MariNH$_3$
Clean, green ammonia
engines for maritime

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Fuel-NOx & Thermal-NOx Estimation by Modelling in Internal Combustion Engines

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University of Birmingham

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

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- N-emissions formation and NO_X Source

University of Birmingham. Experimental

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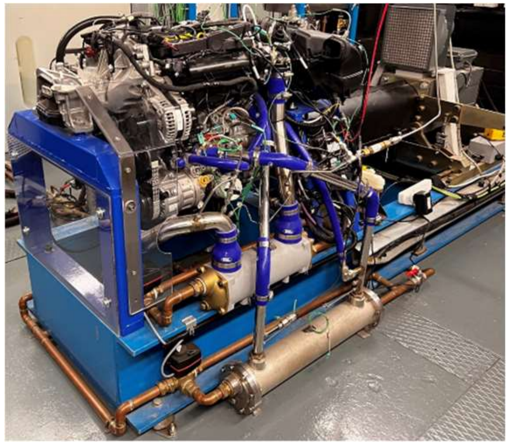
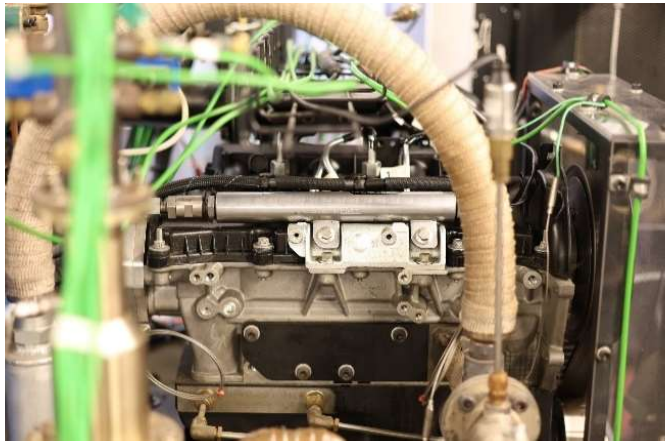
3-Cylinder Gasoline DI Engine



1-Cylinder Diesel Research Engine



Engines Control Room

DRIFT

Bruker VERTEX 70 for Catalysts Characterisation

HSense (V&F)

H_2 Electron Ionization Mass Spectrometer

FTIR MKS MultiGas 2030 (Fourier Transform Infrared Spectroscopy)

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University of Birmingham. Modelling

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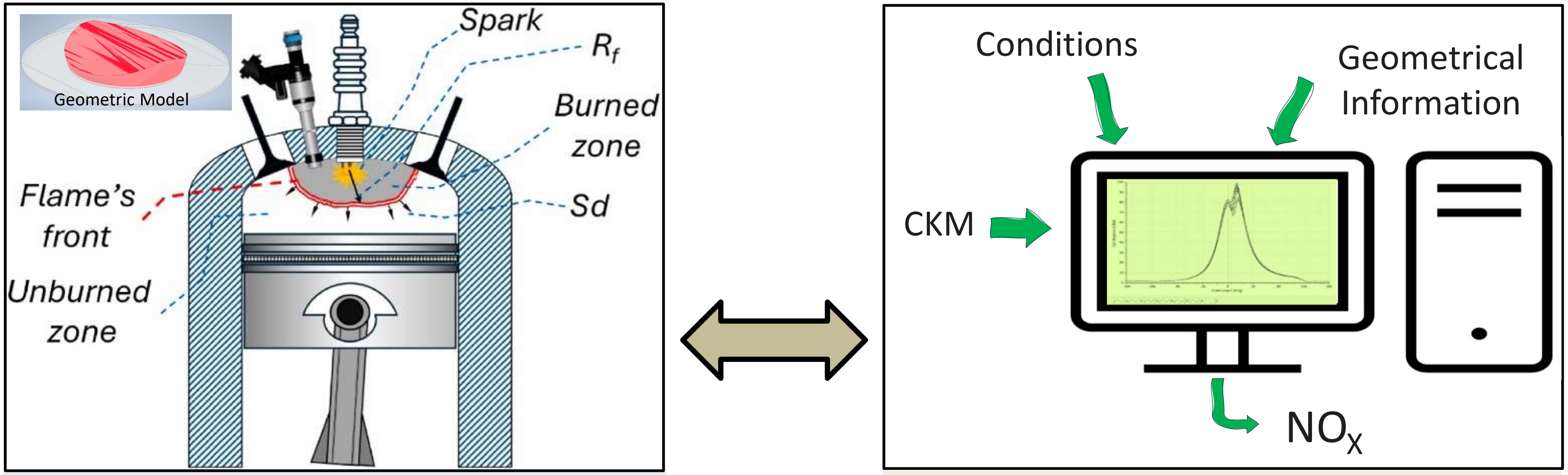

Combustion Propagation of Fuels

- Flame propagation characteristics
- Laminar flame speed (Sl)
- Turbulent combustion speed (St)

Chemical Kinetic Mechanisms (CKM)

- Chemical Reactions
- Thermodynamic properties
- Transport properties

Wu, M. et al. Int J Hydrogen Energy 94, 848-61, 2024. 10.1016/j.ijhydene.2024.11.173
Gabana, P. et al. Fuel 381, 133563, 2025. 10.1016/j.fuel.2024.133563

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NH_3 as a fuel & NH_3 cracking with Heat Recovery

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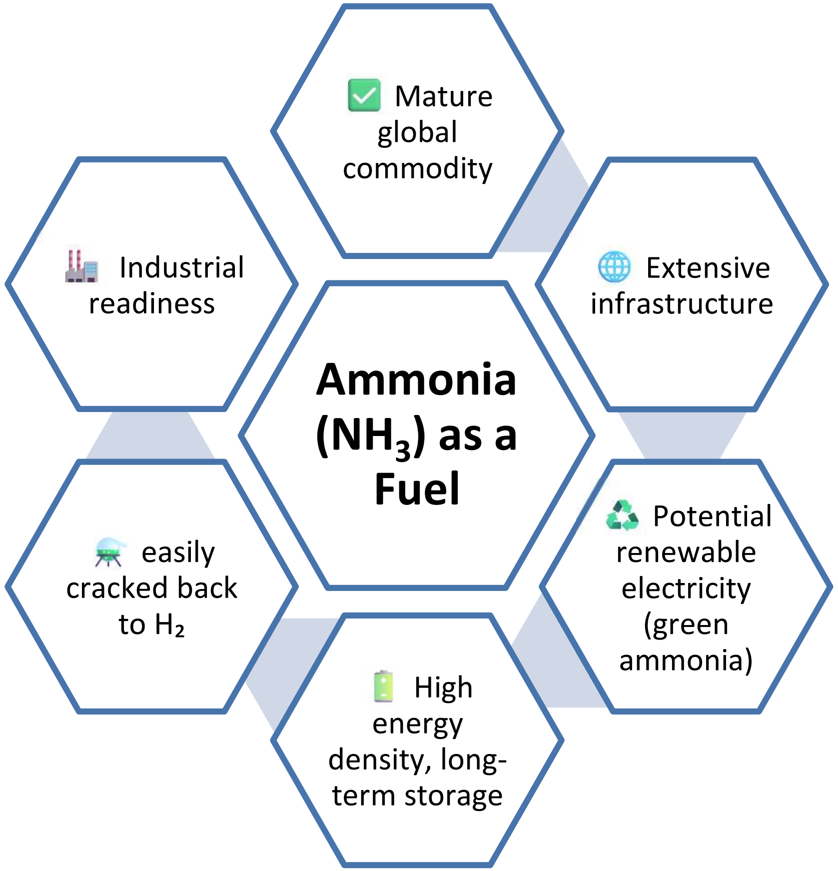

Property	Ammonia (NH_3)	Gasoline
Chemical Formula	NH_3	C_8H_{18} (typical hydrocarbon)
Lower Heating Value (LHV)	~18.6 MJ/kg (5.17 MJ/L)	~44 MJ/kg (32 MJ/L)
Laminar Flame Speed	~7 cm/s	~37 cm/s
Autoignition Temperature	~651°C	~280°C
Flammability Limits (vol%)	15.15–27.35%	~1.4–7.6%
Ignition Energy	~680 mJ	~0.2–0.3 mJ
NO_x Emission Potential	High (due to N-content)	Medium (Temp-dependent)
HC / CO Emissions	None (no C)	High
Greenhouse Gas (GHG) Footprint	Can be near-zero (with green ammonia) attention to N_2O emissions	High CO_2 emissions
Combustion Byproducts	N_2, NO_2, N_2O, NH_3	CO_2, CO, NO_X, HC, PM
Toxicity / Handling	Toxic, pungent, corrosive; requires careful storage	Flammable, volatile; well-established safety

Ammonia is not only a fuel, it's a hydrogen carrier, storage solution, and industrial-ready platform.

NH_3 as a fuel & NH_3 cracking with Heat Recovery

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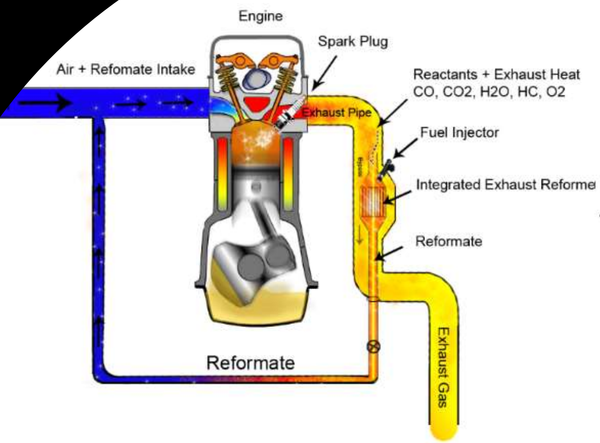
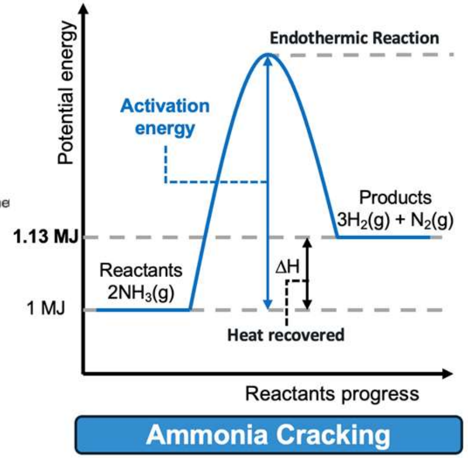
2012 – Assessing the Effects of Partially Decarbonising a Diesel Engine by Co-fuelling with **Dissociated NH_3**
doi.org/10.1016/j.ijhydene.2011.12.137

2013 – NH_3 as Hydrogen Carrier for Transportation; Investigation of the **NH_3 Exhaust Gas Fuel Reforming**
doi.org/10.1016/j.ijhydene.2013.05.144

2015 – Increased NO_2 Concentration in the Diesel Exhaust for Improved Ag/Al_2O_3 **Catalyst** NH_3-SCR Activity
doi.org/10.1016/j.cej.2015.02.067

2021 – **Exhaust Energy Recovery** via Catalytic **NH_3 Decomposition** to H_2 for Low Carbon Clean Vehicles
doi.org/10.1016/j.fuel.2020.119111





$2NH_3 \rightarrow N_2 + 3H_2$, $\Delta H_{298} = +46$ kJ mol^{-1}

Unburnt NH_3 - NOx trade-off?

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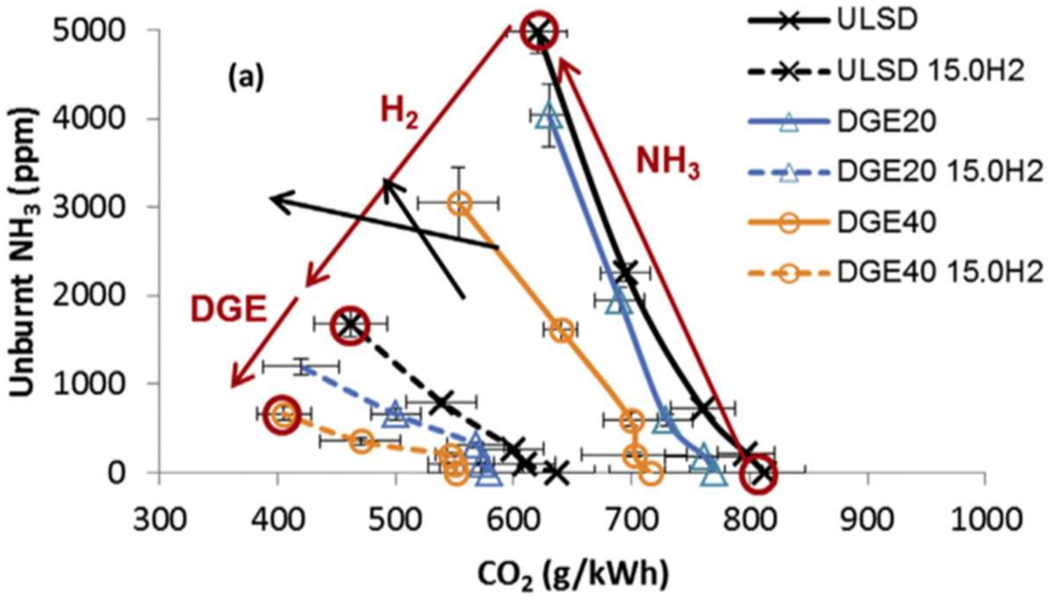

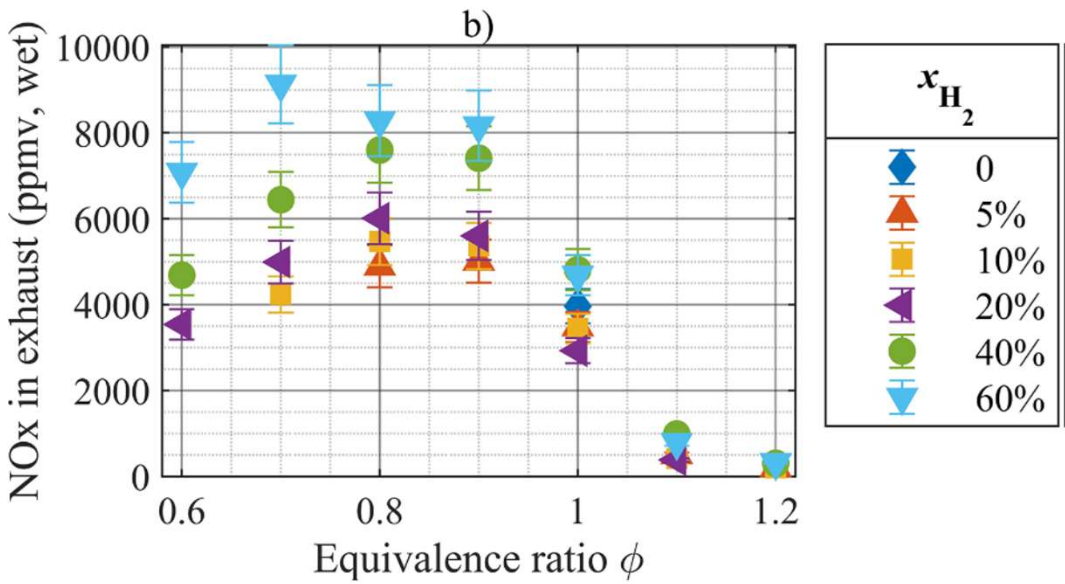

Source: Wang, W. et al. Energy 112, 976, 2016. doi.org/10.1016/j.energy.2016.07.010

Source: Lhuillier, C. et al. Fuel, 269, 117448, 2020. doi.org/10.1016/j.fuel.2020.117448

N-emissions formation and NOx source

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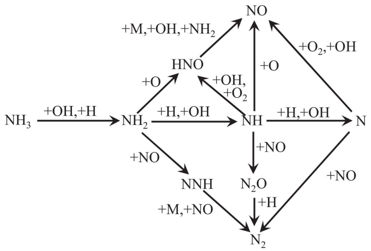
NO_X Formation Pathways



[Miller et al. (2007)](#)

Thermal -NOx

Zel'dovich mechanism

$N_2 + O^\bullet \leftrightarrow \mathbf{NO} + N^\bullet$

$N^\bullet + O_2 \leftrightarrow \mathbf{NO} + O^\bullet$

$N^\bullet + OH^\bullet \leftrightarrow \mathbf{NO} + H^\bullet$

[Lavoie et al. (2007)](#)

NOx

Fuel-NOx

Prompt-NOx

NH_3 oxidation, multiple interconnected pathways

Fenimore mechanism

$N_2 + CH^\bullet \leftrightarrow HCN + N^\bullet$

$HCN + OH^\bullet \leftrightarrow CN^\bullet + H2O$

$CN^\bullet + O_2 \leftrightarrow \mathbf{NO} + CO$

[Fenimore (1971)](#)

Strategic Implications

Strategy	**Technique**
In-Cylinder ($Thermal-NO_X$) ●	EGR, Water Injection, Lean Burn, MILD Combustion
In-Cylinder ($Fuel-NO_X$) ●	Staged Combustion
After-Treatment (NO_X) ●	**SCR**, LNT, TWC, SNCR

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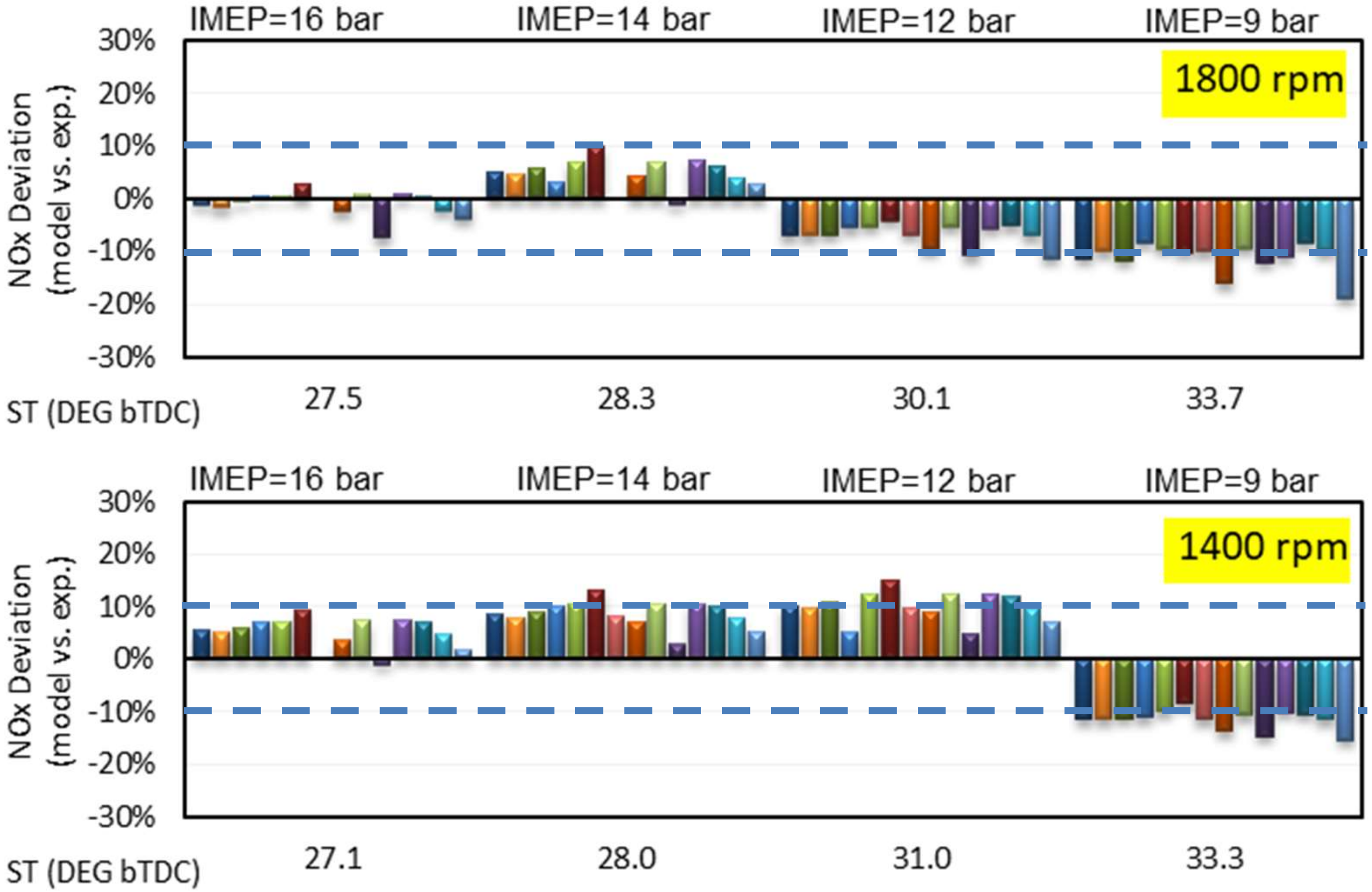

CKM		Author	species/reactions
NAK		Nakamura et al.	33/232
OTO		Otomo et al.	32/213
OKA		Okafor et al.	59/356
STA		Stagni et al.	31/203
BER		Bertolino et al.	31/230
ZHA		Zhang et al	37/263
TAM		Tamaoki et al.	33/228
ZHU		Zhu et al.	43/312
LIU		Liu et al.	30/202
KON		Konnov	127/1207
GLA		Glarborg et al.	151/1397
SHR		Shresta et al.	125/1090
LI		Li et al.	128/957
C3M		C3MechV3.4	3760/16553

Experimental data @ stoichiometry from:

Ambalakatte A, Hegab A, Geng S, Cairns A, Harrington A, Hall J. Bassett M. Evaluation of Ammonia Co-fuelling in Modern Four Stroke Engines. *Johnson Matthey Technology Review* 2024;68:3, 396-411. https://doi.org/10.1595/205651324X17005622661871.

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N-emissions formation and NOx source

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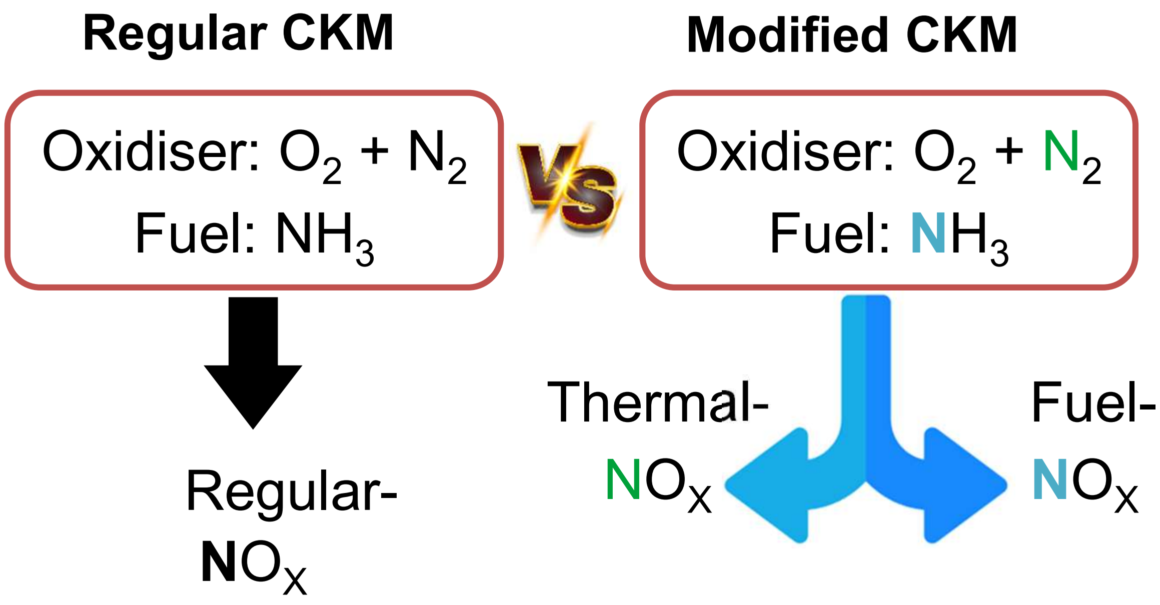
- Nitrogen was decoupled in two "fictitious" nitrogen isotopes N (oxidiser) & N (fuel) is introduced into the CKM.
- By tracking the formation of Regular NO_X and tagged NO_X and NO_X separately, in a modified mechanism:
  - Thermal-NO_X (from atmospheric N_2)
  - Fuel-NO_X (from ammonia's **N**)
- NO_X + NO_X = NO_X vs **N**O_X (Regular)



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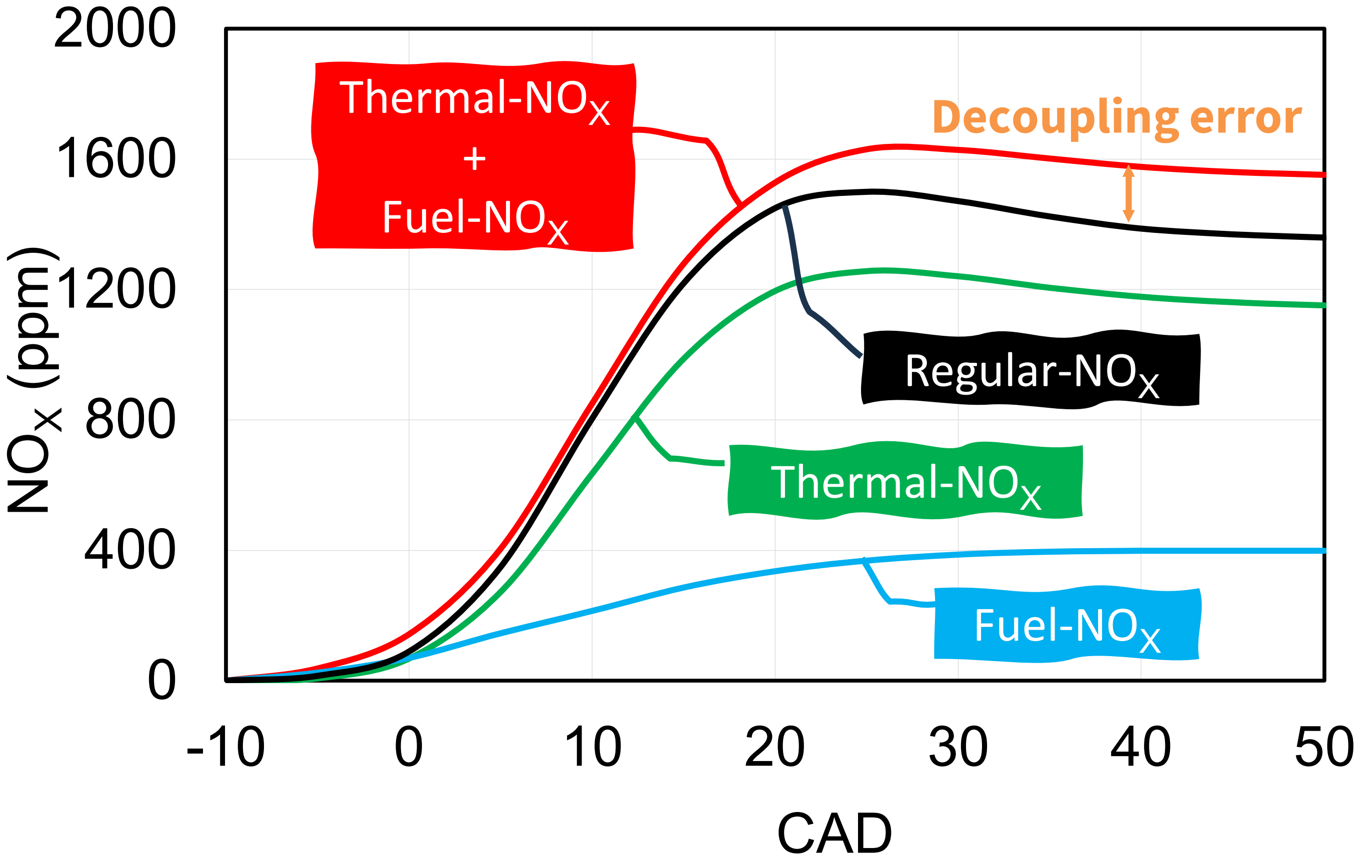
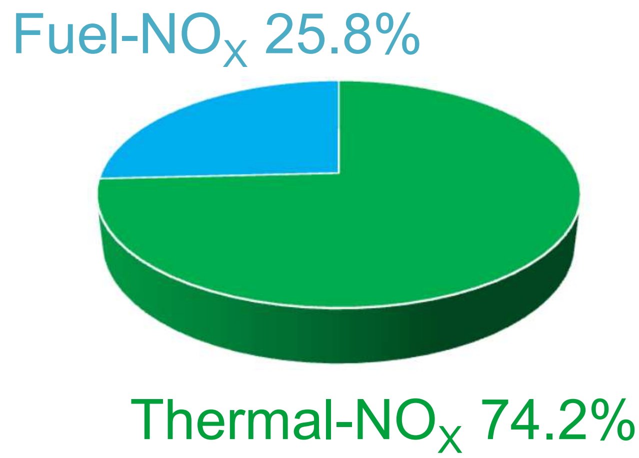


KCM: Otomo, 1800 rpm/12 bar



N-emissions formation and NOx source

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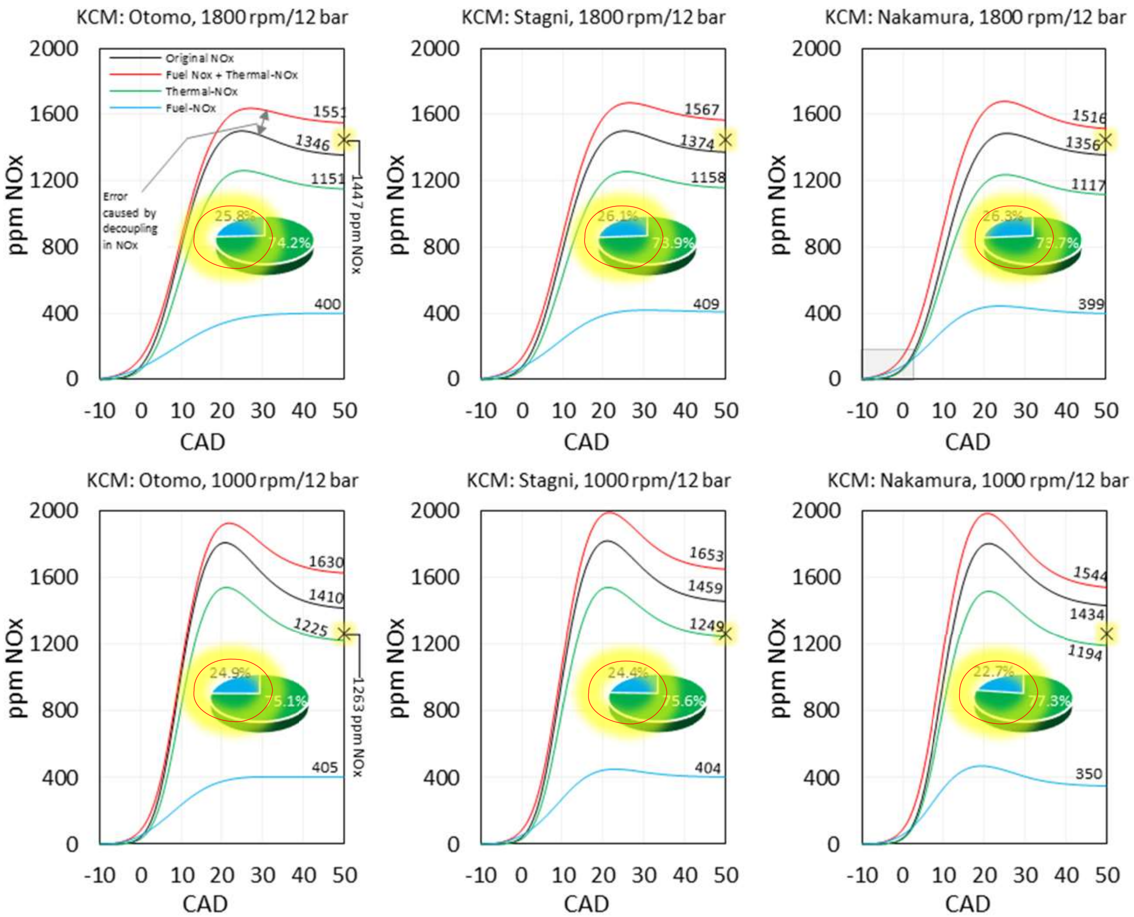

At NH_3 stoichiometric combustion:

- Thermal-NO_X is the dominant pathway (~75% of total NO_X).
- Fuel-NO_X is ~25% of total NO_X).
- The decoupling method overpredicts total NO_X by 10%.

Experimental data @ stoichiometry from:

Ambalakatte A, Hegab A, Geng S, Cairns A, Harrington A, Hall J. Bassett M. Evaluation of Ammonia Co-fuelling in Modern Four Stroke Engines. *Johnson Matthey Technology Review* 2024;68:3, 396-411. https://doi.org/10.1595/205651324X17005622661871.

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Summary

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- Development digital tools calibrated/validated by experimental data
- Evaluation of chemical kinetic mechanisms for **NH_3 → NOx**
- Understanding NO_X Source → %Fuel-NOx vs %Thermal-NOx
- Underpinning solutions to inhibit NOx formation & potential NOx/NH_3 trade-off from NH_3/H_2 combustion

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- EPSRC MariNH3, grant number EP/W016656/1
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- MAHLE Powertrain Ltd
- Johnson Matthey
- University of Valladolid (Spain)

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THANK YOU
ANY QUESTIONS?

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