Engines, Energy and
Environment Group

Synergetic application of 0/1/3D-CFD approaches for hydrogen-fuelled spark ignition engine simulation

GLOBAL GT VIRTUAL CONFERENCE 2021

OCTOBER 19TH – 21ST , 2021

MILLO, F., ROLANDO, L., PIANO, A., ACCURSO, F., GULLINO, F., ROGGIO, S., *Politecnico di Torino*

PESCE, F., VASSALLO, A., *PUNCH Torino*

ROSSI, R., *PUNCH Hydrocells*

BIANCO, A., *POWERTECH Engineering*

21st October 2021

Agenda

- Introduction
- Case study
- Simulation methodology
- Results
- Conclusions

Introduction

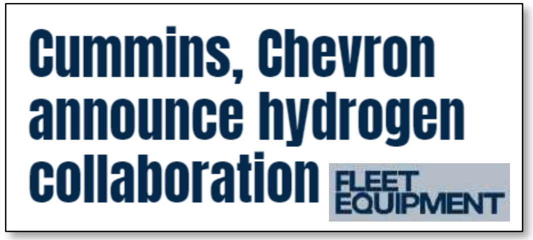
The CO2 challenge, the BEV pain point

Within the framework of policy actions aiming to address the issue of climate change, also the **HD sector** has to **play a major role**.

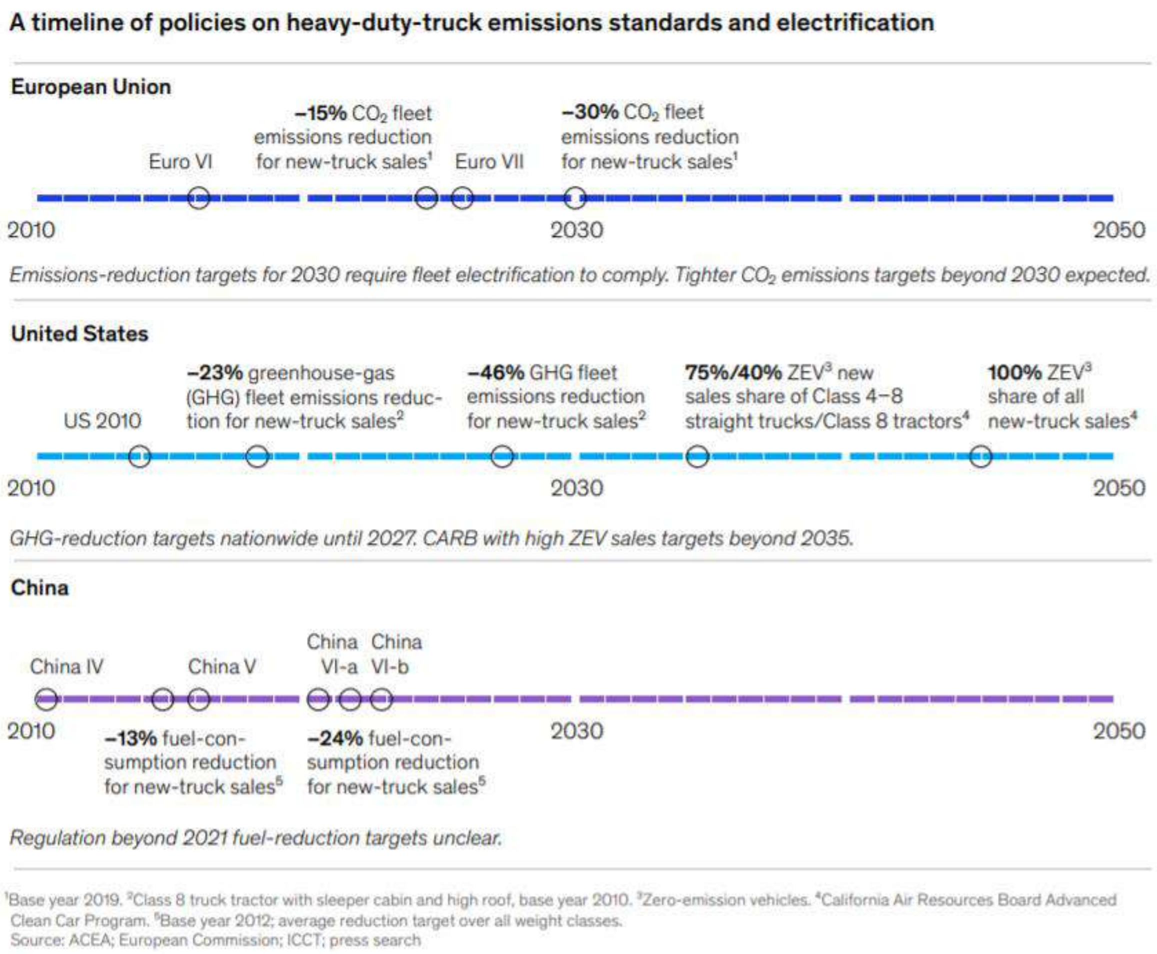
- ❑ **CO2 target** for Heavy Duty (EU reg. 2019/1242)
- ❑ **ZERO EMISSION VEHICLES** procurement **target** (EU directive 2019/1161)
- ❑ Increasing number of US states considering **Low Carbon Fuel Standard**
- ❑ **Long charging time** & payload reduction: pain point of BEV's for Commercial & Heavy Duty

Hydrogen is a viable solution!


Hyundai Motor Group unveils its hydrogen strategy, plans to offer fuel cell versions of commercial cars by 2028


Cummins, Chevron announce hydrogen collaboration


Ricardo advances hydrogen engine to support the decarbonisation of transport


A timeline of policies on heavy-duty-truck emissions standards and electrification

Emissions-reduction targets for 2030 require fleet electrification to comply. Tighter CO₂ emissions targets beyond 2030 expected.

GHG-reduction targets nationwide until 2027. CARB with high ZEV sales targets beyond 2035.

Regulation beyond 2021 fuel-reduction targets unclear.

[1] Base year 2019. [2] Class 8 truck tractor with sleeper cabin and high roof, base year 2010. [3] Zero-emission vehicles. [4] California Air Resources Board Advanced Clean Car Program. [5] Base year 2012; average reduction target over all weight classes.
Source: ACEA; European Commission; ICCT; press search

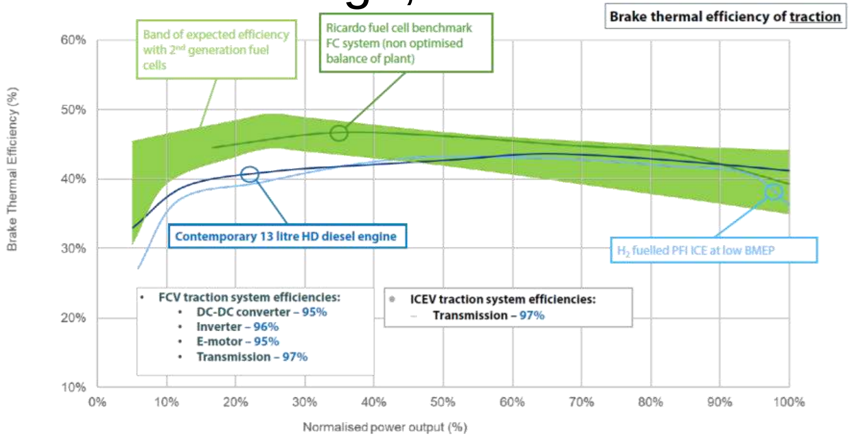
Bernd Heid, Christopher Martens, and Anna Orthofer, "How hydrogen combustion engines can contribute to zero emissions", McKinsey & Company 2021

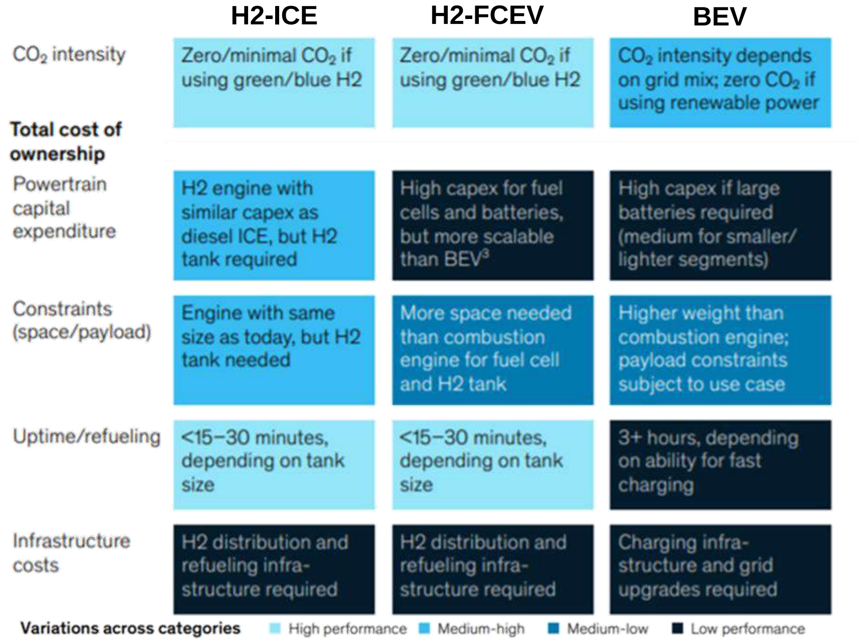
Introduction

Hydrogen ICE strengths

Within the framework of policy actions aiming to address the issue of climate change, also the **HD sector** has to **play a major role**.

- **H2-ICE** for Commercial & Heavy Duty **at similar cost of Diesel engines** (<< of Fuel Cell or Battery)
- **H2-ICE** considered as “**zero-emission vehicle**”
- **No compromise** in driving range, payload and reliability
  Retrofitting of existing vehicle & engine architectures
- **Reuse of existing footprints & skills**, with positive LCA (production & recycle), **quick time to market**
- Improve/keep **sound experience** of existing engines
- Capability to operate at Heavy Duty conditions for prolonged time & in harsh environment
- **Quick refueling time** (like for actual engines)
  Reduced recharging footprint & no grid peak load vs BEV
  Few H2 stations sufficient for hub based specific fleets





	H2-ICE	H2-FCEV	BEV
CO_2 intensity	Zero/minimal CO_2 if using green/blue H2	Zero/minimal CO_2 if using green/blue H2	CO_2 intensity depends on grid mix; zero CO_2 if using renewable power
Total cost of ownership			
Powertrain capital expenditure	H2 engine with similar capex as diesel ICE, but H2 tank required	High capex for fuel cells and batteries, but more scalable than BEV[3]	High capex if large batteries required (medium for smaller/ lighter segments)
Constraints (space/payload)	Engine with same size as today, but H2 tank needed	More space needed than combustion engine for fuel cell and H2 tank	Higher weight than combustion engine; payload constraints subject to use case
Uptime/refueling	<15–30 minutes, depending on tank size	<15–30 minutes, depending on tank size	3+ hours, depending on ability for fast charging
Infrastructure costs	H2 distribution and refueling infra-structure required	H2 distribution and refueling infra-structure required	Charging infra-structure and grid upgrades required

Variations across categories ■ High performance ■ Medium-high ■ Medium-low ■ Low performance

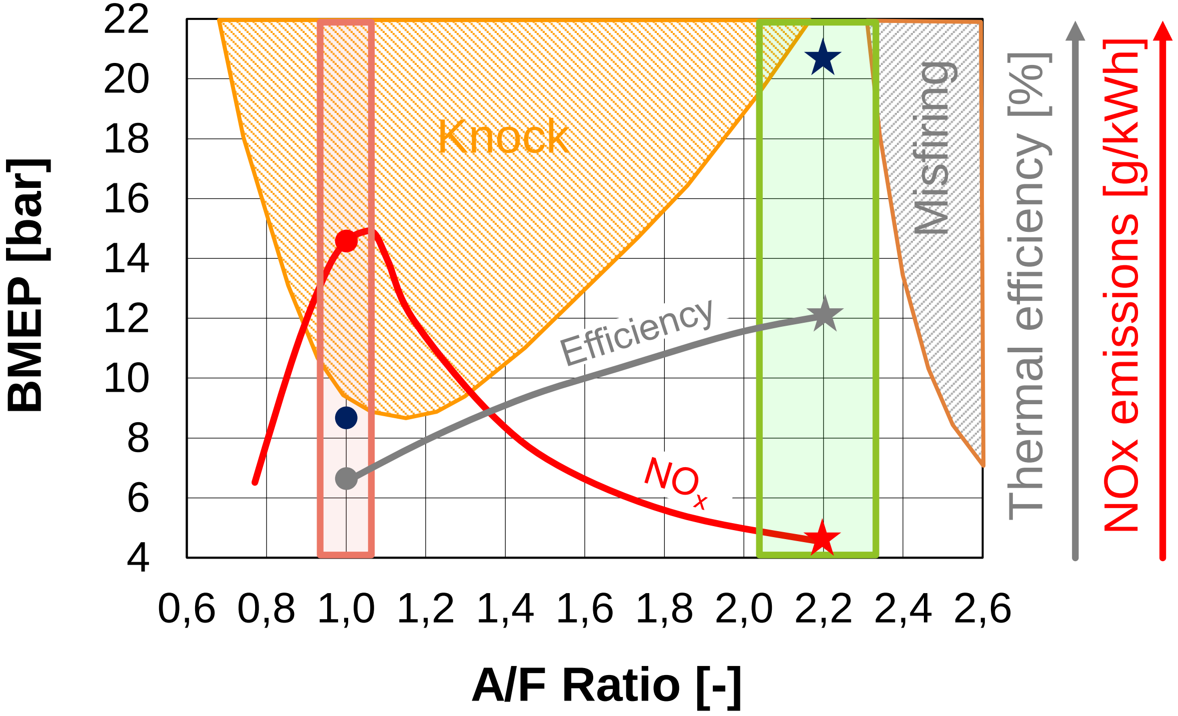
[1] Ricardo Webinar – “Development of Heavy-Duty Hydrogen Powertrains for 2025+”, Nov 24th, 2020
[2] adapted from Bernd Heid, Christopher Martens, and Anna Orthofer, “How hydrogen combustion engines can contribute to zero emissions”, McKinsey & Company 2021

Introduction

H2-ICE key enablers for high efficiency

Recent technological improvements allow lean burn operation w/ significant advantages.

H_2-ICE engine performance



Ultra-lean combustion advantages:

- **Ultra-low emissions**, including NOx
- **High thermal efficiency**, thanks to low heat rejection and faster combustion
- **High knock tolerance** and good performance

Stoichiometric H_2-ICE 🟥

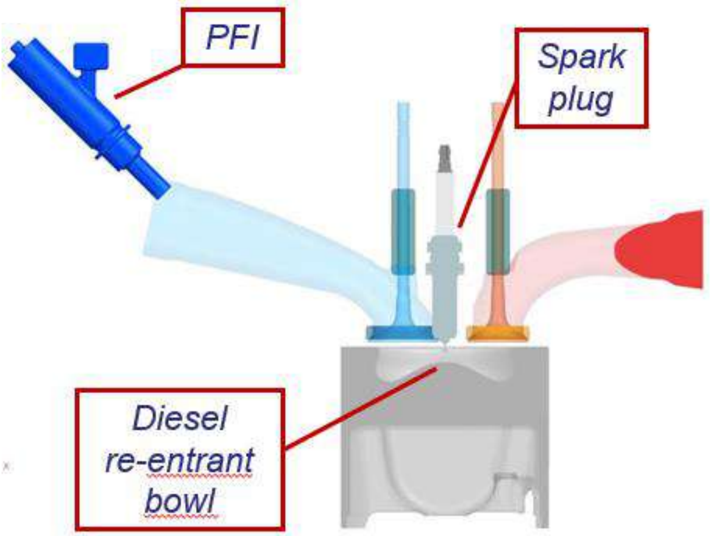
Ultra-lean H_2-ICE 🟩

Introduction

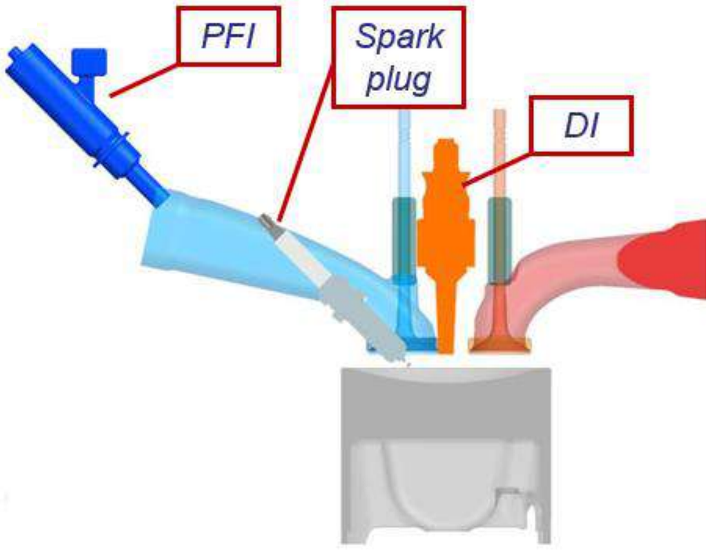
Ultra-lean H2 combustion systems

Different combustions systems could be exploited for lean-burn hydrogen combustion.

PFI solutions

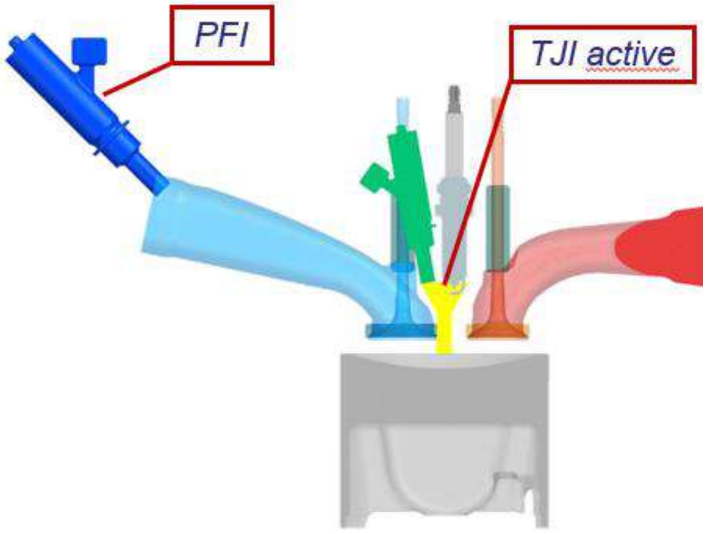


DI solutions



…

TJI solutions



Retrofit benefit

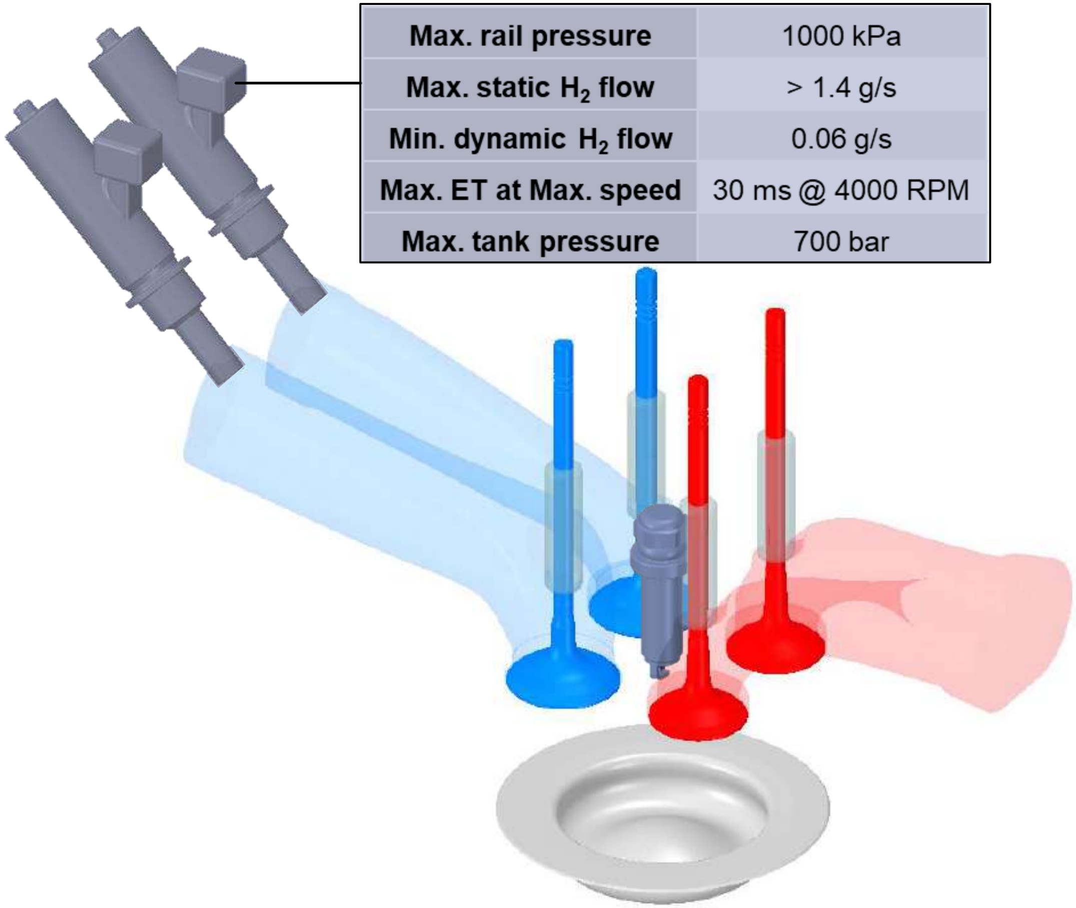
Cost;
Complexity

Aim of the work

A state-of-the-art **low-compression ratio**, **turbocharged**, 3.0L displacement **diesel engine** architecture was selected as case study.

Diesel Engine → Minimum level of cost and complexity → **Hydrogen Engine**

Max. rail pressure	1000 kPa
Max. static H_2 flow	> 1.4 g/s
Min. dynamic H_2 flow	0.06 g/s
Max. ET at Max. speed	30 ms @ 4000 RPM
Max. tank pressure	700 bar



- The original diesel engine block, the swirl-based cylinder head, the turbocharger and the cam timing kept unchanged
- Centrally mounted **Diesel Injector** substituted with a **spark plug**
- Implementation of **PFI system** → re-design of intake system

Case study

Development of a **0/1/3D-CFD synergetic approach** to investigate **H2-ICE potential**.

Synergetic approach among 0/1/3D-CFD numerical tools

3D-CFD simulation

Outcomes used as a reference for calibrating a predictive combustion model in 1D-CFD environment

0/1D-CFD simulation

GT-SUITE combustion model correlation based on the peculiarities of H2

1D-CFD simulation

Preliminary assessment of the engine operating maps for the selected architecture

Simulation methodology

3D-CFD simulation environment

Development of a **0/1/3D-CFD synergetic approach** to investigate **H2-ICE potential**.

Synergetic approach among 0/1/3D-CFD numerical tools

3D-CFD simulation

Outcomes used as a reference for calibrating a predictive combustion model in 1D-CFD environment

0/1D-CFD simulation

GT-SUITE combustion model correlation based on the peculiarities of H2

1D-CFD simulation

Preliminary assessment of the engine operating maps for the selected architecture

- ❑ **RANS**: **K-eps RNG** turbulence model
- ❑ Combustion model: Detailed chemical kinetics solver (**SAGE**)
  - ▪ Predictive and usable also for partially-premixed combustion
  - ▪ Can be used for auto-ignition (knocking)
  - ▪ Well suited for emission modelling

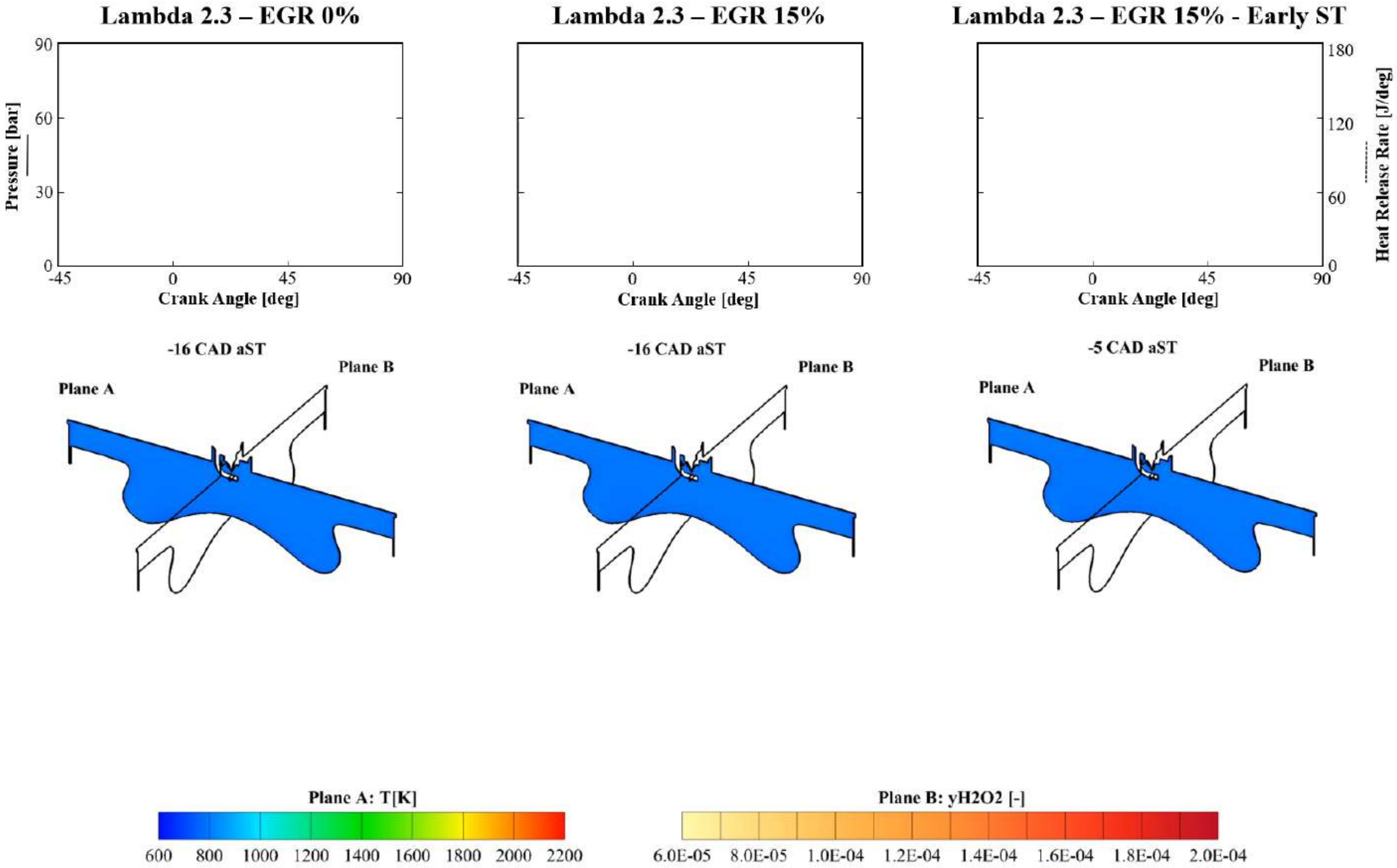
Fuel species	H2/syngas
Mechanism	Zhang et al. (2017)
Species	44
Reactions	251
NOx	Detailed chemistry

[1] Zhang, Y., et al., “Assessing the predictions of a NO x kinetic mechanism on recent hydrogen and syngas experimental data”, DOI: 10.1016/j.combustflame.2017.03.019

[2] Dayma, G., et al., “Effects of air contamination on the combustion of hydrogen-effect of NO and NO2 addition on hydrogen ignition and oxidation kinetics," DOI: 10.1080/00102200600793171.

Simulation methodology

3D-CFD simulation environment – Results



3D-CFD model **predicts the impact** of different engine calibration in terms of **lambda, EGR, ST**

- ☐ At constant spark timing, the **increment of EGR** rate results in a **slower combustion process**
- ☐ **Advanced ST leads to a speed-up of the combustion process** with a comparable combustion duration

Simulation methodology

1D-CFD simulation environment

Development of a **0/1/3D-CFD synergetic approach** to investigate **H2-ICE potential**.

Synergetic approach among 0/1/3D-CFD numerical tools

3D-CFD simulation

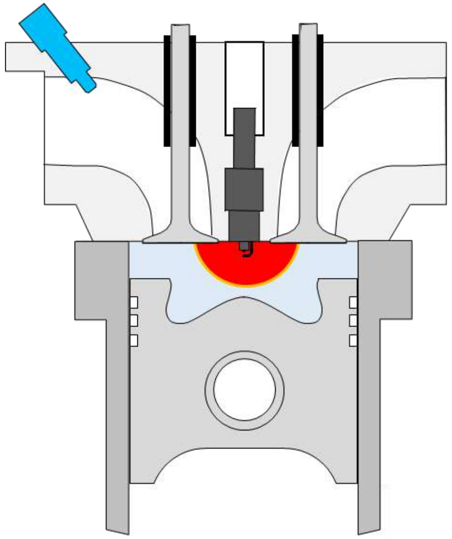
Outcomes used as a reference for calibrating a predictive combustion model in 1D-CFD environment

0/1D-CFD simulation

GT-SUITE combustion model correlation based on the peculiarities of H2

1D-CFD simulation

Preliminary assessment of the engine operating maps for the selected architecture



SITurb Predictive Model:

- ☐ Entrainment and Burn-up approach

$$\frac{dM_e}{dt} = \rho_u A_e (S_T + S_L) \qquad \frac{dM_b}{dt} = \frac{M_e - M_b}{\tau}$$

- ☐ New **Laminar Flame Speed Model** to consider hydrogen properties

$$S_L(\phi, T_u, p_u, x_b) = S_{L0}\left(\frac{T_u}{T_0}\right)^{\alpha}\left(\frac{p_u}{p_0}\right)^{\beta}(1-\gamma x_b)$$

- ☐ Modified **Turbulent Flame Speed Model** to capture flame velocity

$$S_T(p_2, H_2, u') = \mathrm{C_{TFS}}(\mathrm{p_2}, \mathrm{H_2})\ \mathrm{u'}\left(1 - \frac{1}{1 + C_{FKG}\left(\frac{R_f}{L_T}\right)^2}\right)$$

Simulation methodology

1D-CFD simulation environment – Predictive combustion model

New Laminar Flame Speed Model to consider hydrogen properties:

- ☐ Model developed considering Zhang et al. mechanism results
- ☐ Pressure and temperature from low to high load operation, up to ultra-lean and 30% EGR rates (>1600 operating conditions)

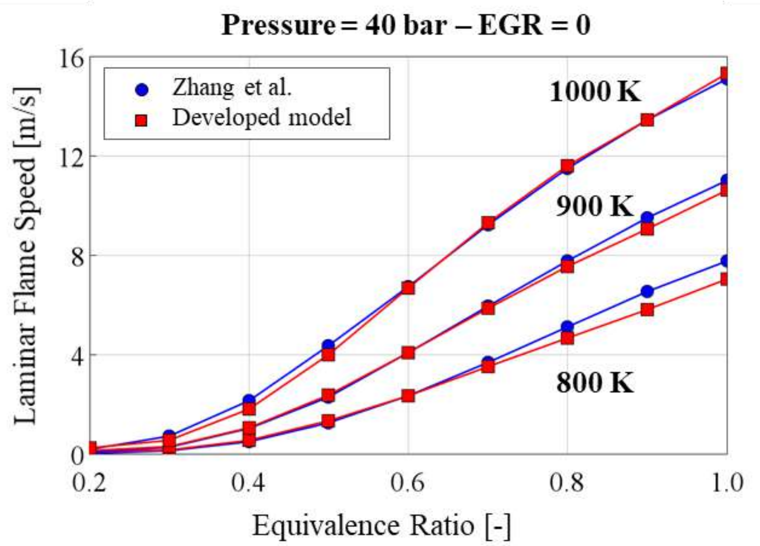
$$\boldsymbol{S_L(\phi, T_u, p_u, x_b) = S_{L0}\left(\frac{T_u}{T_0}\right)^{\alpha}\left(\frac{p_u}{p_0}\right)^{\beta}(1-\gamma x_b)}$$

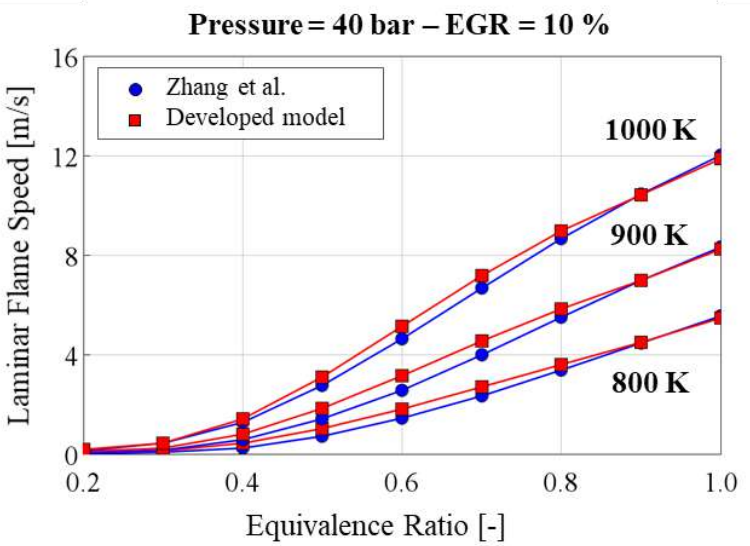
$$S_{L0}(\phi) = k_5\phi^5 + k_4\phi^4 + k_3\phi^3 + k_2\phi^2 + k_3\phi + \mathrm{k}_0$$

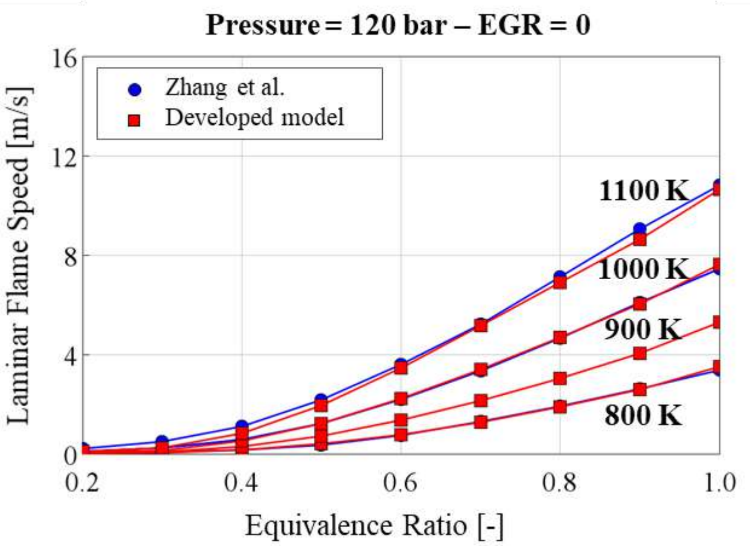
$$\alpha(\phi) = a_2\,\phi^2 + a_1\,\phi + a_0$$

$$\beta(\phi) = \beta_2\,\phi^2 + \beta_1\,\phi + \beta_0$$

$$\gamma(\phi) = \gamma_2\,\phi^2 + \gamma_1\,\phi + \gamma_0$$





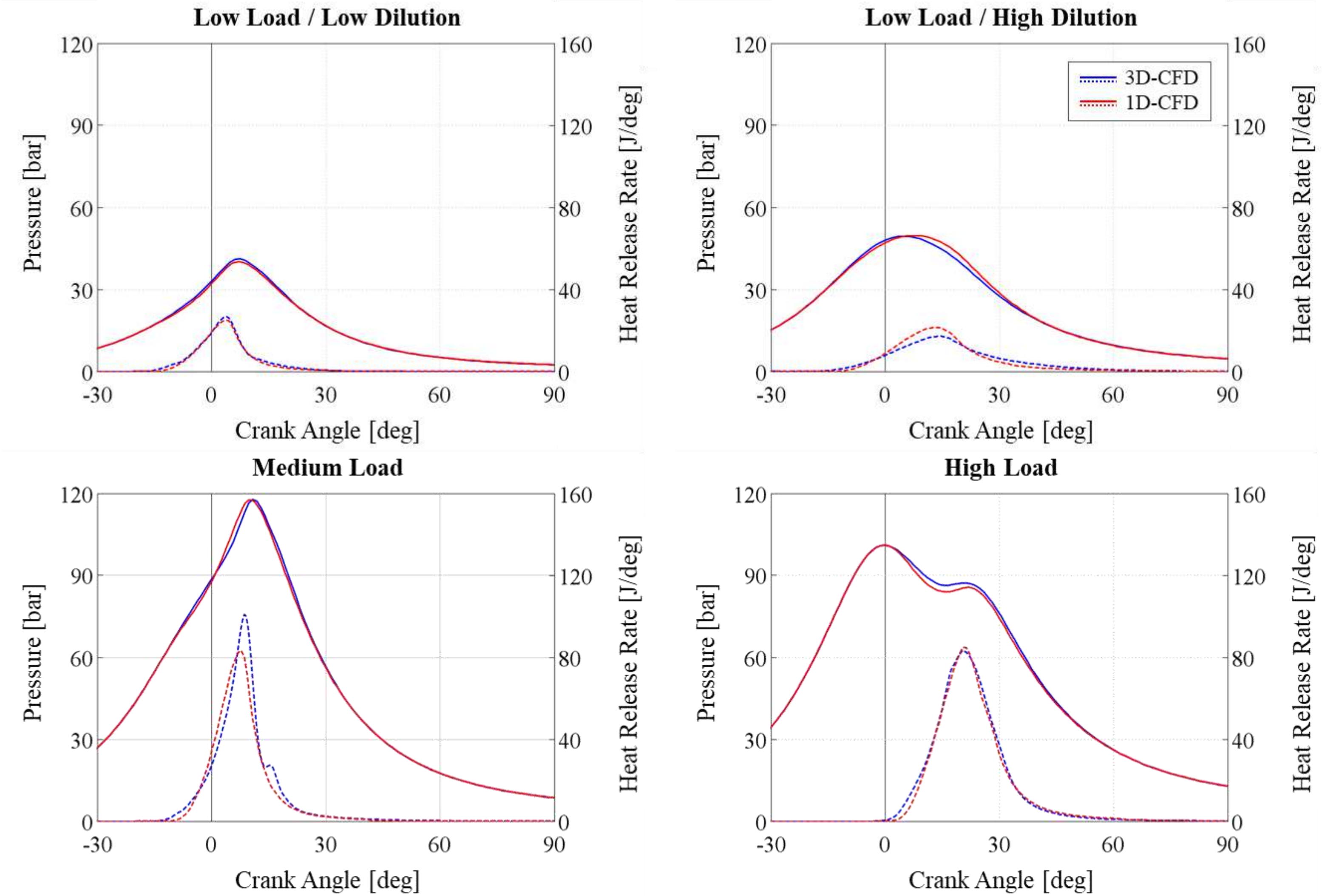


Simulation methodology

1D-CFD simulation environment – Predictive combustion model

Combustion phenomena **well predicted by SITurb**.

- ❑ **Good correlation** between **3D- and 1D-CFD models** for in-cylinder pressure and burn rate.
- ❑ Effect of **lambda and EGR variation captured** by the model
- ❑ **Satisfactory accuracy** level confirmed **at increasing engine load** and in case of retarded spark timings

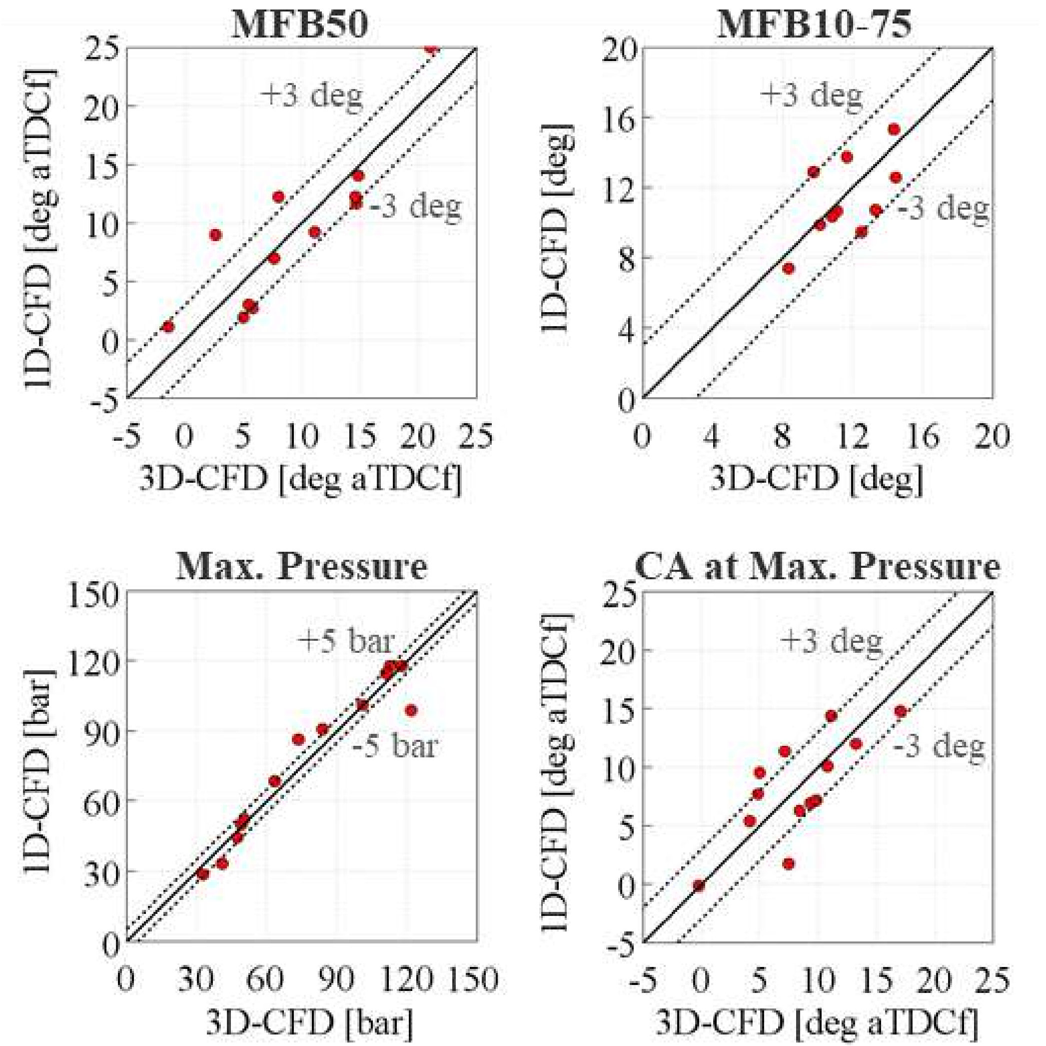


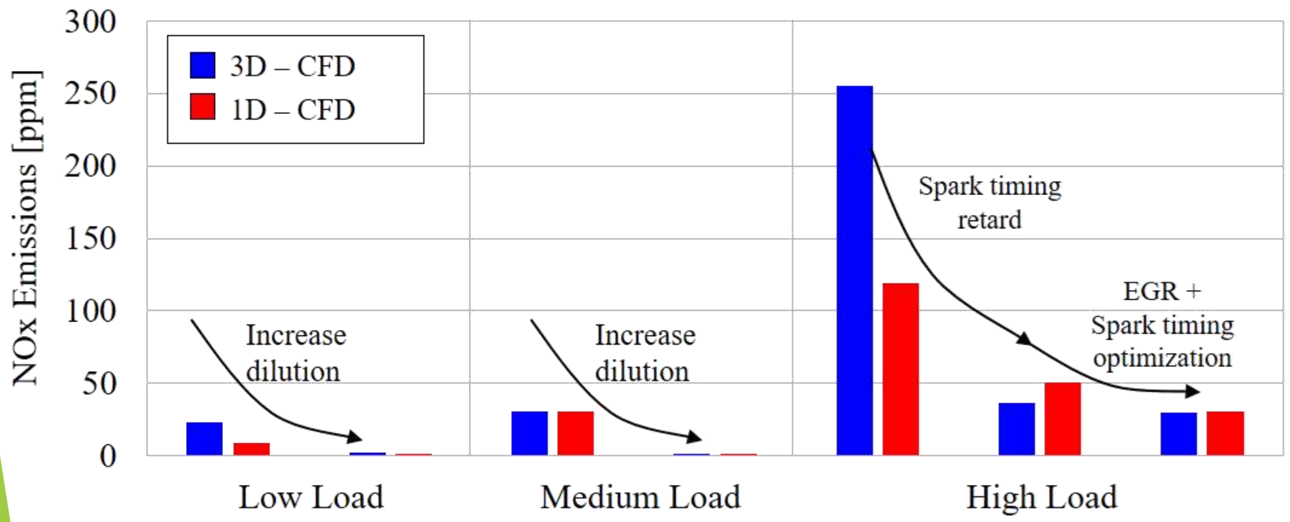
Simulation methodology

1D-CFD simulation environment – Predictive combustion model

Combustion phenomena **well predicted by SITurb**.

- **MFB-50** and **Combustion Duration 10-75 errors lower than 3 deg**
- **Maximum pressure** values and **phasing properly predicted** by the model
- **Good accuracy in terms of NOx** predictions against 3D-CFD results





Simulation methodology

1D-CFD simulation environment

Development of a **0/1/3D-CFD synergetic approach** to investigate **H2-ICE potential**.

Synergetic approach among 0/1/3D-CFD numerical tools

3D-CFD simulation

Outcomes used as a reference for calibrating a predictive combustion model in 1D-CFD environment

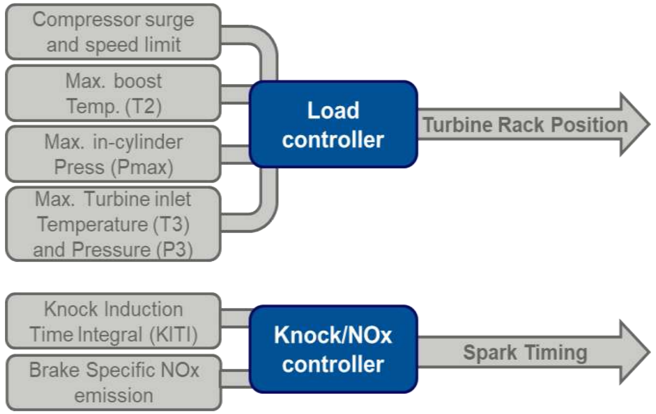
0/1D-CFD simulation

GT-SUITE combustion model correlation based on the peculiarities of H2

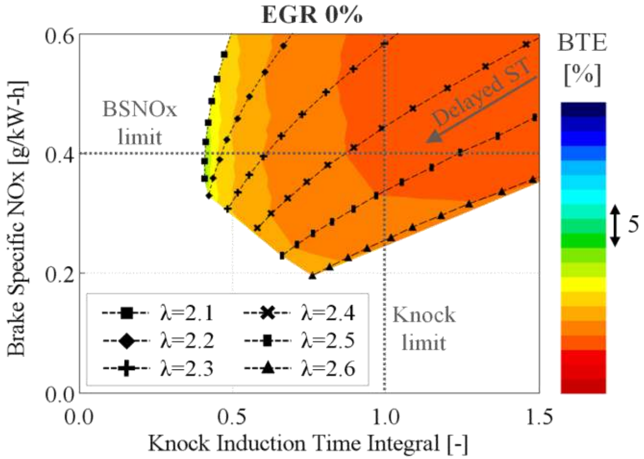
1D-CFD simulation

Preliminary assessment of the engine operating maps for the selected architecture

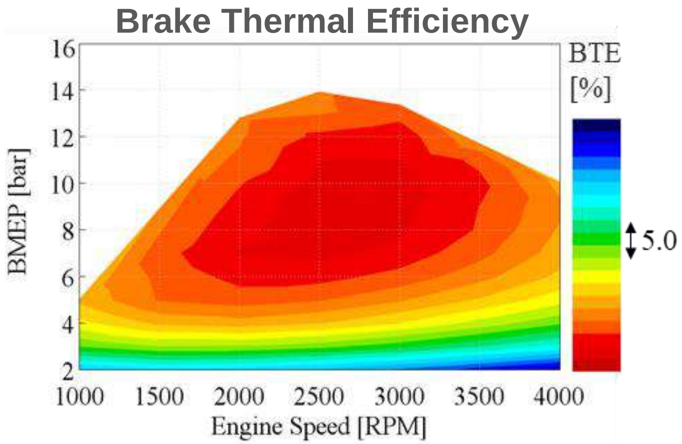
Engine control unit



Preliminary engine calibration



Engine Maps

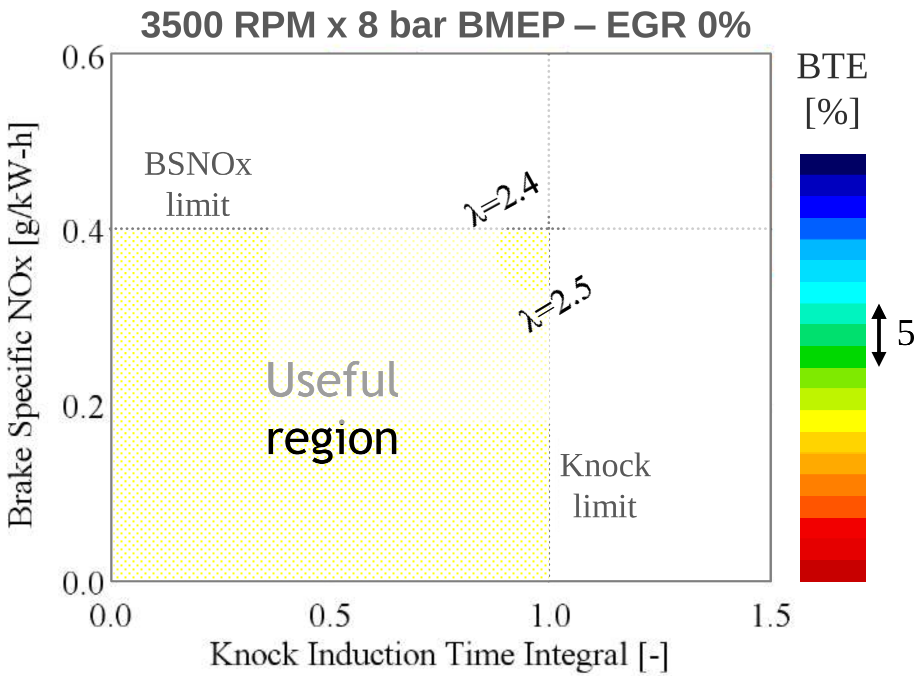


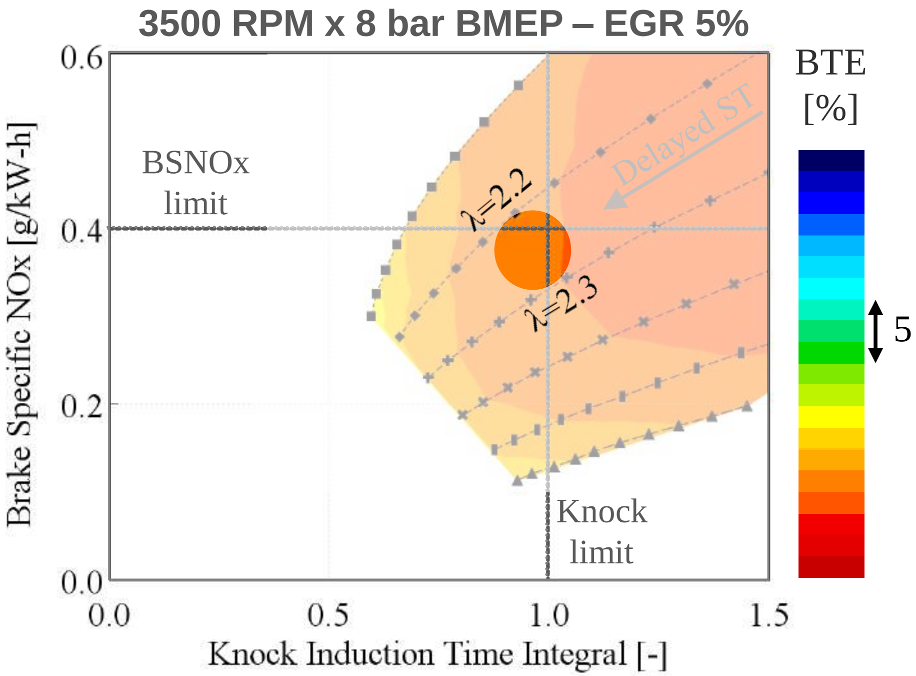
Simulation methodology

1D-CFD simulation environment – Engine controls for map definition

A preliminary **optimization of the main calibration parameters**, as spark timing, boost pressure, lambda and EGR percentage was performed over the entire engine operating map.

- A **DoE methodology** was adopted **to select the optimal combination of lambda and EGR ratio** to maximize the Brake Thermal Efficiency (BTE)
- **Higher EGR content** implied an increment of the in-cylinder temperature (↑**knock likelihood**), thus requiring a more delayed combustion (↓**BTE**)



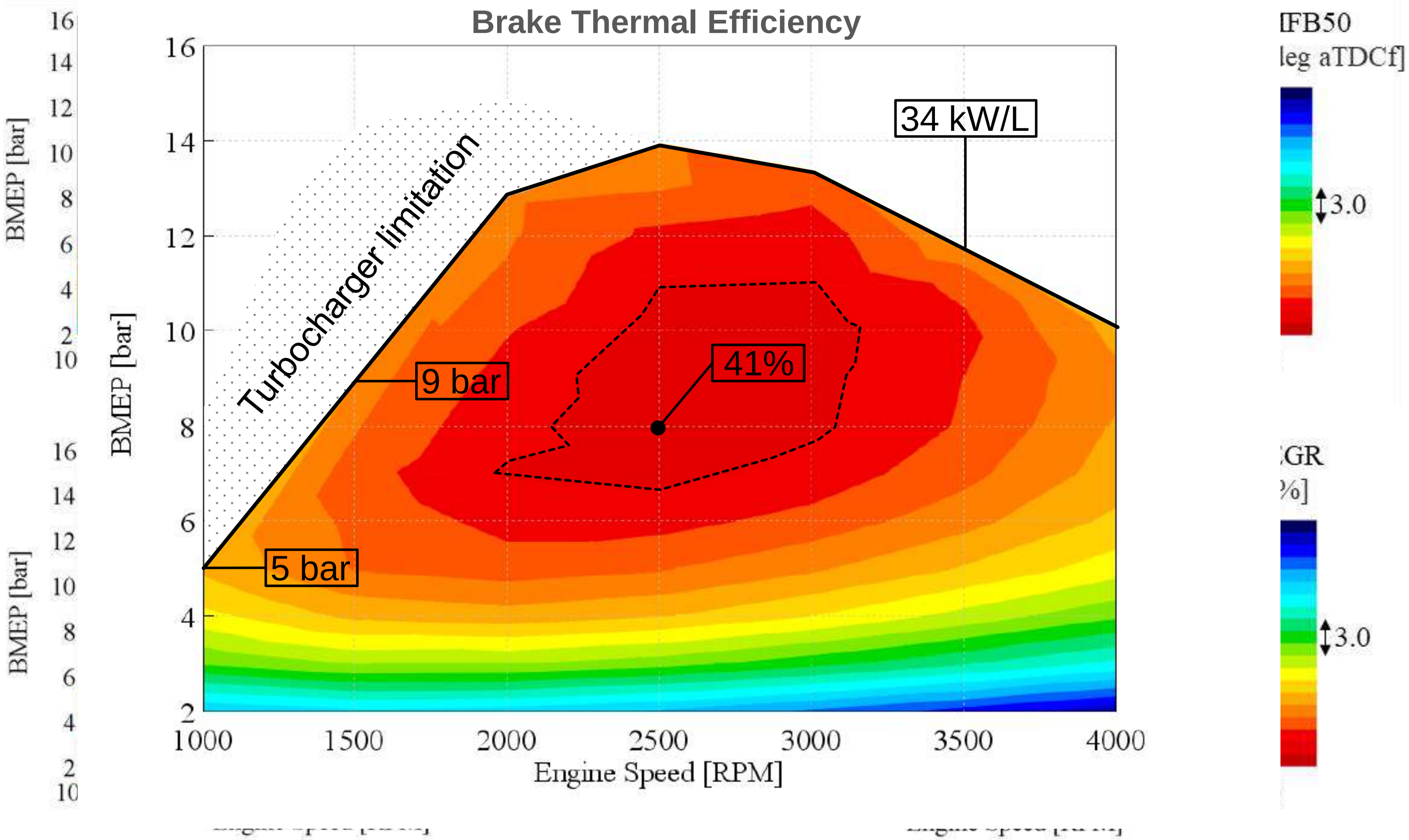


Results

Engine maps

The **complete engine model** was exploited to assess the performance of the hydrogen fueled engine on the complete operating map.

- ☐ A maximum **power density** of **34 kW/L** can be achieved at 3500 RPM
- ☐ **Low-End Torque region** strongly **limited by turbocharger** system
  - high boost requirement due to the poor volumetric efficiency caused by the low-density hydrogen injected in the intake ports
- ☐ A wide high-**BTE** area was achieved with a maximum level of **41%** at 2500 RPM x 8 bar BMEP
- ☐ Exploitation of **high dilution** in the **low-load region**

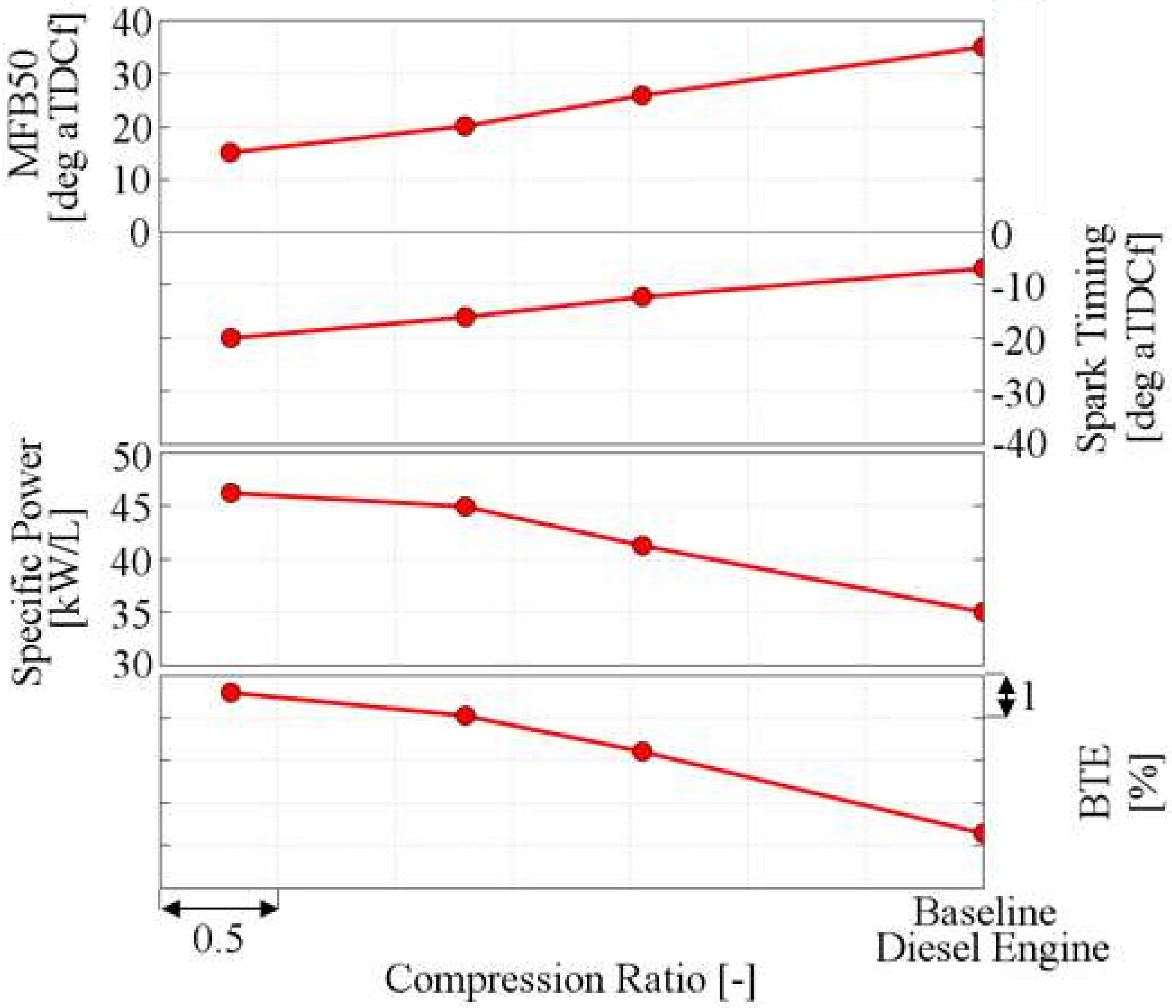


Results

Compression Ratio sensitivity analysis

To evaluate potential benefits in terms of power density a sensitivity analysis to the Compression Ratio was carried out.

- **Significant spark timing advance** at lower CR **due to the reduced knock** likelihood
- **Advanced MFB-50 as a results of the spark timing advance** and the lower combustion duration
- Potential **engine efficiency improvement of +2.5%** with a CR reduction of ~3
- Significant **improvement of the power density (+11 kW/L)**



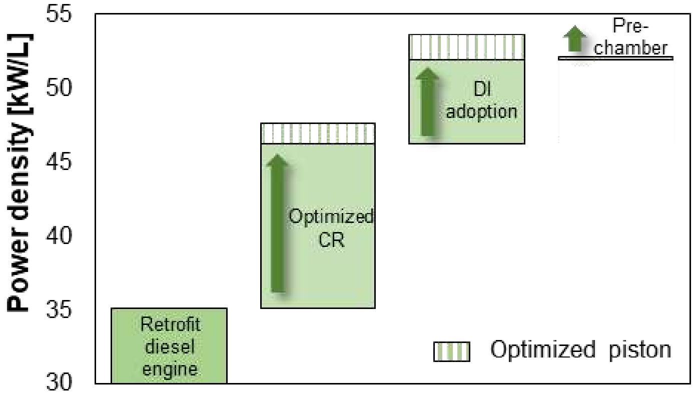
Conclusions

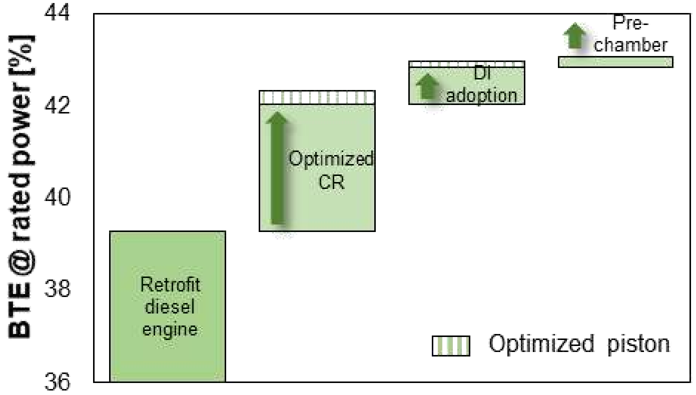
A comprehensive methodology based on the **synergetic use of 0/1/3D-CFD** numerical simulations to assess the performance of a **new generation of hydrogen fueled engines.**

A **PFI retrofitted** state-of-the-art low compression ratio, turbocharged, 3.0L displacement diesel engine was selected as a first test case achieving **41% peak BTE and 34 kW/l specific power output**.

Main features of the proposed methodology include:

- ☐ Coupling among 0/1/3D simulation platforms
- ☐ 3D-CFD **combustion modelling** based on **detailed chemistry scheme**
- ☐ **Specific laminar flame speed** correlation, **modified turbulence flame speed** and **ignition delay maps** to capture H2 combustion peculiarities





Already **ongoing activities** are focusing on the assessment of more complex architectures including **DI, TJI and dual-fuel operations.**

Acknowledgments

PWT
POWERTECH ENGINEERING

PUNCH

Politecnico
di Torino
1859

CONVERGE
CFD SOFTWARE

GT Gamma
Technologies

Synergetic application of 0/1/3D-CFD approaches for hydrogen-fuelled spark ignition engine simulation

Thank you for your kind attention!

The work presented was already submitted to SAE International Journal of Engine for publication:

Millo, F., Rolando, Piano, A., Accurso, F., Gullino, F., Roggio, S., Pesce, F., Vassallo, A., Rossi, R., Bianco, A., *“Synergetic application of 0/1/3D-CFD approaches for hydrogen-fuelled spark ignition engine simulation”*

Contact:
Federico Millo
Energy Department (DENERG)
Politecnico di Torino
C.so Duca degli Abruzzi, 24
ITALY – 10129 Turin
@ federico.millo@polito.it


e3 - Engines Energy Environment | Research Group of Politecnico di Torino
Centri di ricerca
Torino, Italia · 574 follower
Researching efficient uses of energy in automotive powertrains to minimize their CO2 and pollutants emissions.

…and remember to follow our LinkedIn page to be updated on our latest research works!

e3 - Engines Energy Environment