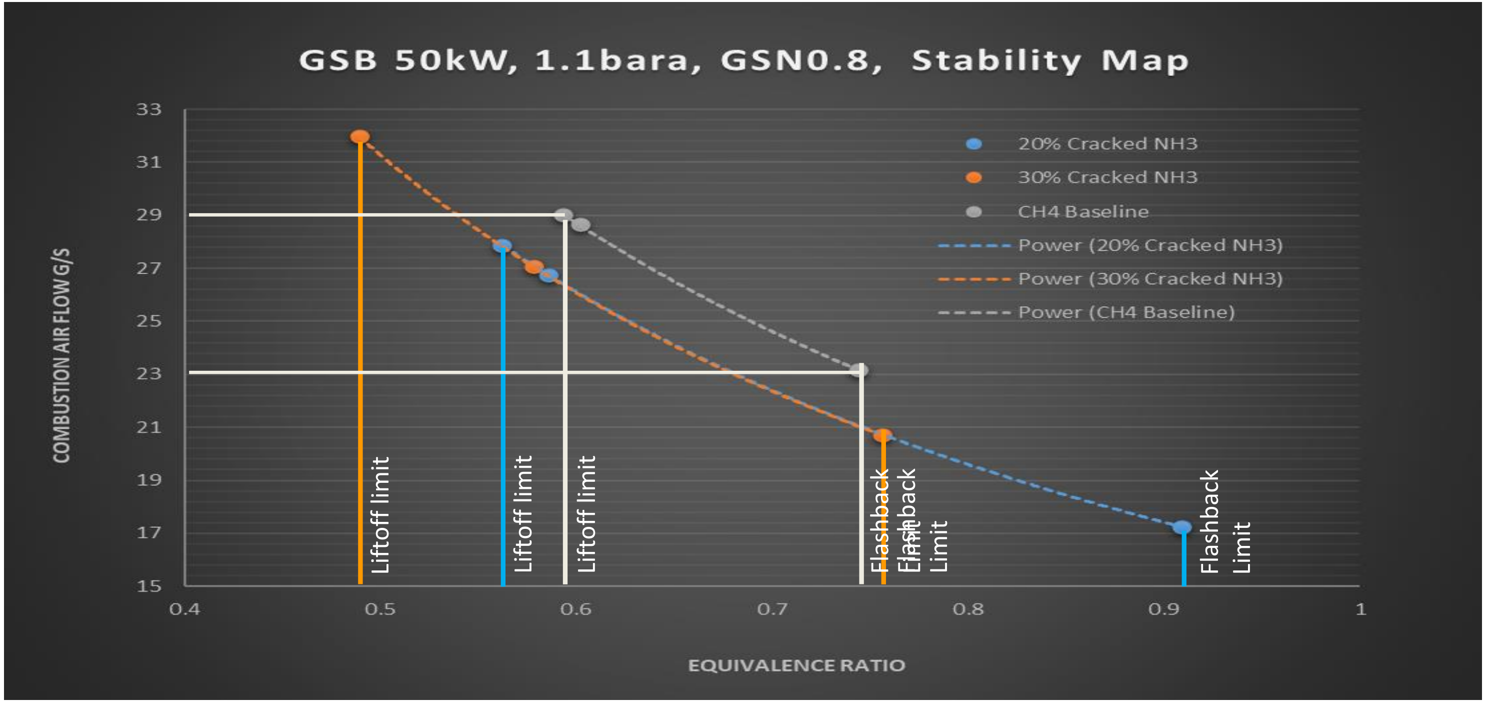
Developments – Gas Turbines



Operability limits using cracked ammonia compared to methane.

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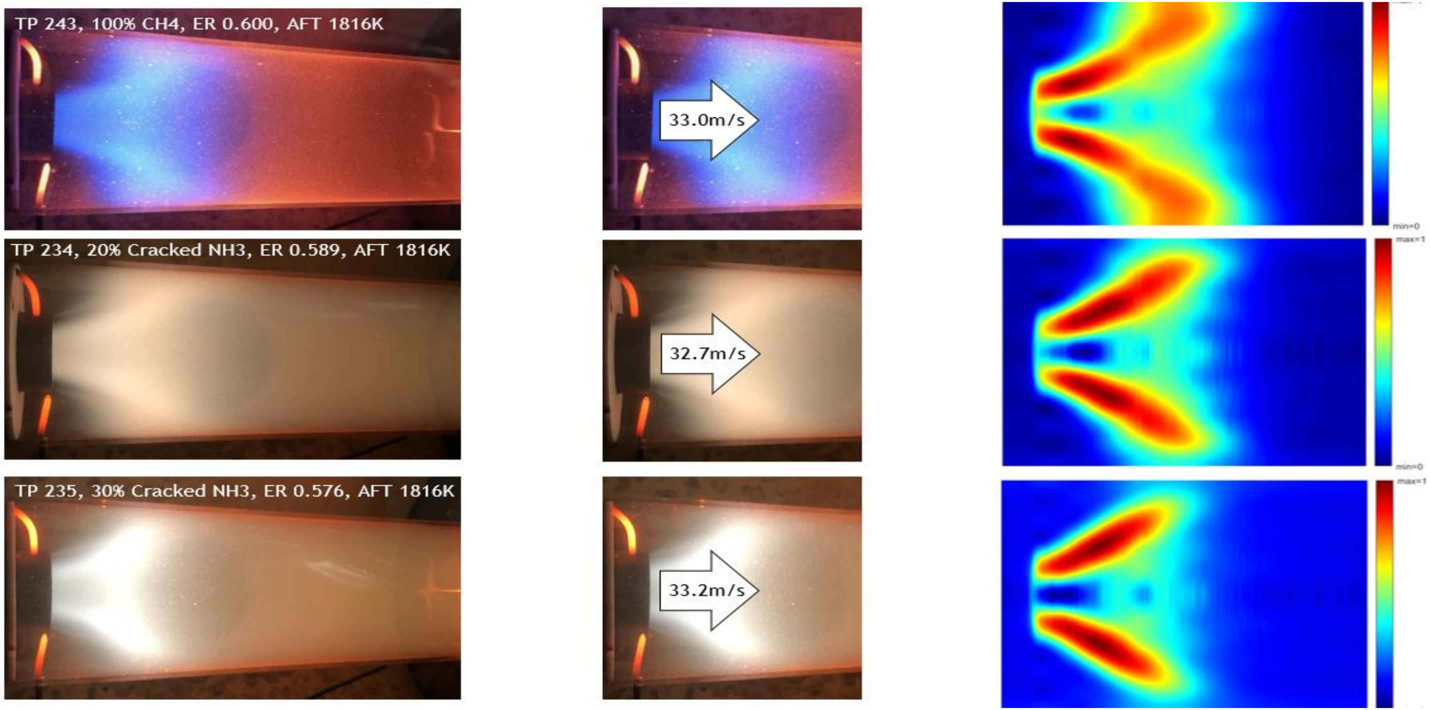
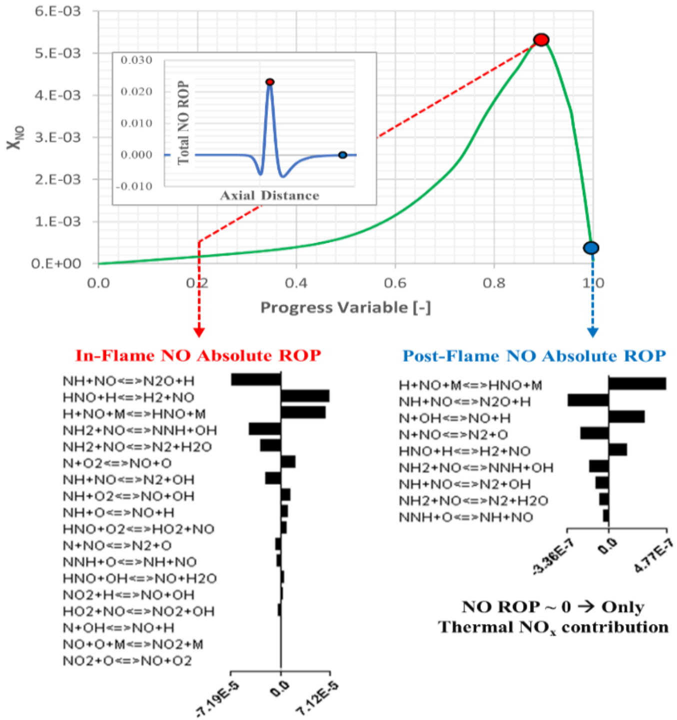
Developments – Gas Turbines

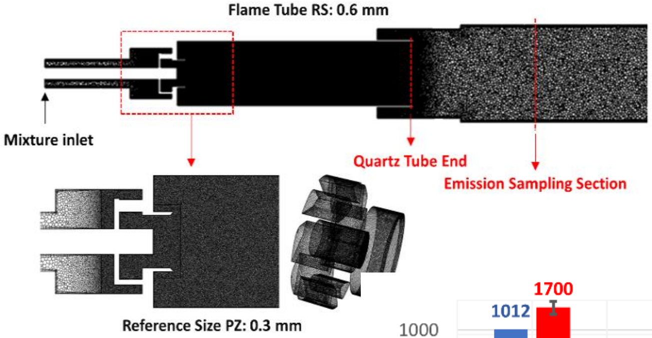


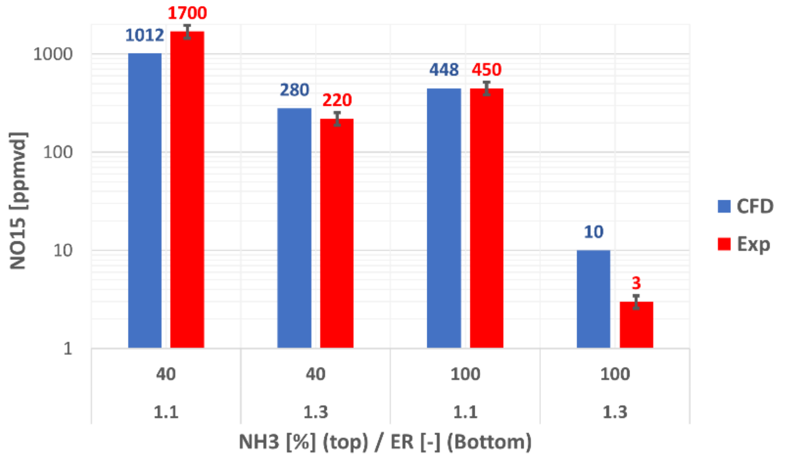
Photographs and OH*Chemi. 50kW,1.1bara, 538K

This Project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement N. 884157

Developments – Gas Turbines







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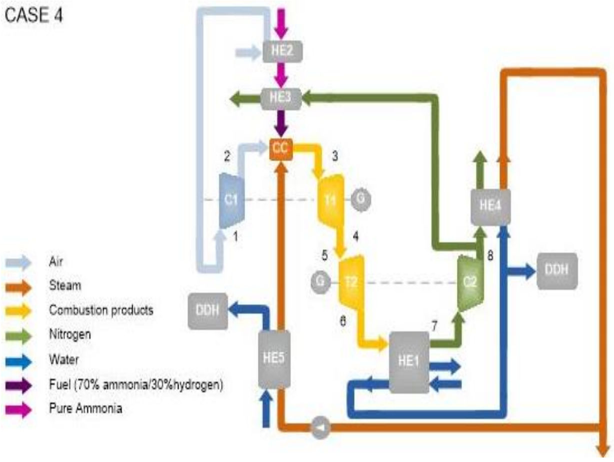
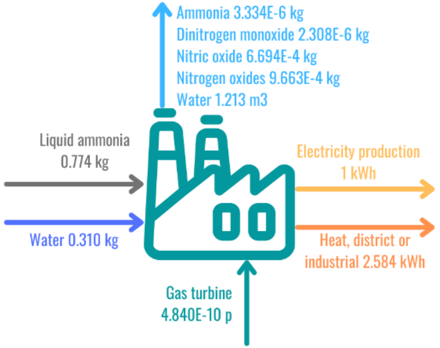
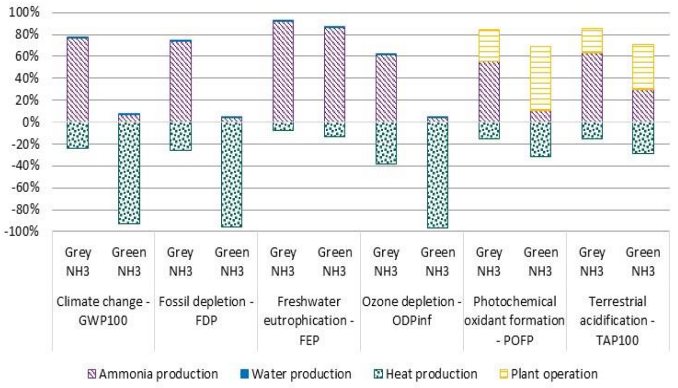


Modified Brayton Cycle
Inlet temperature 1260K
Outlet temperature 827K
Supplied heat 10.45MWth
Power 3.56MWe
Plant efficiency 34%

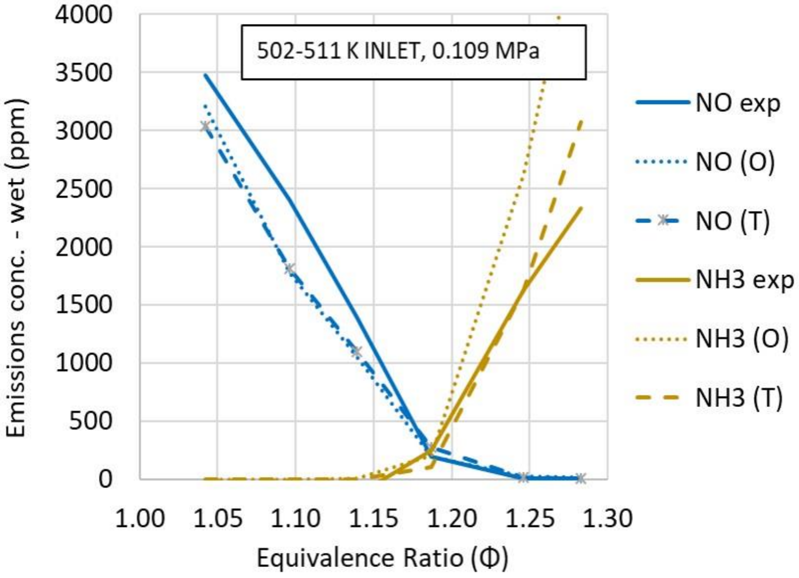
Trigeneration Cycle
Cooling+Power+Heating
Initial calculations: 62.5% (compared to ~80%)

Similarly, LCA shows the superior environmental advantages of green NH3

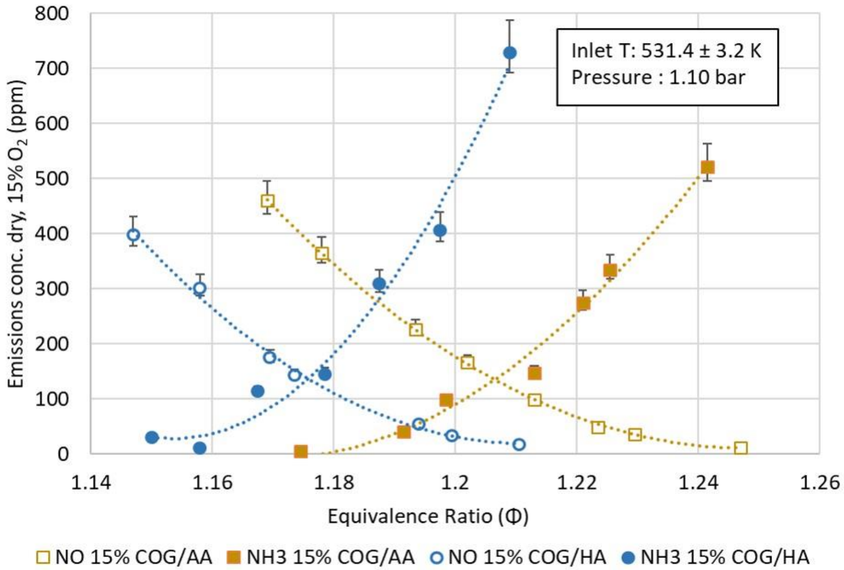




Developments – Boilers/Furn.

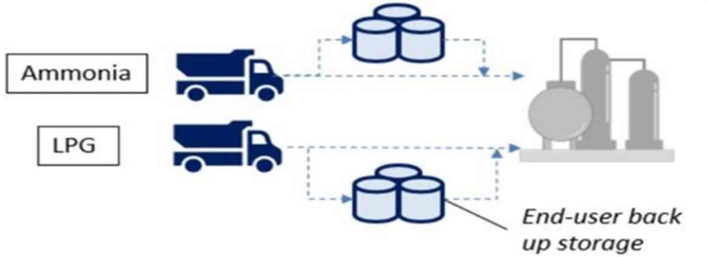


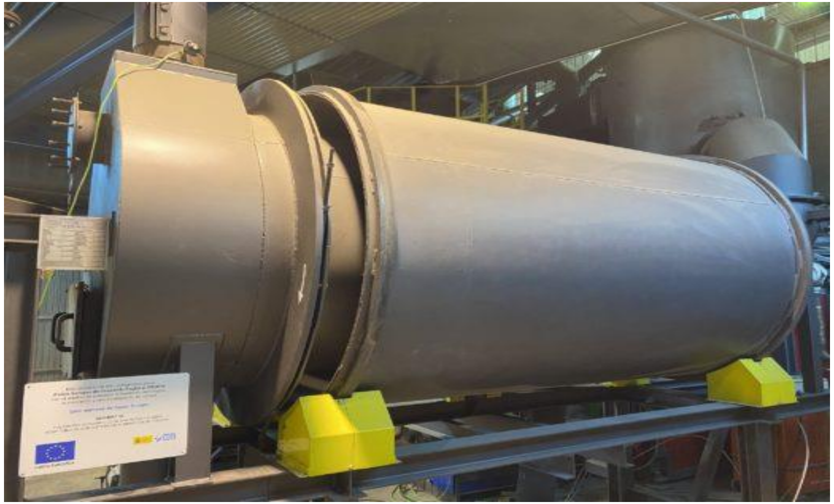
Correlation between experimental and numerical models [Tian and Okafor] using COG (20%) and Ammonia [Hewlett S, 2022]



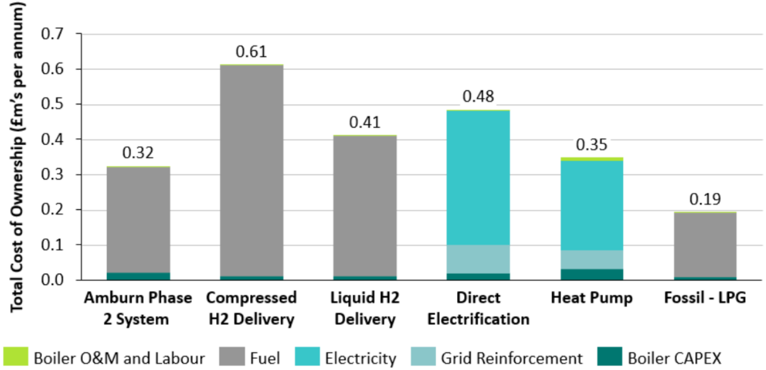
Shift in the reaction by using Humidified (60% water) ammonia blends [Hewlett S, 2022]

Developments – Boilers/Furn.



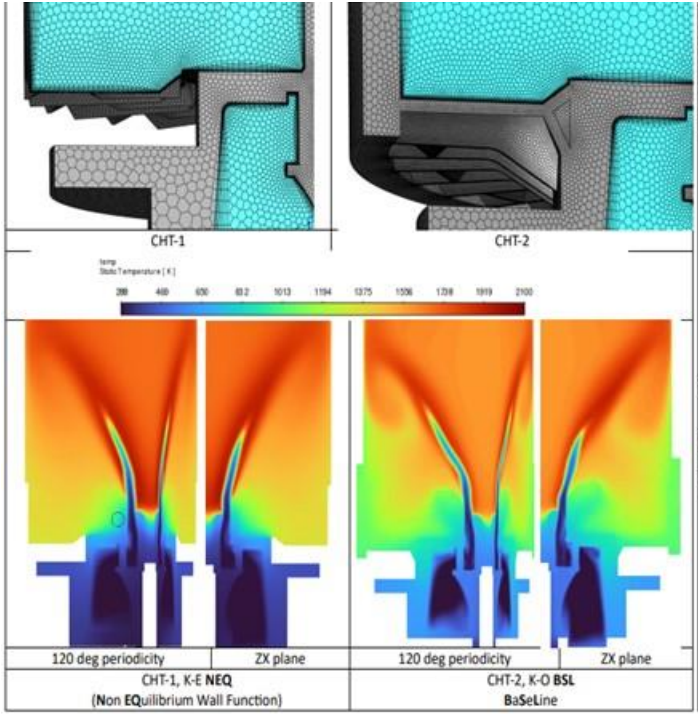


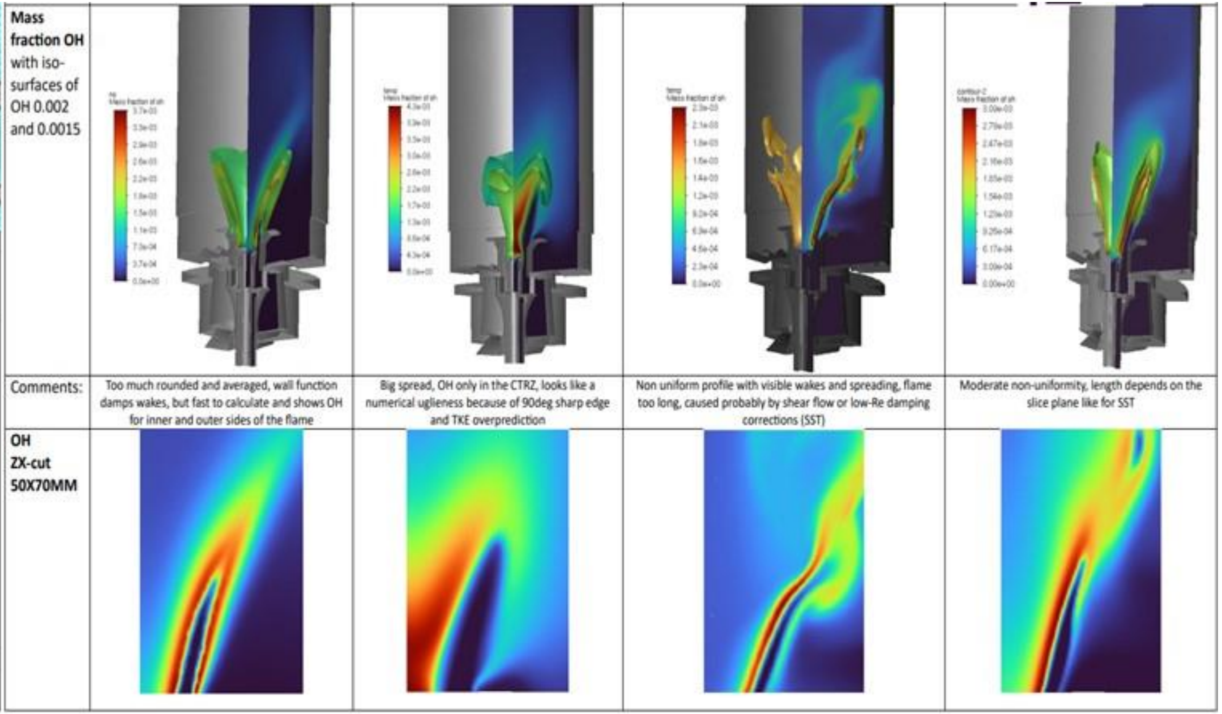
Pure and Residual ammonia can be used for extra power



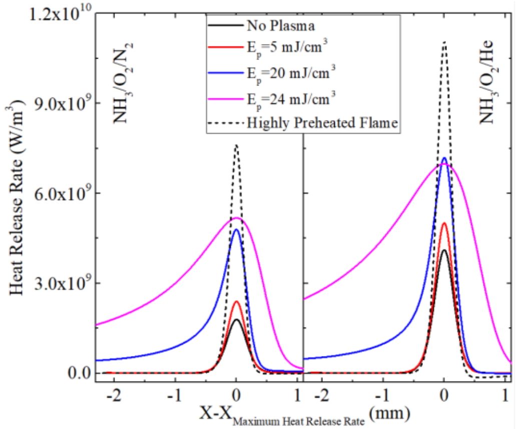
- Works in collaboration with TATA steel and the South Wales Industry have led to the recognition of several streams, product of waste gases, from which ammonia can be recovered for additional power generation via engines, gas turbines or furnaces.
- Current work is taking place with FloGas for new burners running up to **2MW**.

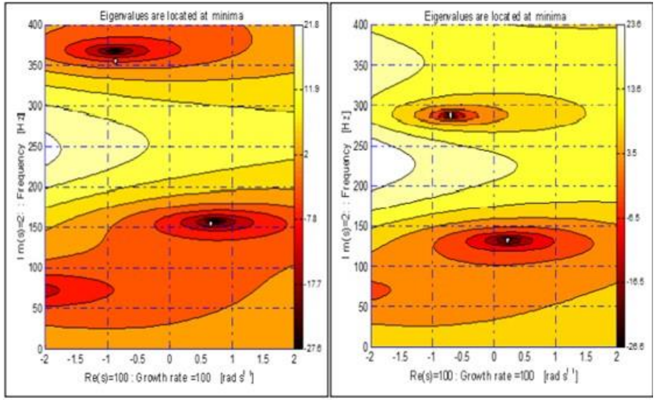
Developments – Boilers/Furn.

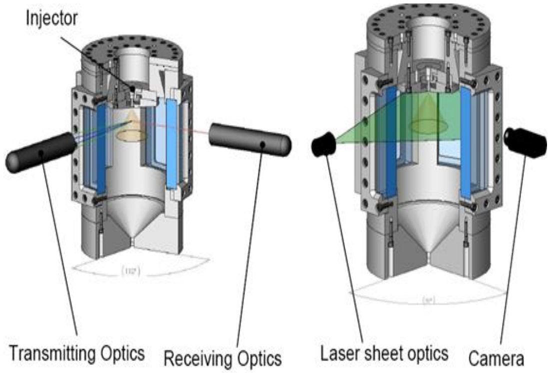


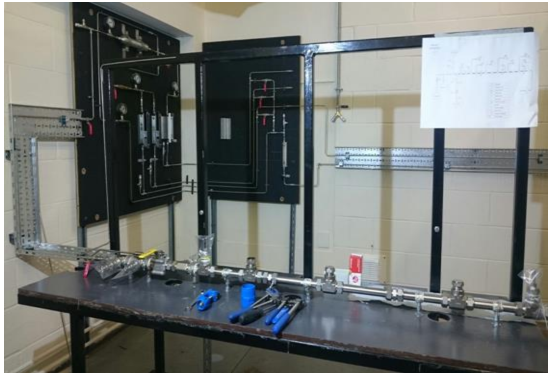


Developments – Other areas









Experimental Additions

Plasmas Combustion (Nox reduction)

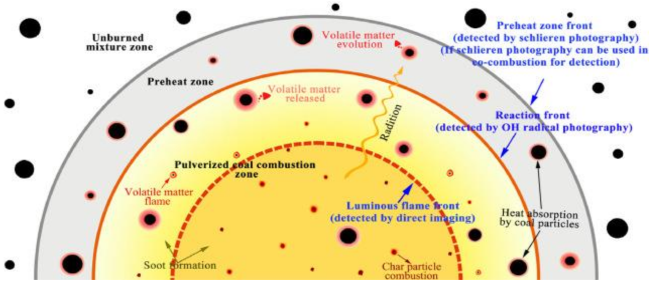
Thermoacoustics (flames stability)

Multi-phase injection (fuel replacement)

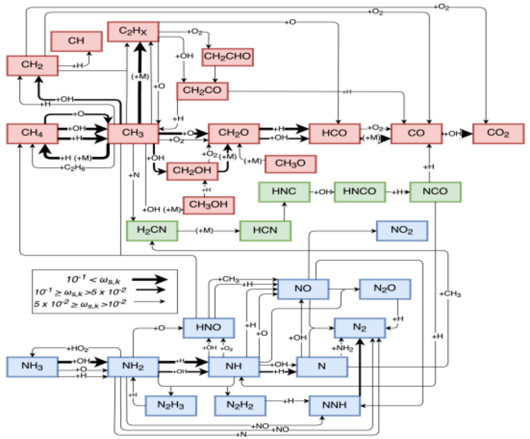
Direct ammonia injection (liquid spray)

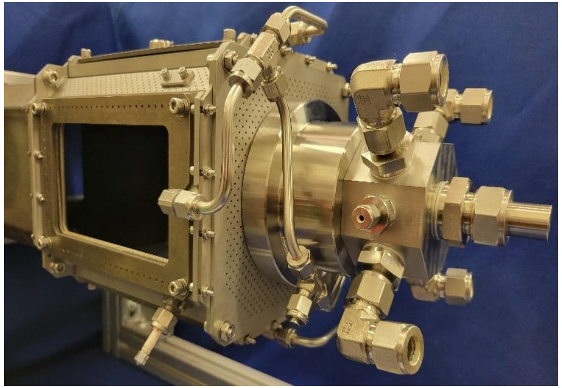
Pulse detonation (explosions)

Developments – Other areas



Assumption of co-combustion flame structures [Xia et al. 2021]





Experimental Additions

Jet Injection (in collaboration with Nottingham)

Materials Analyses

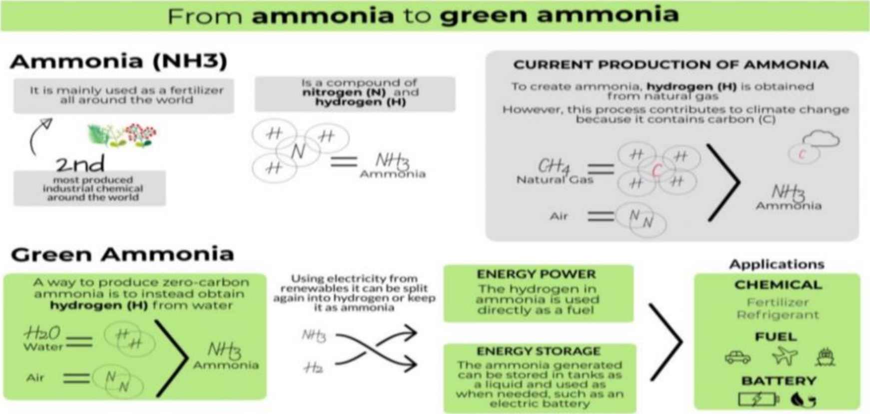
Multi-phase Injection

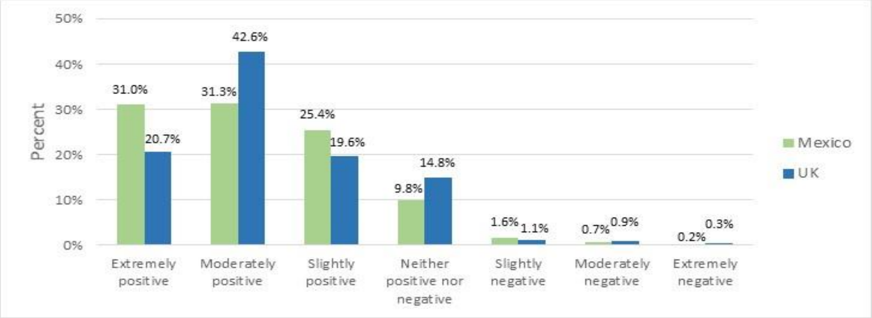
Coal-ammonia co-firing

Additional molecules (ie. cyanide) in reaction pathways

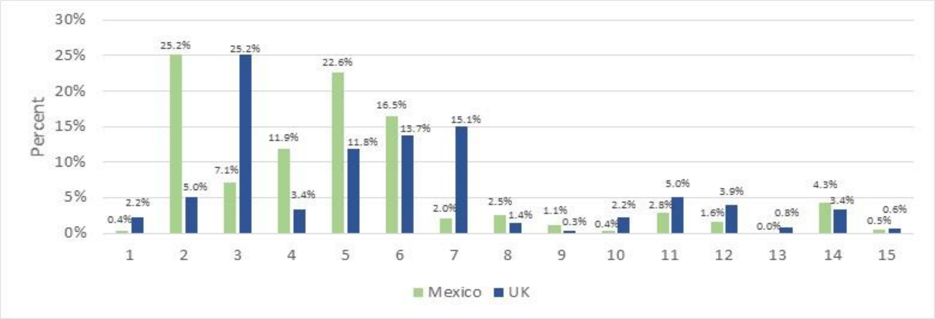
Radiation studies

Developments – H&S/Envirn.

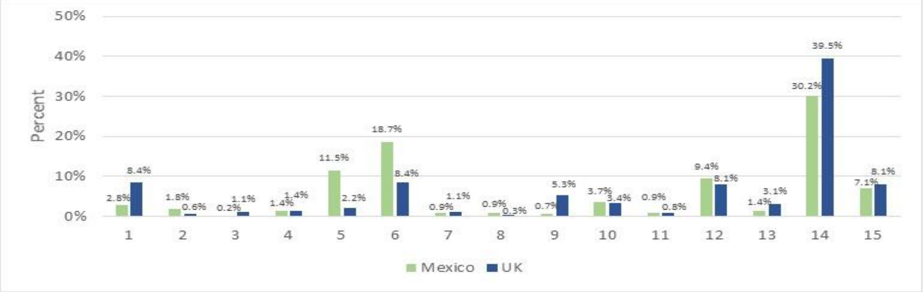




Percent of responses for opinion of green ammonia technology (920 individuals – 357 UK, 563 Mexico).



Percentages for most common answers by country of first associations of ammonia. (1) Nothing/Don't know (2) Poison/toxic (3) Smell (4) Safety (5) Chemical (6) Cleaning products (7) Urine/manure (8) Pollutant (9) Death/killing (10) Fuel (11) Fertilizer/refrigerant (12) Other products (13) Negative (14) Substance (15) Confusion with other chemicals.



Percentages for most common answers by country of perception of green ammonia. (1) Nothing/Don't know (2) Poison/toxic (3) Smell (4) Safety (5) Solution/alternative (6) Novel concept (7) Cost (8) Pollutant (9) Complex/confusing (10) Need more information (11) Water (12) Positive for the environment (13) Negative (14) Generic positive (15) Sceptical.

Conclusions

- Ammonia blends can be used efficiently, with low NOx, and production of species that can be used for combined processes.
- However, ammonia will be only useful for some niche applications.
- Reaction mechanisms need to be accurate and include a variety of complex processes still requiring vast research.
- There are still many points in the combustion of ammonia that require further research, with a lot of input from Public Perception.

THANKS FOR YOUR ATTENTION

FURTHER INFORMATION: VALERAMEDINAA1@CARDIFF.AC.UK