Computational analysis of a zero-carbon hydrogen fuelled thermal engine for heavy duty transport applications

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Aim

Perform a feasibility study (TRL1), using simplified numerical models, of a new zero-carbon hydrogen-based technology that will allow the fast decarbonisation of trucks and ships.

Outline

- Motivation
- Green ignition promoter
- Aim – Objectives
- Results
- Remaining work
- Acknowledgements

Motivation

- The electrification of heavy-duty applications (e.g., trucks, ships) is currently not very attractive (size of the batteries, charging times).
- UK government (Net zero emission strategy, Oct 2021):
  - by 2040, all HGVs will be zero-emission
  - for maritime, net zero as early as feasible
- Key role of hydrogen:

"Hydrogen is likely to be fundamental to achieving net zero in transport, potentially complementing electrification across modes of transport such as buses, trains and heavy goods vehicles (HGVs). It is also likely to provide solutions for sectors that will not be able to fully decarbonise otherwise, including aviation and shipping. Low carbon hydrogen can provide an alternative to petrol, diesel and kerosene as it can be used directly in combustion engines…"

UK Hydrogen Strategy, Aug 2021

"As set out clearly in the recent Hydrogen Strategy and Transport Decarbonisation Plan, hydrogen is likely to play a significant role in transport applications, particularly where energy density requirements or refuelling times make it the most suitable low carbon energy source. Our dedicated hydrogen R&D funding and support is focussed on heavier applications, such as rail, maritime, aviation and heavy road freight, where hydrogen offers in-use advantages and the largest global market potential."

Net zero emission strategy, Oct 2021

Motivation

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- Can we decarbonise heavy-duty applications using hydrogen, ideally through retrofitting?
- Ships and trucks are predominantly powered currently with compression ignition (CI) engines.
- So, why don't we use hydrogen instead of diesel to fuel these engines?
- Not so simple…
- Fundamental operation of CI engines: air is compressed and close to the top dead center (TDC) the fuel is injected; ignition achieved due to the increased temperature of the heated air.
- The thermodynamic conditions achieved in the engine cylinder must be suitable to allow ignition.
- Autoignition temperatures: **diesel - 483 K**, kerosene - 428 K, **hydrogen - 852 K**

Motivation

Three strategies for using hydrogen in CI engines:

1) Increased compression ratios (> 30) $\Longrightarrow$ engine redesign (typical $CRs = 15 - 20$).
2) Charge/Air preheating (glow plug) $\Longrightarrow$ (scarce literature) decrease of the engine performance, abnormal combustion
3) Dual fuel strategy (use of a pilot fuel to initiate ignition) $\Longrightarrow$ predominantly diesel used as pilot fuel; offers unique flexibility for engine operation

- ❖ **What if we used a non-carbon-based fuel as pilot fuel?**
- ❖ **Ideally, this fuel should exist in the market already (existing logistics support).**

Green ignition promoter

<u>Hydrogen peroxide (H_2O_2)</u>

- ❖ Used as rocket propellant since the 1940s.
- ❖ Research studies for transport applications, used with other carbon-based fuels, e.g., diesel, natural gas etc, for ignition promotion purposes.
- ❖ Can be produced from renewable sources.
- ❖ Existing logistics mechanism;
  - o medical-grade hydrogen peroxide (<10% v/v) can be found in any supermarket
  - o food-grade hydrogen peroxide (<35% v/v) used for cleaning, disinfecting, manufacturing, etc.
  - o industrial use (<90% v/v)

Objectives

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- By examining both a low temperature combustion (LTC) strategy such as the **Homogeneous Charge Compression Ignition (HCCI)** and a conventional dual fuel CI mode, the current project will allow for:
  - The investigation of the effect of H_2O_2 and H_2O addition on the engine performance characteristics.
  - The identification of the sweet spots of the addition of H_2O_2 and H_2O at different engine load and speed conditions.
  - The identification of the associated limitations and challenges, particularly related to the in-cylinder pressure rise rate and NOx emissions, in terms of the mixture composition, the thermodynamic conditions and the injection strategy.
  - The investigation of the effect of the injection strategy on the engine performance characteristics.

Material and Methods

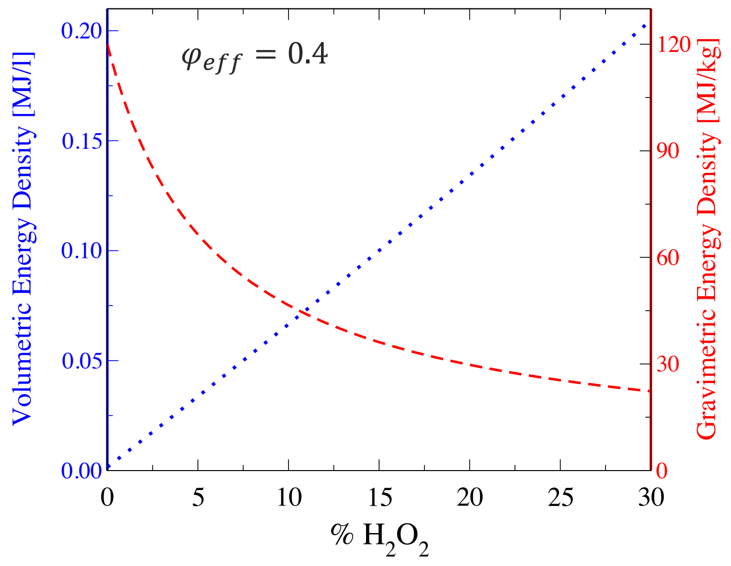
- Zero-dimensional single zone HCCI engine model (Chemkin Pro-ANSYS).
- Species& energy equations plus an additional equation for volume (piston movement).
- Chemical mechanism: Aramco 3 for hydrogen + Glarborg et al. 2018 for nitrogen

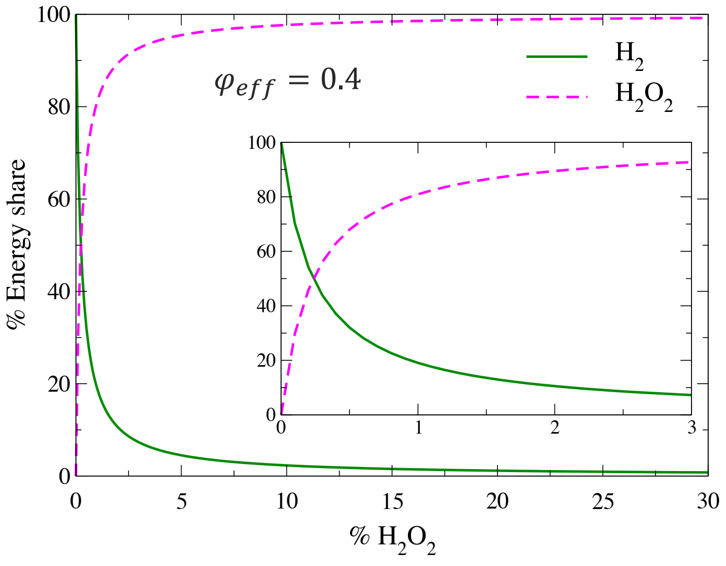
Engine speed	1000, 2000, 3000 rpm
Engine compression ratio	14–20
Bore	100 mm
Stroke	105 mm
Connecting Rod to Crank Radius Ratio	3.714 286
Intake pressure	1 atm
Intake temperature	320 K
Displaced/Swept volume	0.824 6 l

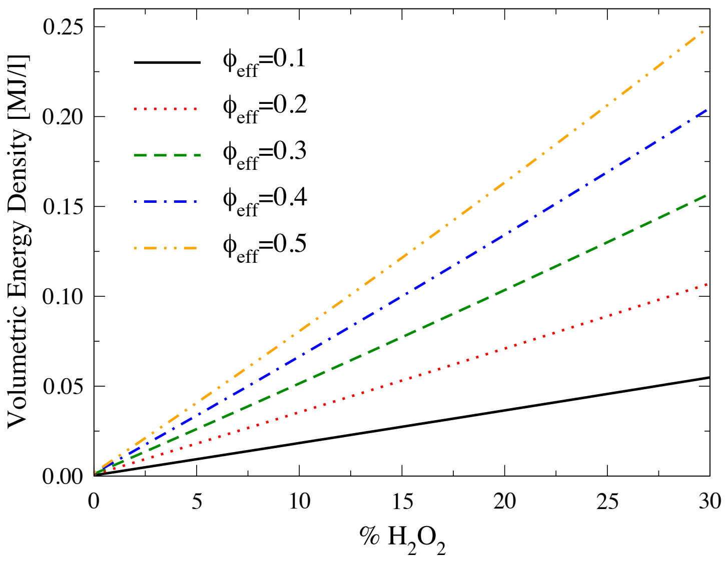
- Conventional definition of the equivalence ratio, no longer valid for H_2/H_2O_2 mixtures.
- Use of effective equivalence ratio: $\varphi_{eff} = \frac{X_{H_2}/(0.5X_{H_2O_2} + X_{O_2})}{(X_{H_2}/X_{O_2})_{st}}$

Material and Methods

- Gravitational energy density: Hydrogen 120 MJ/kg, Hydrogen peroxide 3 MJ/kg
- Volumetric energy density: Hydrogen 0.0104 MJ/l, Hydrogen peroxide 4.4128 MJ/kg
- Addition of hydrogen is performed on a volume basis.
- Hence, in the mixture: the volumetric energy density increases and the gravimetric energy density drops.







Results

- H_2/H_2O_2 blends (adiabatic)

  Iliana D. Dimitrova, Thanos Megaritis, Lionel Christopher Ganippa, Efstathios-Al Tingas, *Int. J. Hydrog. Energ. 47 (2022) 10083-10096*

  - Comparison against "glow plug" approach
  - Effect of H_2O_2 addition on the engine performance
  - Constant (low) load investigation

- H_2/H_2O_2 blends with steam dilution

  Oliver Fernie, Thanos Megaritis, Lionel Christopher Ganippa, Efstathios-Al Tingas, *Fuel (Under review)*

  - Comparison against "glow plug" approach
  - Effect of both H_2O_2 and H_2O addition on the engine performance
  - Constant (high) load investigation

Results - H_2/H_2O_2 blends (adiabatic)

Comparison against "glow plug" approach

	Speed	% H2O2	T_{in}	CAD_{ign}	CAD90	IMEP	Power	Torque	n_{th}	T_{max}	NOx	P_{max}
	Rpm		K	CAD aTDC	CAD aTDC	bar	J/sec	N · m		K	Ppmvd	bar
φ_{eff}=0.1	1000	0.00%	386.1	1.89	2.02	2.12	1458.1	13.9	0.609	1462.7	0.33	67.5
	1000	12.00%	320.0	1.89	4.32	2.75	1891.5	18.1	0.618	1301.3	0.11	70.5
	2000	0.00%	401.4	1.97	2.13	2.03	2791.6	13.3	0.607	1496.0	0.39	66.3
	2000	28.00%	320.0	1.97	4.54	2.96	4071.2	19.4	0.618	1316.6	0.11	71.4
	3000	0.00%	407.3	3.95	4.16	1.99	4109.2	13.1	0.604	1498.3	0.40	64.0
	3000	40.00%	320.0	3.97	6.65	3.09	6374.9	20.3	0.612	1309.4	0.09	69.5
φ_{eff}=0.2	1000	0.00%	374.9	1.84	1.84	4.11	2824.0	27.0	0.596	1779.7	1.21	83.3
	1000	4.25%	320.0	1.84	1.85	5.01	3441.4	32.9	0.606	1672.2	0.81	91.8
	2000	0.00%	390.3	1.69	1.69	3.93	5402.4	25.8	0.594	1812.7	1.43	81.5
	2000	10.00%	320.0	1.70	1.71	5.17	7102.7	33.9	0.607	1688.2	0.92	92.9
	3000	0.00%	399.2	1.85	1.85	3.83	7901.1	25.2	0.592	1831.0	1.57	80.4
	3000	17.00%	320.0	1.86	1.87	5.36	11 055.7	35.2	0.607	1707.1	1.00	94.1
φ_{eff}=0.3	1000	0.00%	369.3	1.49	1.49	5.89	4051.0	38.7	0.583	2068.3	78.68	96.7
	1000	2.50%	320.0	1.49	1.49	7.00	4811.8	45.9	0.592	1975.6	18.51	106.7
	2000	0.00%	383.5	1.75	1.75	5.65	7768.7	37.1	0.581	2096.8	56.15	94.3
	2000	5.50%	320.0	1.75	1.75	7.12	9791.7	46.8	0.591	1986.8	9.97	107.3
	3000	0.00%	393.0	1.51	1.51	5.50	11 341.0	36.1	0.579	2116.5	50.11	92.9
	3000	9.50%	320.0	1.52	1.52	7.29	15 031.9	47.8	0.591	2002.8	8.73	108.5

Results - H_2/H_2O_2 blends (adiabatic)

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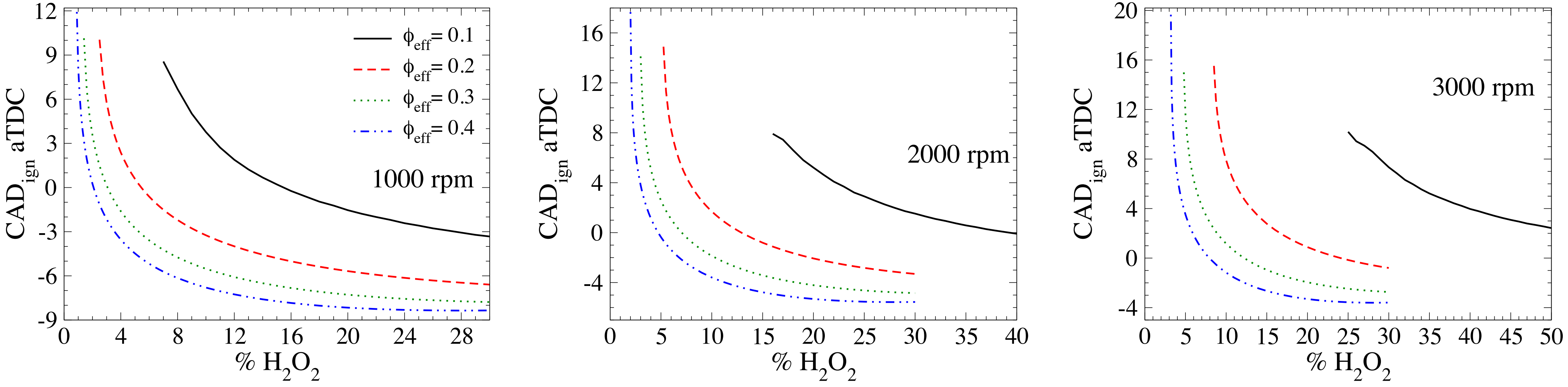
Comparison against "glow plug" approach

- At $\varphi = 0.1$:
  - the required addition of H_2O_2 is 12% - 40% (1000 – 3000 rpm)
  - IMEP, Power and Torque increase significantly (29% - 55%)
  - small increase of the thermal efficiency (~1.5%)
  - impressive NOx decrease (67% - 78%)
- At $\varphi = 0.2$:
  - the required addition of H_2O_2 drops to 4.25% - 17% (1000 – 3000 rpm)
  - IMEP, Power and Torque still increase considerably but less (22% - 40%)
  - small increase of the thermal efficiency (~2.0%)
  - great NOx decrease (33% - 36%)
- At $\varphi = 0.3$:
  - the required addition of H_2O_2 drops further to 2.5% - 9.5% (1000 – 3000 rpm)
  - IMEP, Power and Torque still increase but even less (19% - 33%)
  - small increase of the thermal efficiency (~2.0%)
  - significant NOx decrease (77% - 83%)

Results - H_2/H_2O_2 blends (adiabatic)

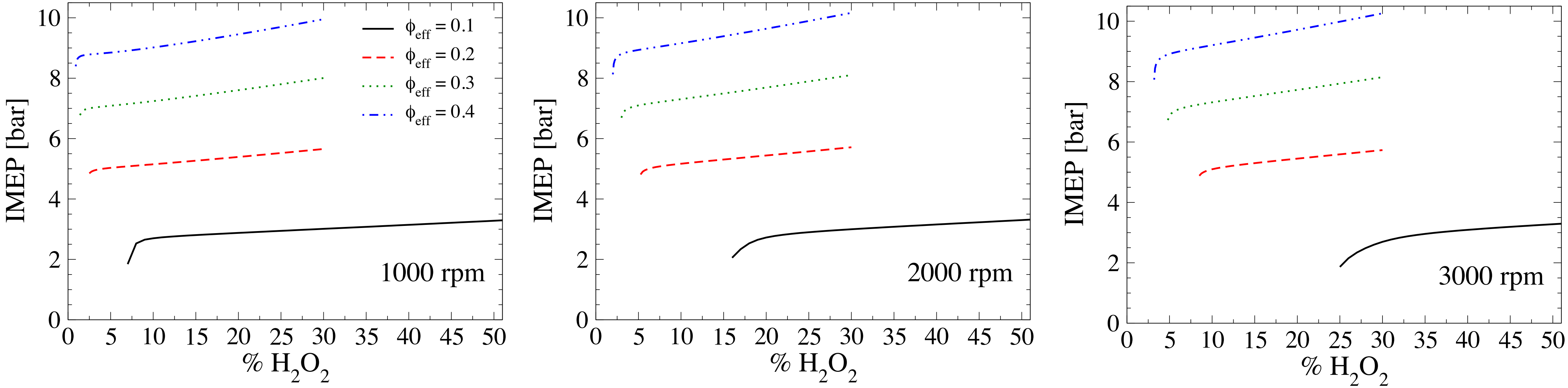
Effect of H_2O_2 addition on the engine performance



- The addition of H_2O_2 results initially in drastic reduction of the CAD_{ign} and further addition has negligible effect on the ignition promotion.
- As the mixture becomes richer and regardless the engine speed, the effect of H2O2 addition on the ignition promotion becomes more pronounced.

Results - H_2/H_2O_2 blends (adiabatic)

Effect of H_2O_2 addition on the engine performance



- ❖ The addition of H_2O_2 increases the IMEP, power, torque for all engine speeds and effective equivalence ratios.
- ❖ H_2O_2 induces linear change
- ❖ As the mixture becomes richer the effect of H_2O_2 addition on IMEP, power and torque becomes stronger at a gradually smaller rate.

Results - H_2/H_2O_2 blends (adiabatic)

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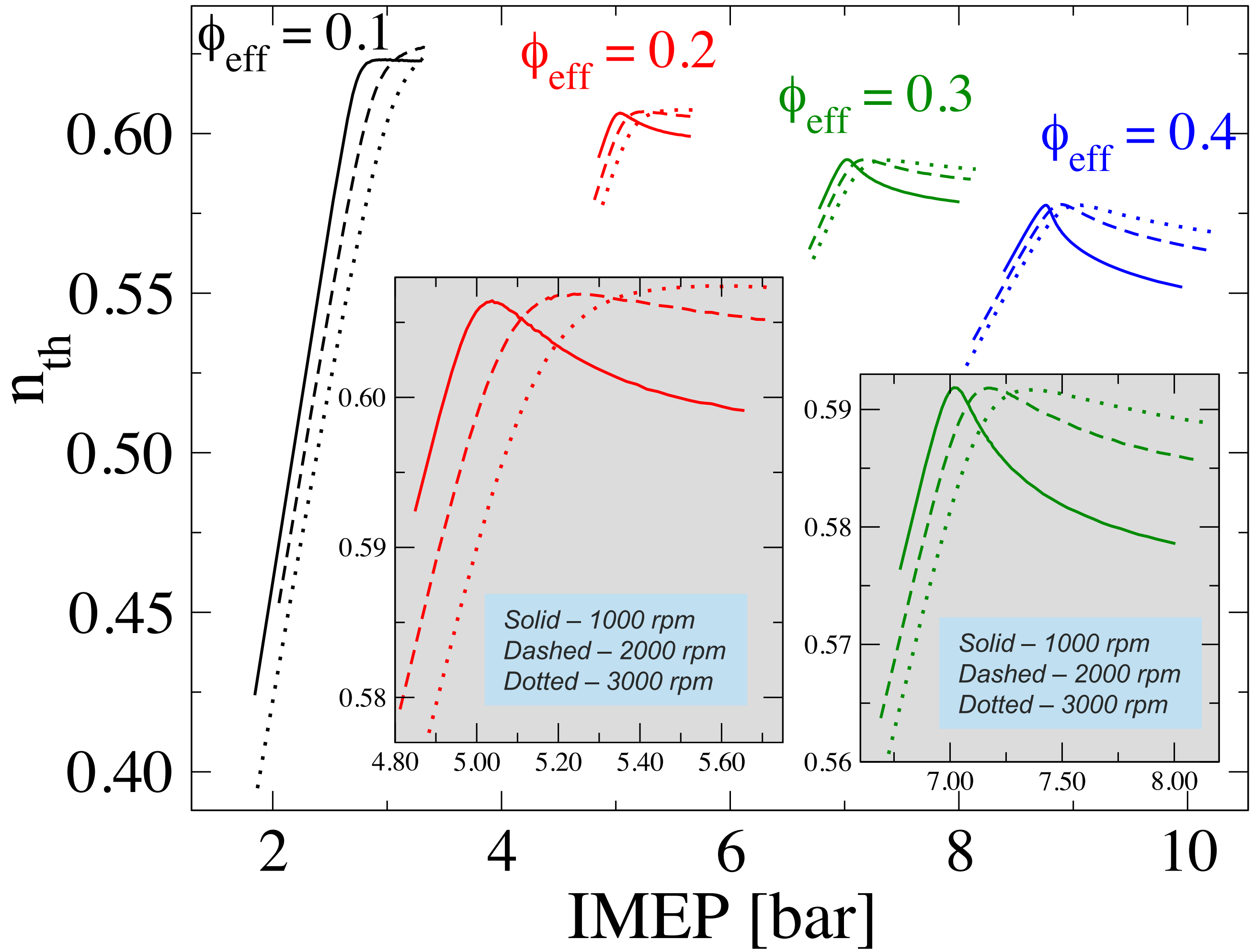
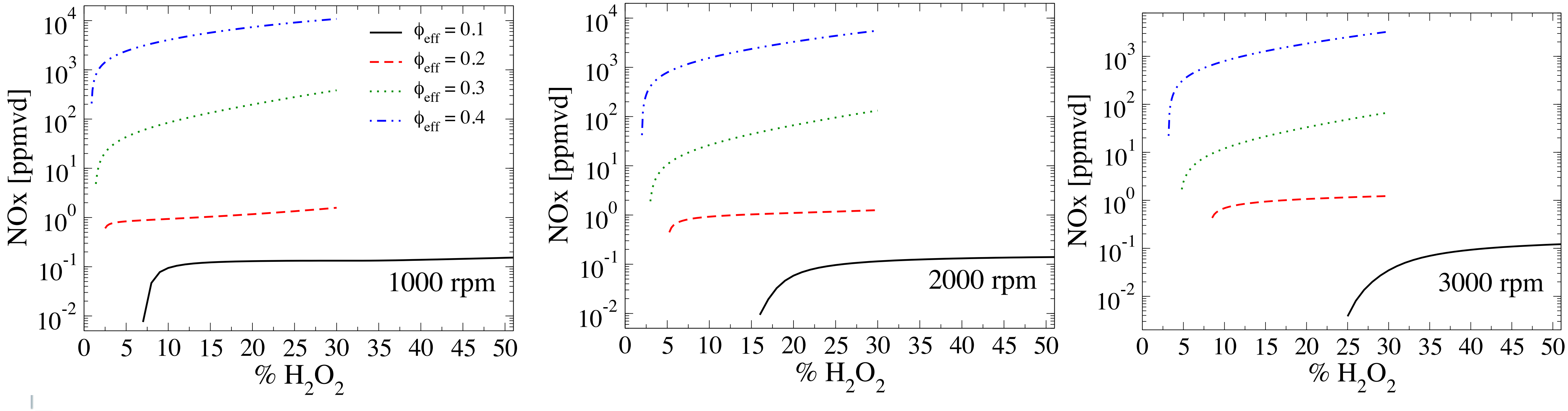
Effect of H_2O_2 addition on the engine performance



- The max n_{th} for each case of φ_{eff} and rpm does not coincide with the max load value.
- At constant φ_{eff} and low loads, the engine speed appears to move the curve to the right, i. e, the same n_{th} is achieved by the same IMEP difference between two speeds.
- As the engine load is increased further (beyond the threshold corresponding to the max n_{th}) and n_{th} starts dropping at constant φ_{eff}, there is great variation in the response of the n_{th} due to the engine speed.
- These load and n_{th} values are significantly higher than those reported in the earlier experimental works.

Results - H_2/H_2O_2 blends (adiabatic)

Effect of H_2O_2 addition on NOx



- At sufficiently low effective equivalence ratios, e.g., $\varphi_{eff} = 0.1$ or 0.2, NOx emissions are so low that would not require any after-treatment.
- The main reason for the decreased NOx emissions at sufficiently low φ_{eff} values is the low maximum temperatures reached (1,380 - 1,750 K).

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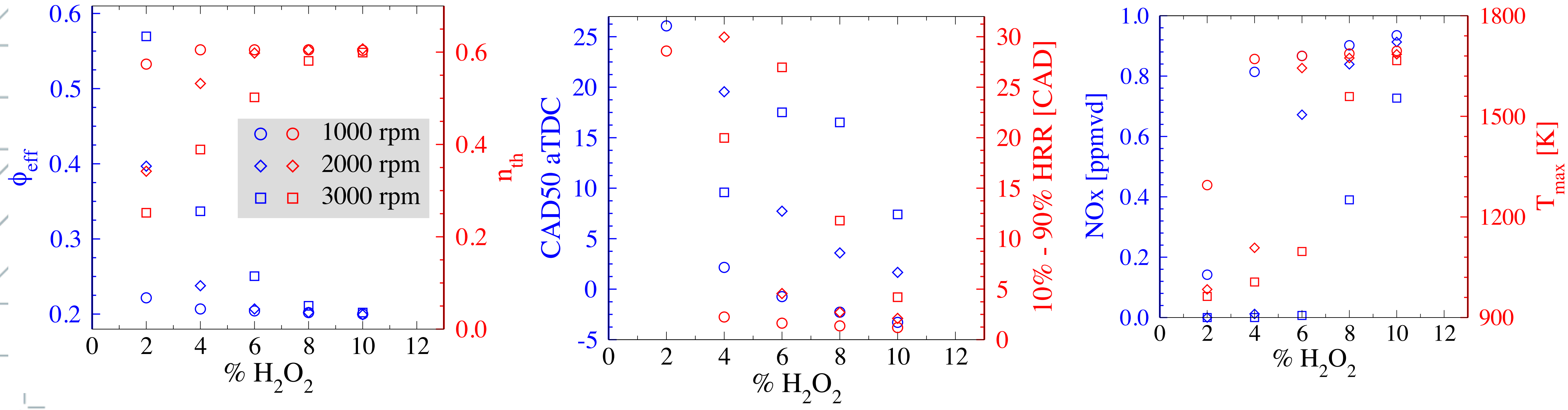
Results - H_2/H_2O_2 blends (adiabatic)

Constant (low) load ($33.8\ N \cdot m$) investigation



- Strong effect of H_2O_2 addition (especially at 2000 and 3000 rpm). In view of n_{th} the H_2O_2 addition has practical value for percentages equal or larger than **4%** ($\varphi_{eff} = 0.2068$) at 1000 rpm, **6%** ($\varphi_{eff} = 0.2068$) at 2000 rpm and **8%** ($\varphi_{eff} = 0.211$) at 3000 rpm.
- NOx emissions are extremely low ($< 1\ ppmvd$) at all cases of H_2O_2 addition and engine speeds which is attributed to the generally low maximum temperatures (1500 - 1700 K).

Results

- H_2/H_2O_2 blends (adiabatic)

  Iliana D. Dimitrova, Thanos Megaritis, Lionel Christopher Ganippa, Efstathios-Al Tingas, *Int. J. Hydrog. Energ. 47 (2022) 10083-10096*

  - Comparison against "glow plug" approach
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- H_2/H_2O_2 blends with steam dilution

  Oliver Fernie, Thanos Megaritis, Lionel Christopher Ganippa, Efstathios-Al Tingas, *Fuel (In progress)*

  - Comparison against "glow plug" approach
  - Effect of both H_2O_2 and H_2O addition on the engine performance
  - Constant (high) load investigation

Results - H_2/H_2O_2 blends with steam dilution

Comparison against "glow plug" approach (adiabatic)

ϕ_{eff}	Speed rpm	% H_2O	% H_2O_2	T_{in} K	T_{max} K	P_{max} bar	NOx ppmvd	IMEP bar	Torque $N \cdot m$	n_{th}	RBA CAD
$\phi_{eff}=0.3$	1000	0	1.78	320	1962	102	11.67	6.93	45.5	0.588	1.41
		0	0.00	364	2046	94	41.64	5.96	39.1	0.581	0.37
		5	2.55	320	1886	99	3.39	6.58	43.2	0.585	1.69
		5	0.00	370	1979	89	13.92	5.51	36.2	0.576	0.49
		10	3.67	320	1815	95	1.31	6.24	41.0	0.582	1.92
		10	0.00	377	1916	85	4.79	5.10	33.5	0.572	0.62
		15	5.34	320	1749	92	0.79	5.93	38.9	0.580	2.11
		15	0.00	383	1855	81	1.86	4.70	30.8	0.568	0.77
$\phi_{eff}=0.4$	2000	0	2.73	320	2238	115	341.4	8.76	57.5	0.575	0.84
		0	0.00	373	2329	102	994.0	7.26	47.6	0.565	0.20
		5	3.95	320	2148	111	98.60	8.35	54.8	0.572	0.97
		5	0.00	381	2247	97	345.0	6.72	44.1	0.561	0.28
		10	5.79	320	2066	107	28.29	7.97	52.3	0.569	1.06
		10	0.00	388	2168	92	114.0	6.21	40.8	0.558	0.37
		15	8.76	320	1991	104	8.65	7.63	50.1	0.567	1.11
		15	0.00	394	2092	88	36.40	5.73	37.6	0.554	0.48
$\phi_{eff}=0.5$	3000	0	3.27	320	2479	125	3615.0	10.34	67.9	0.559	0.50
		0	0.00	378	2567	110	7256.4	8.37	54.9	0.547	0.12
		5	4.82	320	2380	121	1250.4	9.91	65.1	0.558	0.57
		5	0.00	386	2472	104	3073.8	7.79	51.1	0.547	0.17
		10	7.32	320	2289	117	413.3	9.52	62.5	0.557	0.60
		10	0.00	393	2380	99	1119.0	7.21	47.3	0.544	0.24
		15	11.90	320	2213	114	148.8	9.23	60.6	0.554	0.59
		15	0.00	400	2293	94	374.0	6.66	43.7	0.542	0.32

The hydrogen peroxide strategy results in:

- Higher (16-39%) engine performance (IMEP, power, torque), favored as steam dilution or effective equivalence ratio increase.
- Negligible increase (~2%) of the thermal efficiency.
- Remarkable decrease (50%-76%) of NOx emissions, favored as the steam dilution decreases.

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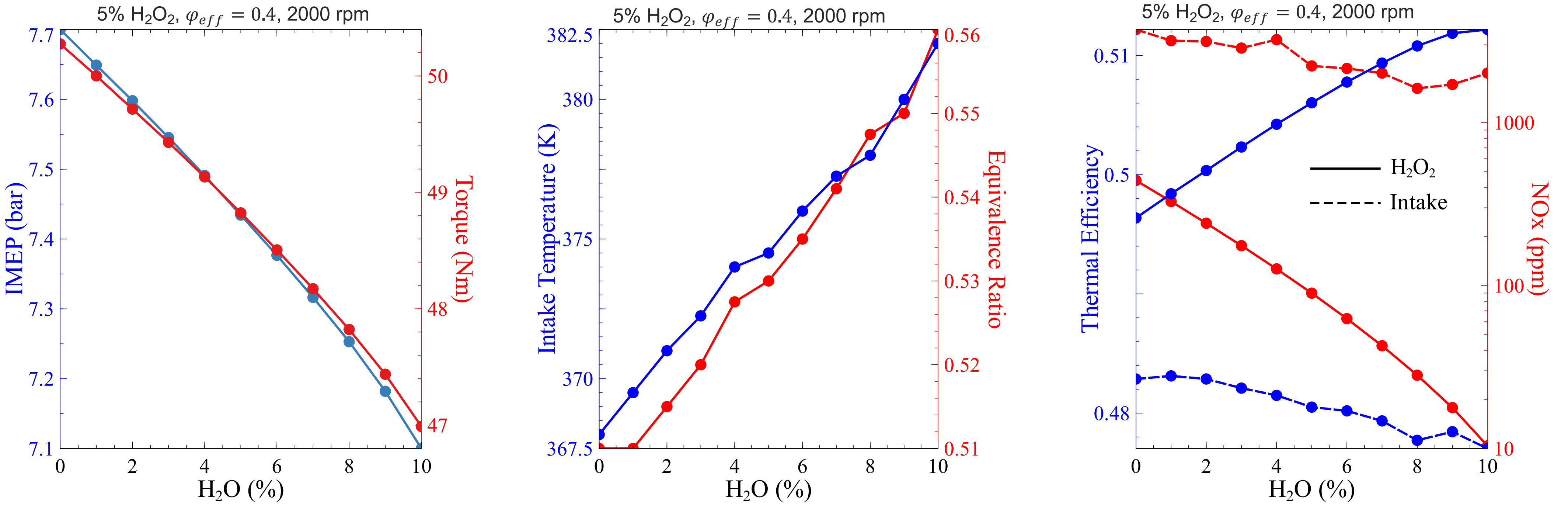
Results - H_2/H_2O_2 blends with steam dilution

Comparison against "glow plug" approach (non-adiabatic)

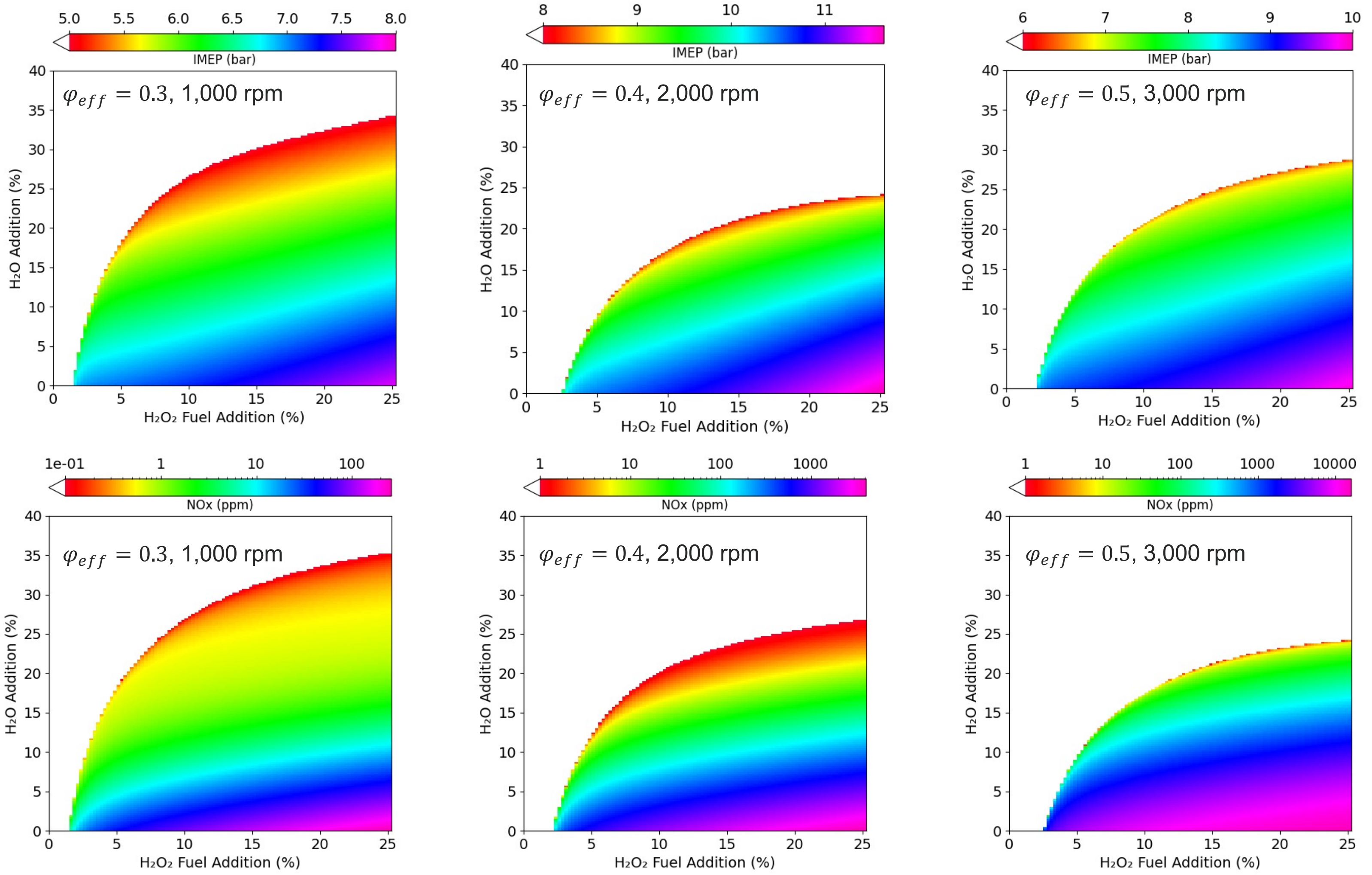


- Achieving the same load output (2000 rpm) with two approaches, while increasing the steam dilution from 0 to 10%: 5% H_2O_2, $T_{in} = 320\ K$ and $\varphi_{eff} = 0.4$ **versus** 0% H_2O_2 and increasing T_{in} and φ_{eff}.

- For both n_{th} and NOx, the difference between the 2 approaches becomes more pronounced as steam dilution increases.

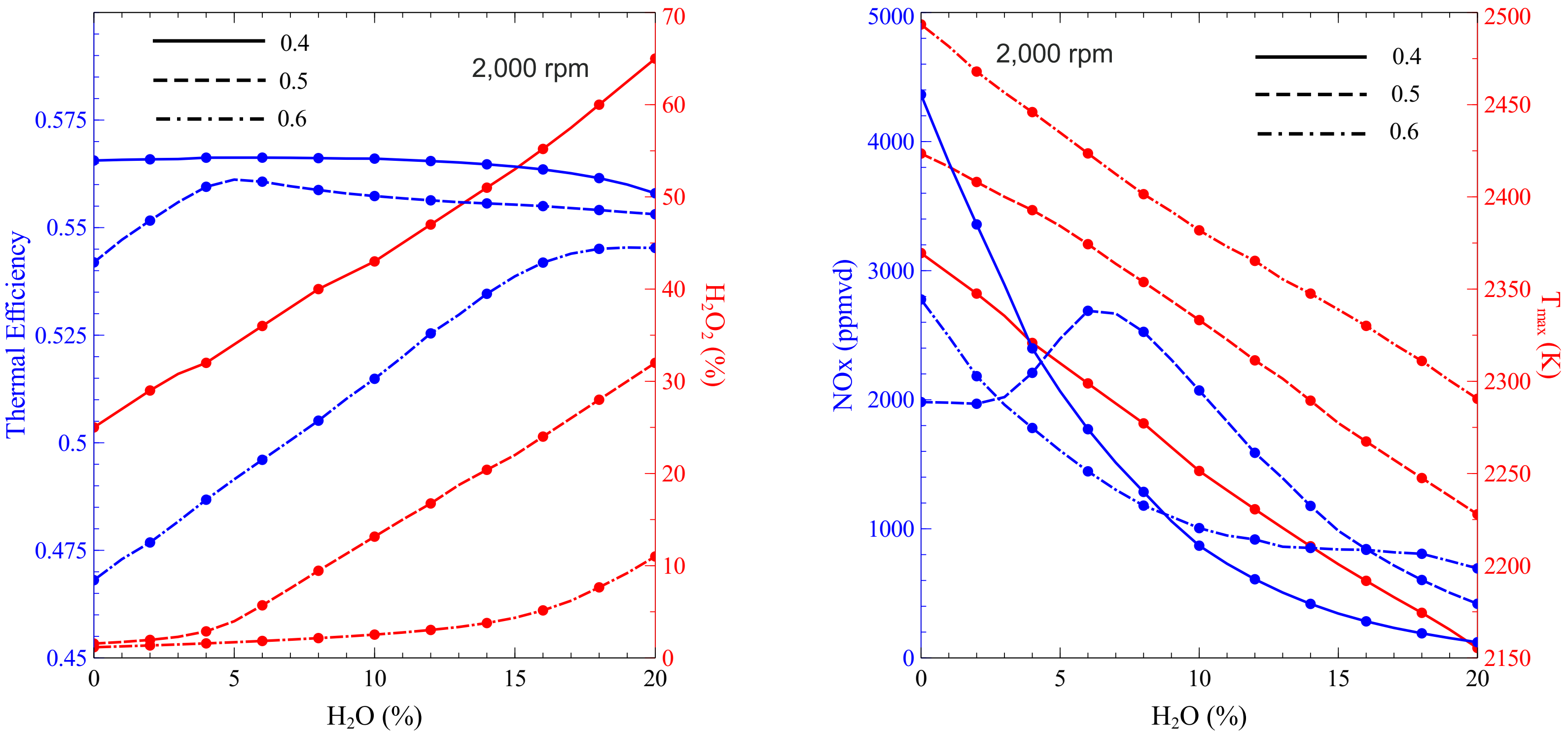
Results - H_2/H_2O_2 blends with steam dilution

Effect of H_2O_2 and H_2O addition on the engine performance



Results - H_2/H_2O_2 blends with steam dilution

Constant (high) load (65 $N \cdot m$) investigation



- ❖ For high load conditions and 2000 rpm, the best approach would be to use a relatively high equivalence ratio, e.g., 0.6, and ample steam dilution (~20%).
- ❖ This leads to very low NOx emissions and only ~10% of H_2O_2 is required.

Summary

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- The use of H_2O_2 as an ignition promoter instead of inlet preheating proved to provide substantially better engine performance and reduced NOx emissions.
- The addition of H_2O_2 leads to significant increase of IMEP, torque and power, small increase of the thermal efficiency and considerable decrease of NOx.
- Steam dilution can be an invaluable tool in minimizing NOx emissions with the proposed technology.
- In fact, balancing the equivalence ratio and the steam dilution, the hydrogen peroxide can be maintained to lower than 10-12% per hydrogen volume.

Remaining work

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- CI engine model development and validation with a benchmark dataset.
- An analysis on of the CI engine performance and NOx emission based on the injection strategy of H_2O_2.
- An analysis on the effects of H_2O/H_2O_2 blends injected in the H_2/air CI engine in view of the engine performance characteristics and NOx emissions.

- HCCI engine operation maps in view of the maximum desired pressure rise rate and the minimum desired combustion efficiency. These maps will additionally reflect other engine performance characteristics (IMEP, torque, thermal efficiency, NOx) in the acceptable range of engine operation.

Funding

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Awarded

- EPSRC Network-H2, (2021), £40k
- Royal Society of Edinburgh (2020), £65k

In preparation (EPSRC, responsive mode)

- One bid with Imperial College London and University of Cambridge, ~£2m (fundamental research on gas turbines and CI engines).
- One bid with Brunel University London and University of Cambridge, ~£1.5m (CI engine experiments and high-fidelity numerical simulations).

Thank you!

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