Politecnico
di Torino

The supporting role of numerical simulation for innovative H2-ICE development

Giornata di studio AIMSEA '*Idrogeno e tecnologie per la generazione energetica e la propulsione nei trasporti green*'

Genova, Italy – January 25, 2024

PROF. FEDERICO MILLO (Politecnico di Torino, Italy)

Agenda

- Introduction
- Supporting role of CFD in H2ICE development
    - 3D-CFD driven design optimization
    - 1D-CFD predictive models for virtual calibration
- Conclusions

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- **Introduction**

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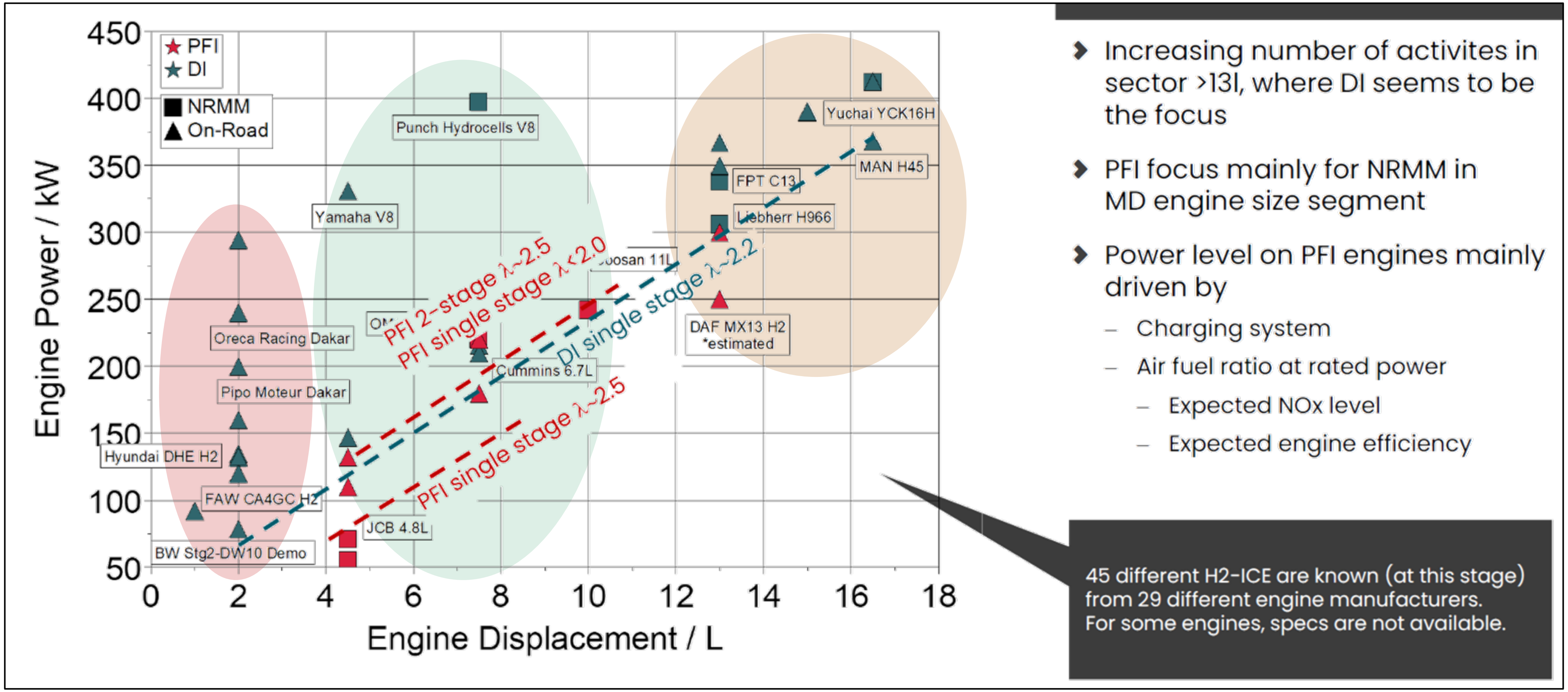
Introduction

Benchmark of existing hydrogen demo engines

45 different H2ICE are known (at this stage) from 29 different engine manufacturers.



- Increasing number of activites in sector >13l, where DI seems to be the focus
- PFI focus mainly for NRMM in MD engine size segment
- Power level on PFI engines mainly driven by
  - Charging system
  - Air fuel ratio at rated power
    - Expected NOx level
    - Expected engine efficiency

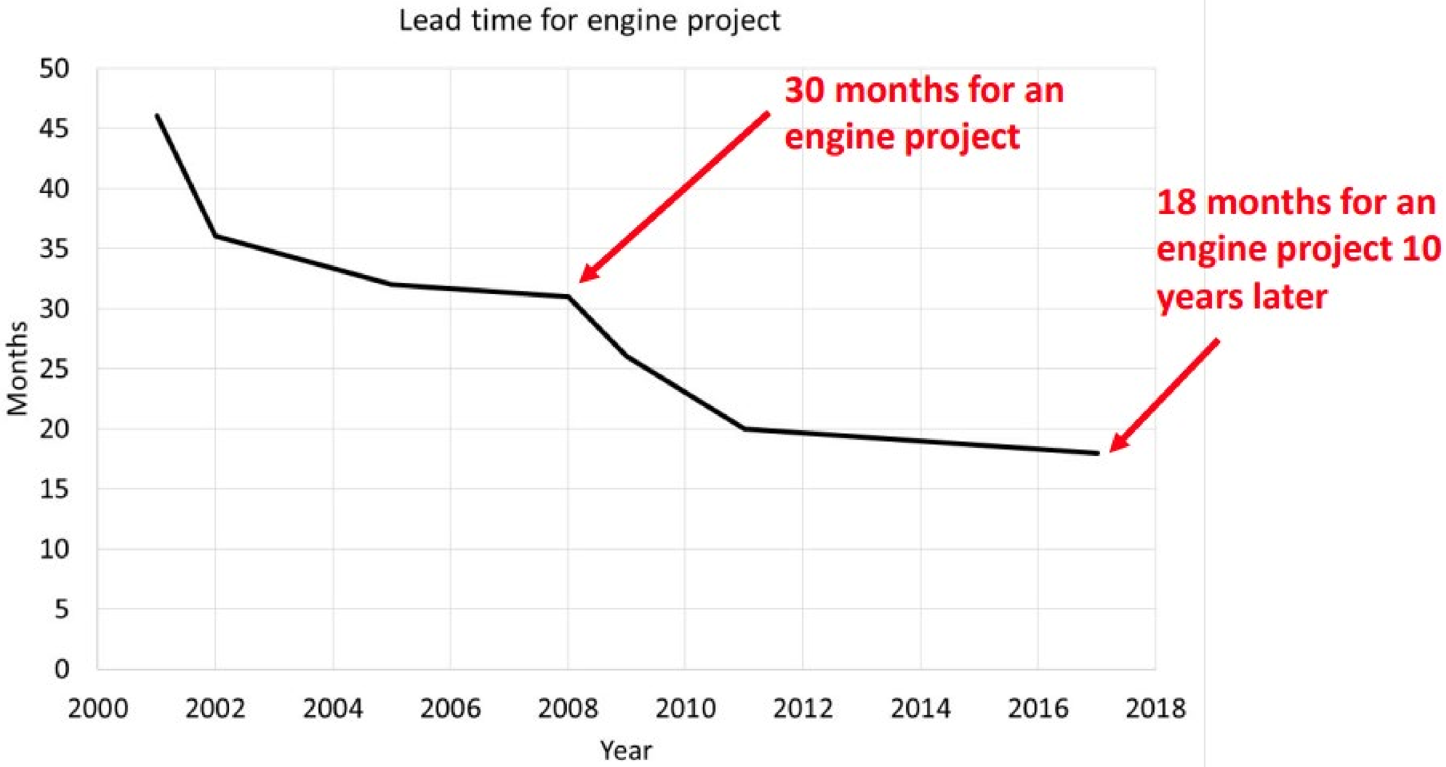
45 different H2-ICE are known (at this stage) from 29 different engine manufacturers. For some engines, specs are not available.

Source: F. Mallamo, “FEV’s perspective on H2-Fueled Current and Future ICEs”, Hydrogen for Sustainable Mobility Forum, Turin, 2023

Introduction

Engine development process duration

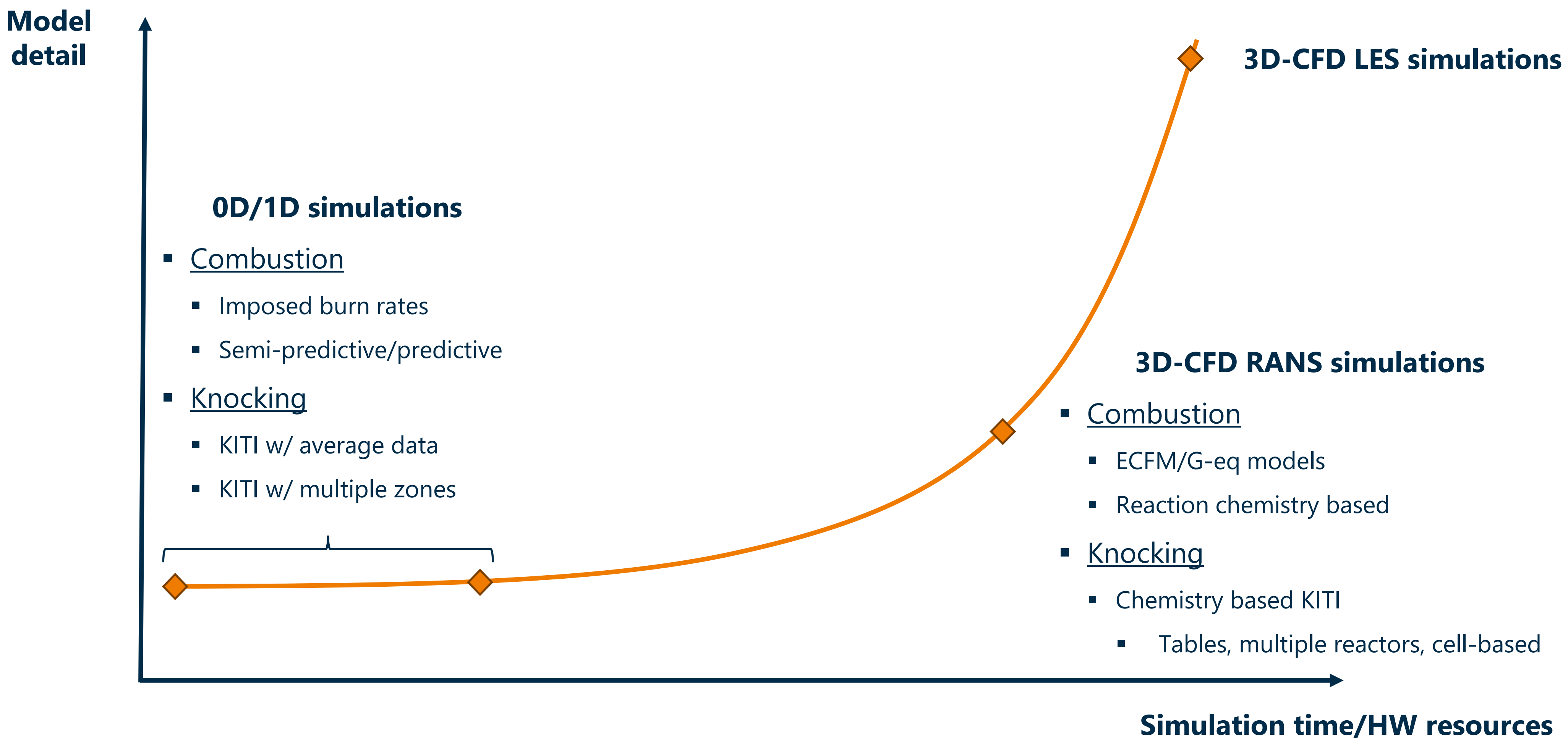
During the years, the lead time for an engine project has been remarkably reduced. For this reason, the supporting role of numerical simulation is becoming even more crucial for the design and optimization of the engine.



Source: F. Ravet, "Crucial needs for efficient simulations in automotive industry", CONVERGE User Conference 2019

Introduction

Different approaches for modeling of hydrogen combustion



0D/1D simulations

- Combustion
  - Imposed burn rates
  - Semi-predictive/predictive
- Knocking
  - KITI w/ average data
  - KITI w/ multiple zones

3D-CFD RANS simulations

- Combustion
  - ECFM/G-eq models
  - Reaction chemistry based
- Knocking
  - Chemistry based KITI
    - Tables, multiple reactors, cell-based

3D-CFD LES simulations

Introduction

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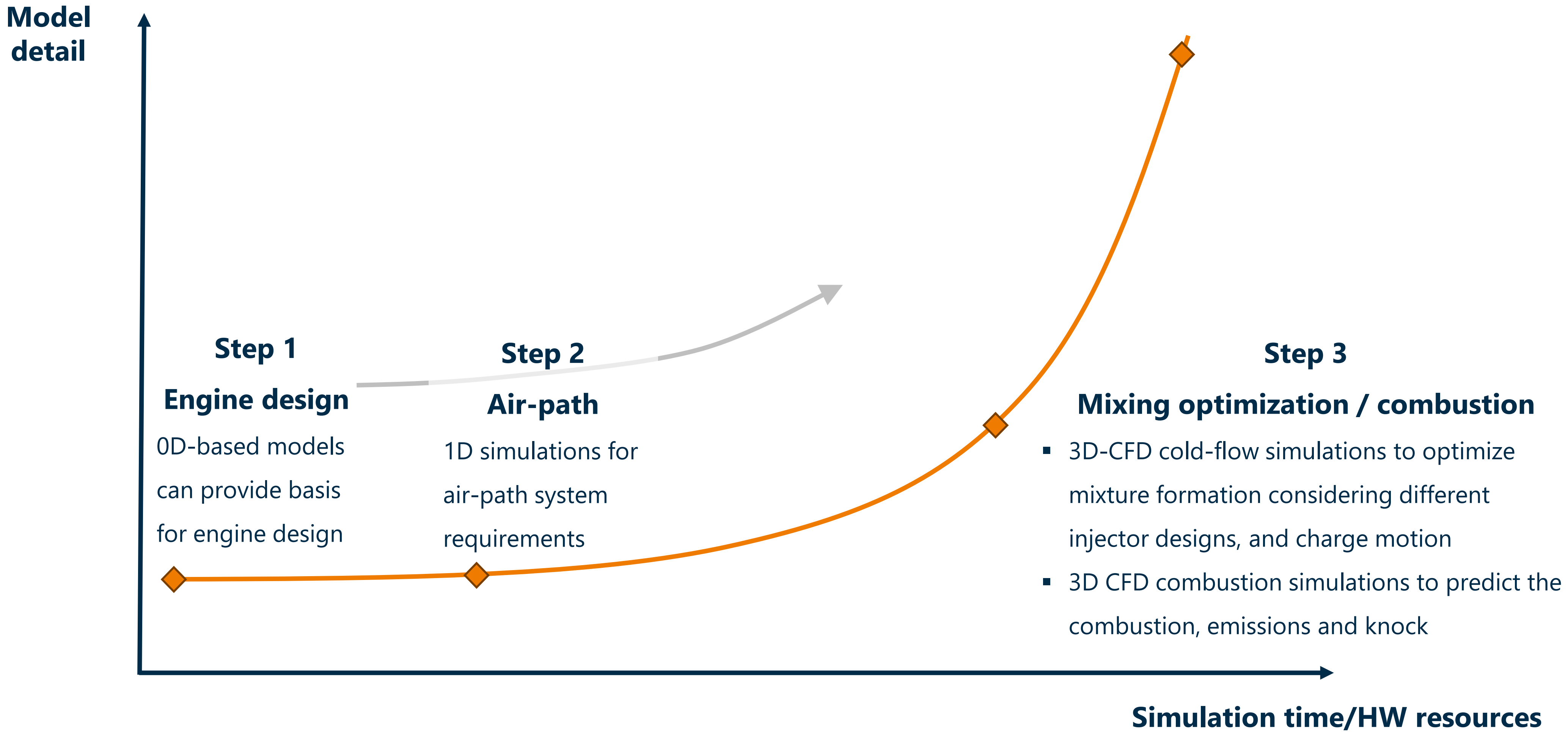

Step 1

Engine design

0D-based models can provide basis for engine design

Step 2

Air-path

1D simulations for air-path system requirements

Step 3

Mixing optimization / combustion

- 3D-CFD cold-flow simulations to optimize mixture formation considering different injector designs, and charge motion
- 3D CFD combustion simulations to predict the combustion, emissions and knock

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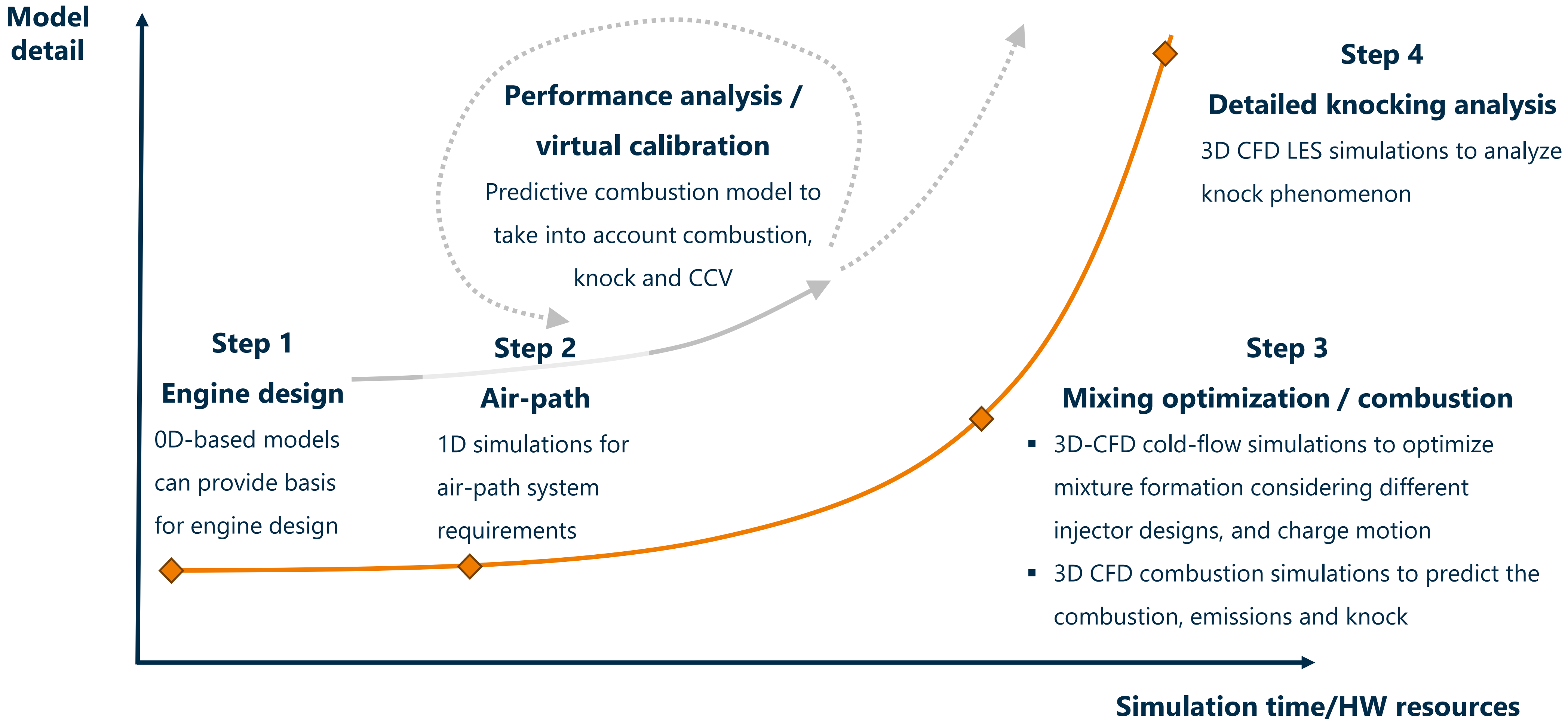

Model detail

Performance analysis / virtual calibration

Predictive combustion model to take into account combustion, knock and CCV

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Step 4

Detailed knocking analysis

3D CFD LES simulations to analyze knock phenomenon

Simulation time/HW resources

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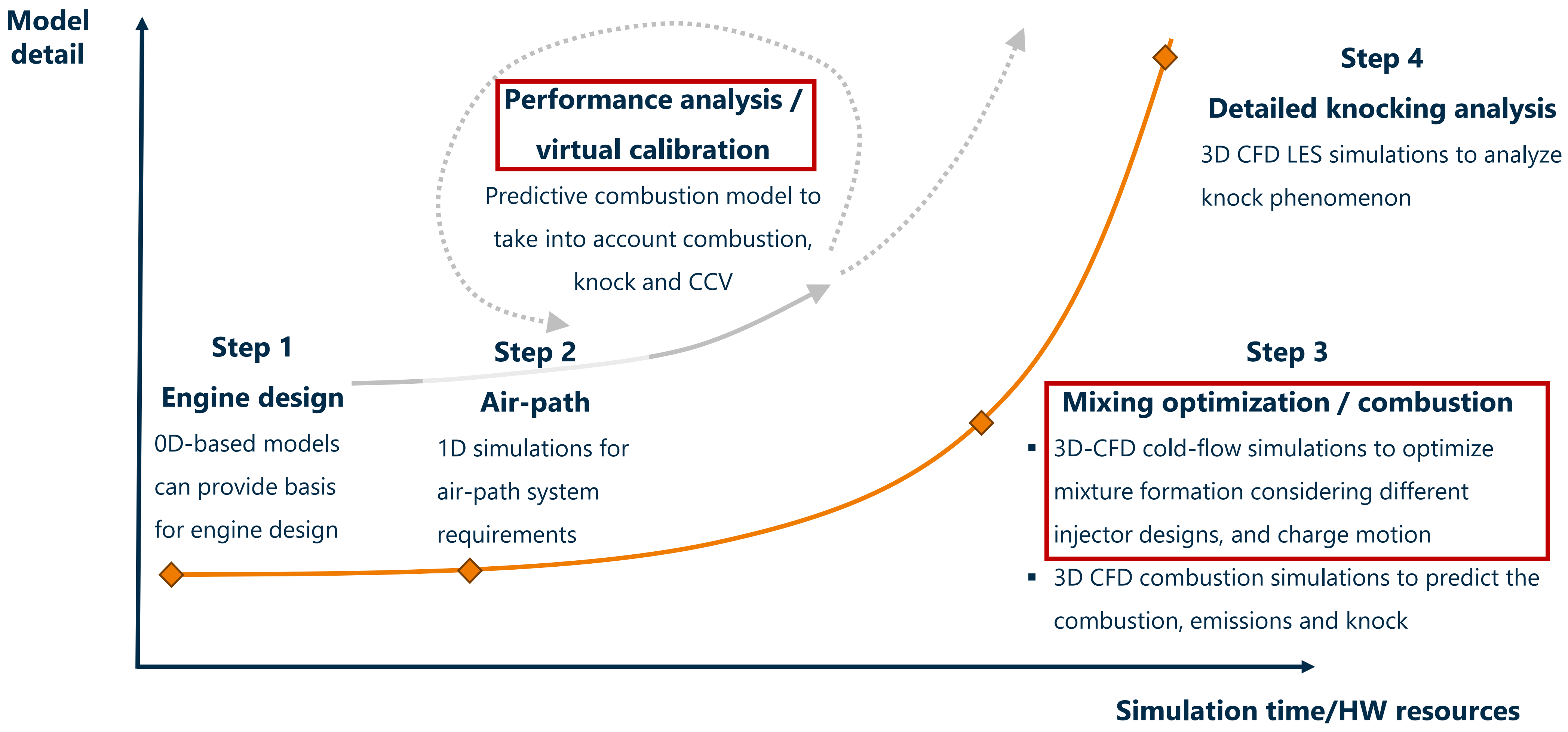
Different approaches for modeling of hydrogen combustion



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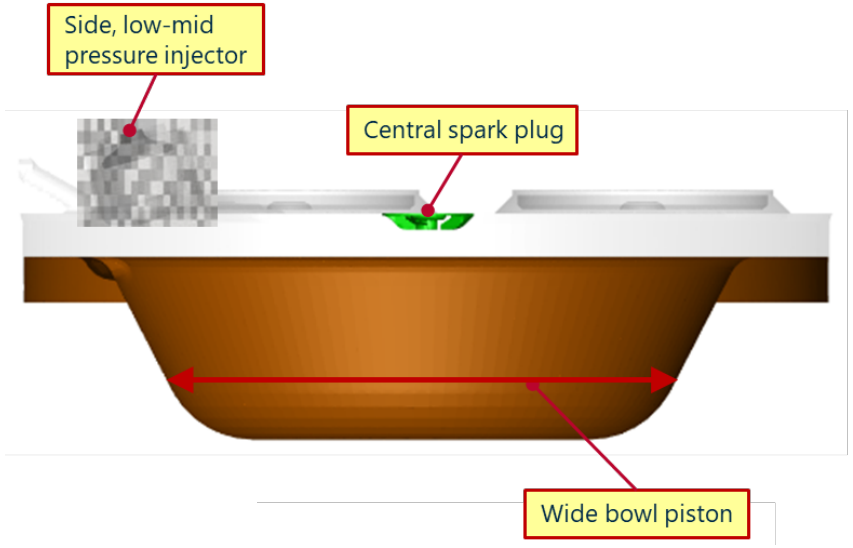
3D-CFD driven design optimization

Aim: Optimization of the mixture formation process in a small-displacement (Vdispl ~ 0.5L/cyl.) DI H2-ICE (retrofitted from a diesel engine for off-road applications) through 3D-CDF simulations.

Constraints

- ☐ Piston bowl shape because of manufacturing, cooling requirements
  - ☐ Target compression ratio (~11) achievement
- ☐ Injector position (side) to avoid interference with already existing components and additional machining of the cylinder head
  - ☐ Injector type → DI low pressure (20 bar < p_{inj} < 40 bar)



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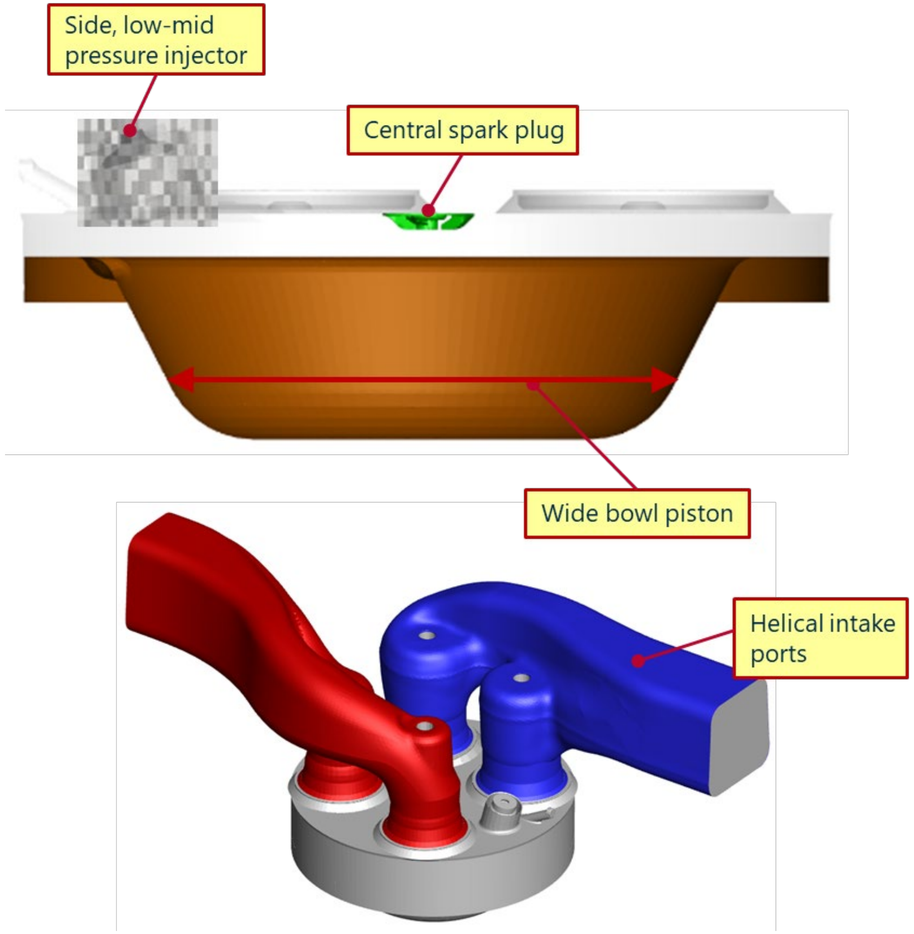
- Intake ports design



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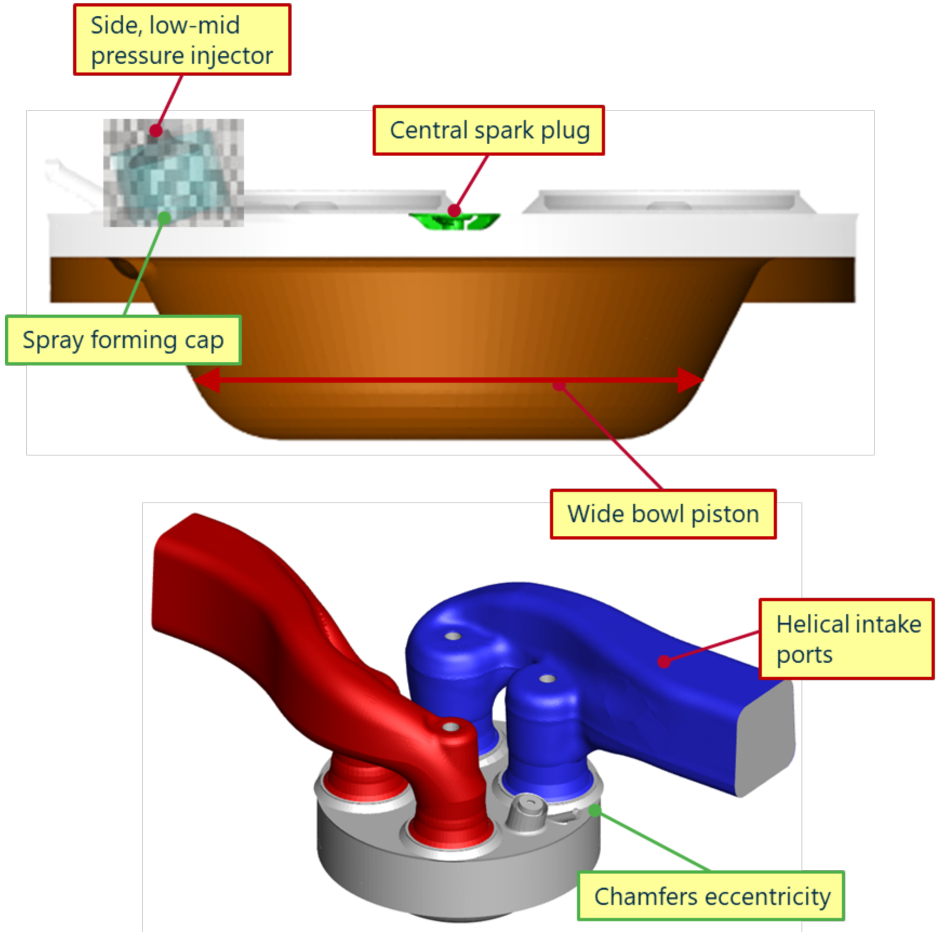
Degrees of freedom

- Injection timing
- Spray forming cap
- Port swirl induced

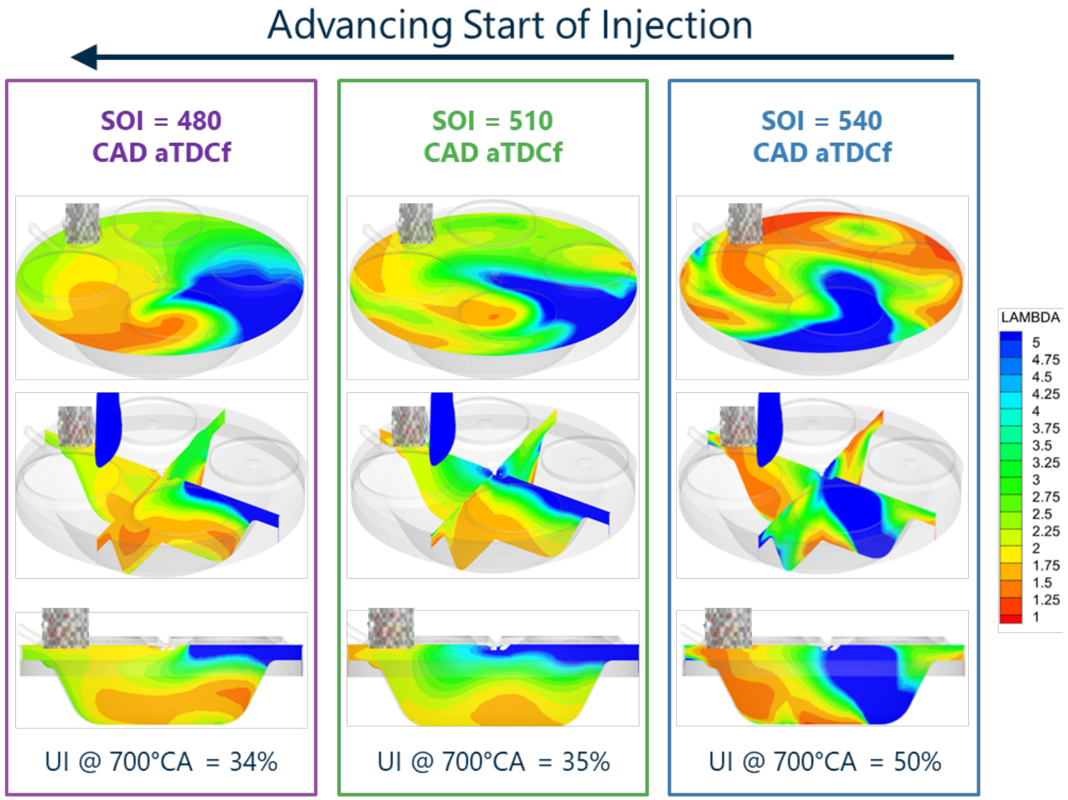
Optimization of the mixture properties through a suitable control of the charge motion



3D-CFD driven design optimization

Results: Injection Timing Sweep

- ☐ Injection timing has a sensible impact on mixture properties
- ☐ Mixture homogeneity improvement is not linear with the start of injection advance



Advancing Start of Injection

SOI = 480 CAD aTDCf

UI @ 700°CA = 34%

SOI = 510 CAD aTDCf

UI @ 700°CA = 35%

SOI = 540 CAD aTDCf

UI @ 700°CA = 50%

Uniformity Index (UI) = σ_{Φ}/Φ_{av}

3D-CFD driven design optimization

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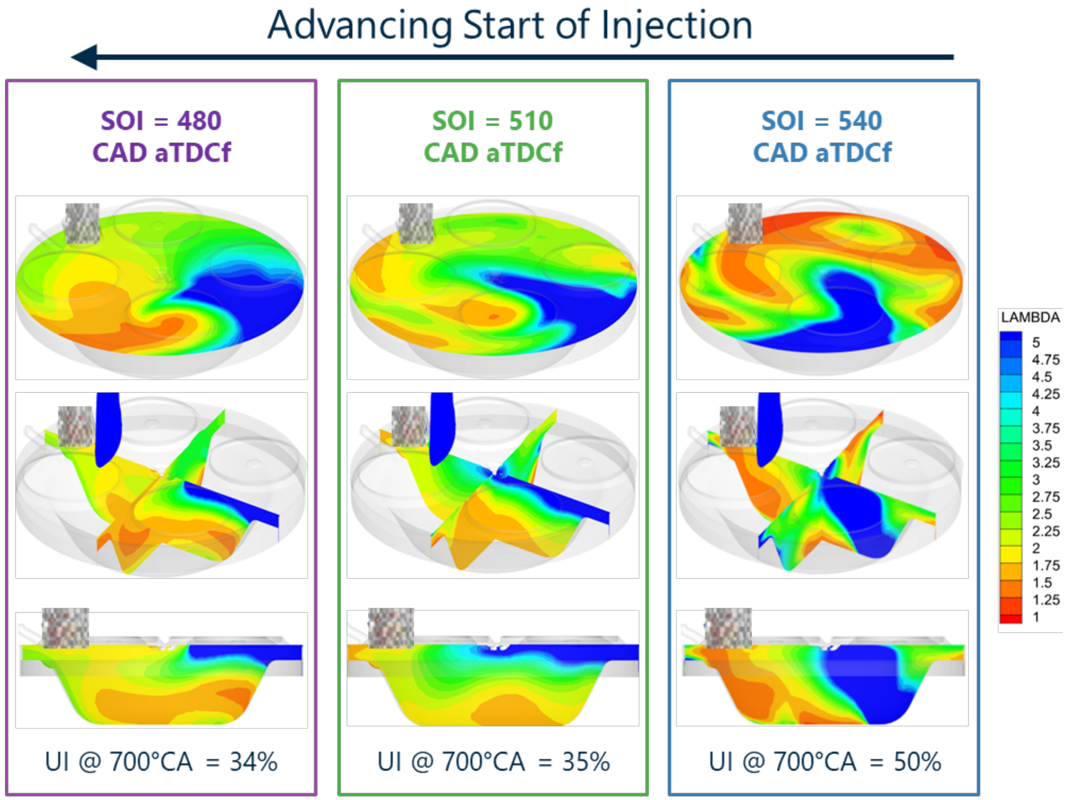
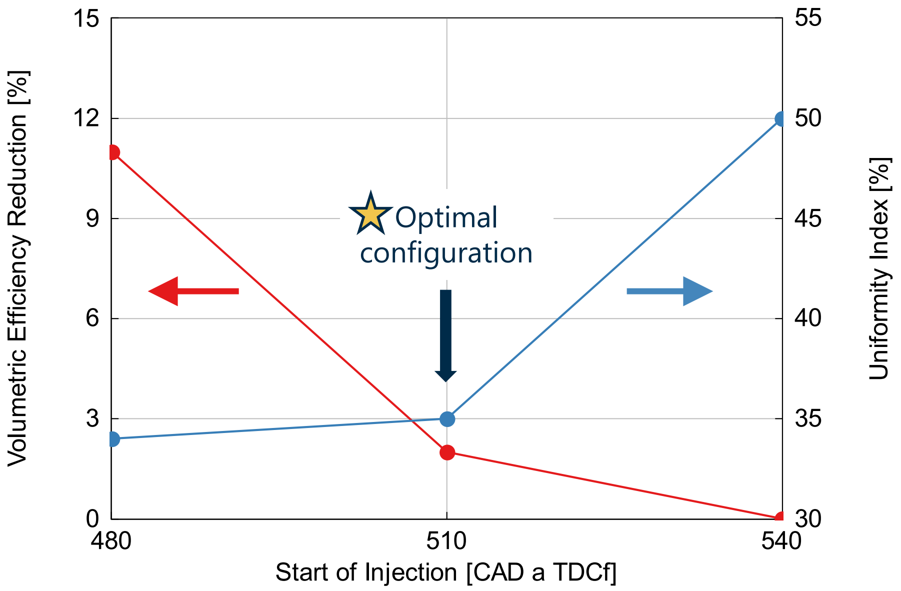


Uniformity Index (UI) = σ_{Φ}/Φ_{av}

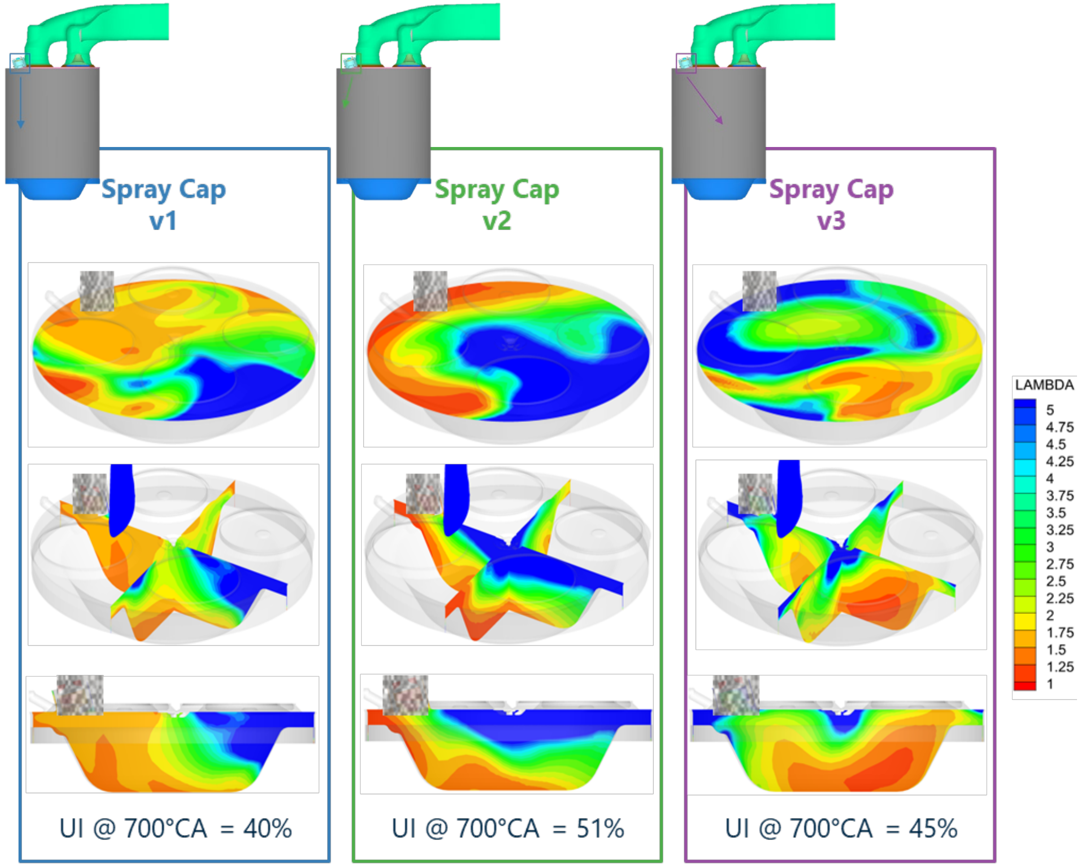
The best trade-off between volumetric efficiency reduction and mixture homogeneity is obtained with SOI = 510 CAD aTDCf



3D-CFD driven design optimization

Results: Spray cap variation

Spray cap has a sensible impact on mixture properties.



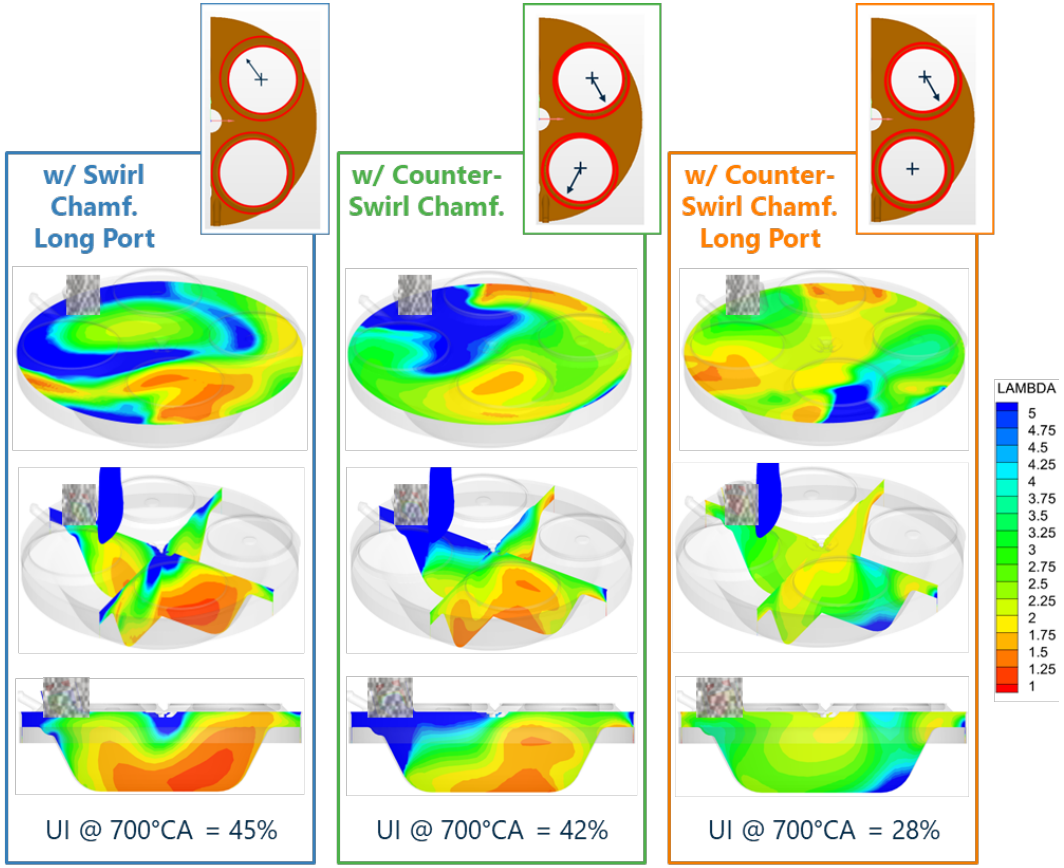
Uniformity Index (UI) = σ_{Φ}/Φ_{av}

- ❑ The best performance in terms of uniformity index is achieved by the Cap v1, thanks to the split of the injected H_2 generated by the cap
- ❑ Spray Cap v3 seems to be the most promising since:
  - ❑ Part of the H_2 is not locked by the swirl, thus the scavenging of the guiding cap is intrinsically favored
  - ❑ The injected gas does not impinge directly on the liner, reducing the risk of oil dilution

3D-CFD driven design optimization

Results: Swirl chamfer variations

- ❑ Swirl intensity was varied by acting on the swirl chamfers, to reduce the strong swirl intensity derived from the original diesel design that hinders the spread of the injected hydrogen.



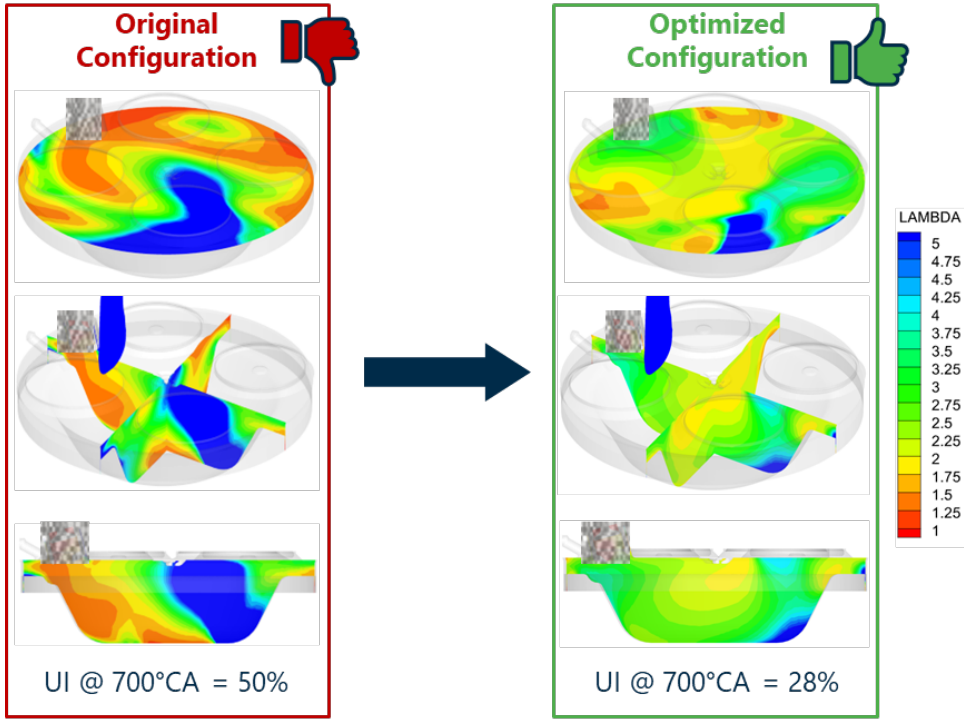
Uniformity Index (UI) = σ_Φ/Φ_{av}

- ❑ The configuration w/ counter-swirl chamfers on the long port leads to an enhanced mixture homogeneity

3D-CFD driven design optimization

Results: Final design

- ☐ A 3D-CFD analysis was performed to assess the impact of the injection timing and of the geometrical configuration of the combustion system on the mixture formation process in a DI H2-ICE.
- ☐ By acting on these parameters a large improvement in terms of H2 distribution was achieved



Uniformity Index (UI) = $\sigma_{\Phi} / \Phi_{av}$

- ☐ An optimal injection window, capable of maximizing mixture uniformity, without a sensible impact on the volumetric efficiency was defined
- ☐ Several spray guiding caps were tested
- ☐ The impact of swirl intensity on the mixture formation process was assessed by acting on the swirl chamfers configuration

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    - **1D-CFD predictive models for virtual calibration**

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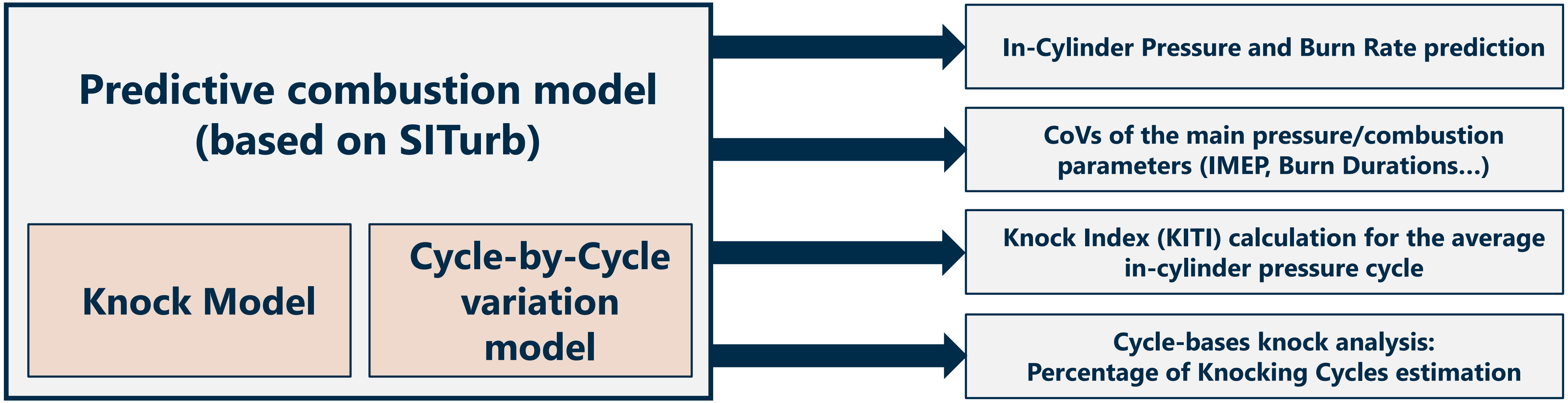
1D-CFD predictive models for virtual calibration

Aim: development of a reliable simulation tool to drive and speed up the development process of H2-fuelled ICE.

In this regard, the developed comprehensive combustion model must be able to:

- predict burn rate and in-cylinder average pressure cycle, as well as to mimic CCV
- estimate the knock likelihood considering both the average pressure cycle and cycle-basis knock indexes



Predictive combustion model (based on SITurb)

Knock Model

Cycle-by-Cycle variation model

In-Cylinder Pressure and Burn Rate prediction

CoVs of the main pressure/combustion parameters (IMEP, Burn Durations…)

Knock Index (KITI) calculation for the average in-cylinder pressure cycle

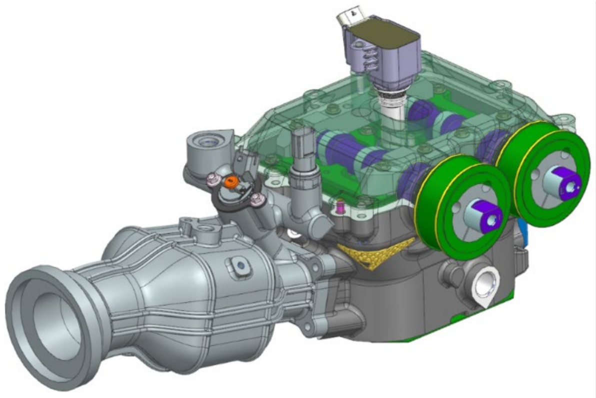
Cycle-bases knock analysis:
Percentage of Knocking Cycles estimation

1D-CFD predictive models for virtual calibration

Case study

The engine selected as case study is representative of a retrofitting of a state-of-the-art low-compression ratio diesel engine.

Engine type	Single Cylinder Engine (SCE)
Bore	83 mm
Stroke	90.4 mm
Displacement	0.5 L
Compression ratio	12.0:1
Piston type	Hemi-spherical bowl
Fuel system	Port Fuel Injection (PFI)



Single-cylinder head

Hemi-spherical piston

Two engine operating conditions have been analyzed.

- ☐ 2000 RPM x Full Load
- ☐ 2000 RPM x Partial Load

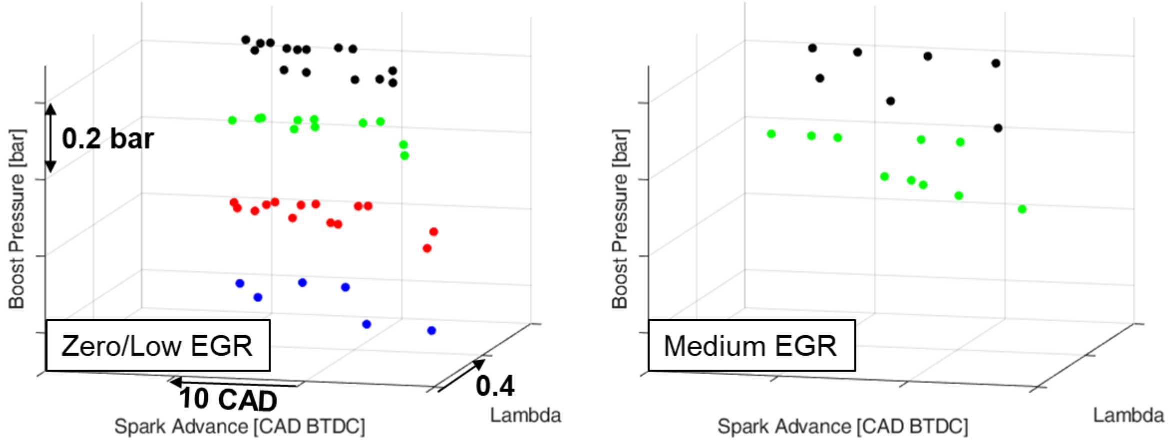
1D-CFD predictive models for virtual calibration

Experimental campaign

A wide experimental campaign has been performed on two engine operating conditions.

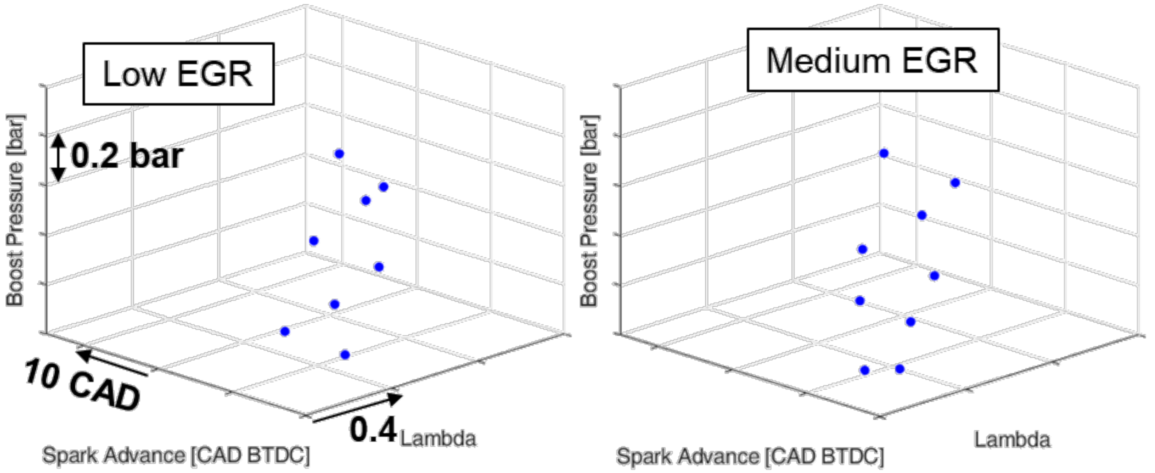
☐ 2000 RPM x Full Load

Parameter	Lower Limit	Upper Limit
Spark Advance [CAD]	<10	>30
Lambda [-]	>1.2	>2
Boost Pressure [bar]	>2.0	>3.2
EGR [%]	0	>10
65 tested combinations		



☐ 2000 RPM x Partial Load

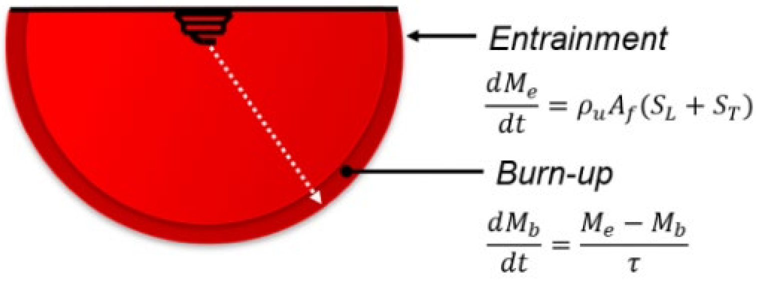
Parameter	Lower Limit	Upper Limit
Spark Advance [CAD]	<5	>30
Lambda [-]	>1.3	>2.5
Boost Pressure [bar]	>1.1	>1.7
EGR [%]	0	>10
31 tested combinations		



1D-CFD predictive models for virtual calibration

Predictive combustion model

The combustion model is based on the already available SITurb combustion model. A single equivalent flame is modeled by adopting a classical entrainment and burn-up approach in which the flame propagation is triggered from a fixed location inside the cylinder.



As the flame brush propagates, it entrains unburned gasses, which are then burned behind the flame over a characteristic timescale.

☐ **Unburned mixture entrainment into the flame front**:

$$\frac{dm_e}{dt} = \rho_u A_e (S_L + S_T)$$

- ρ_u is the unburned mass density
- A_e is the effective flame area

☐ **Burn rate of entrained gas:**

$$\frac{dm_b}{dt} = \frac{m_e - m_b}{\tau}$$

ratio between the actual unburned mass entrained by the flame and a characteristic burning timescale

$$\tau = \frac{\boldsymbol{C_{TLS}}\lambda}{S_L} = \frac{\boldsymbol{C_{TLS}} \cdot L_i / Re_T}{S_L}$$

☐ **Turbulent flame speed**

Turbulent flame speed is computed considering the turbulent intensity and the integral length scale

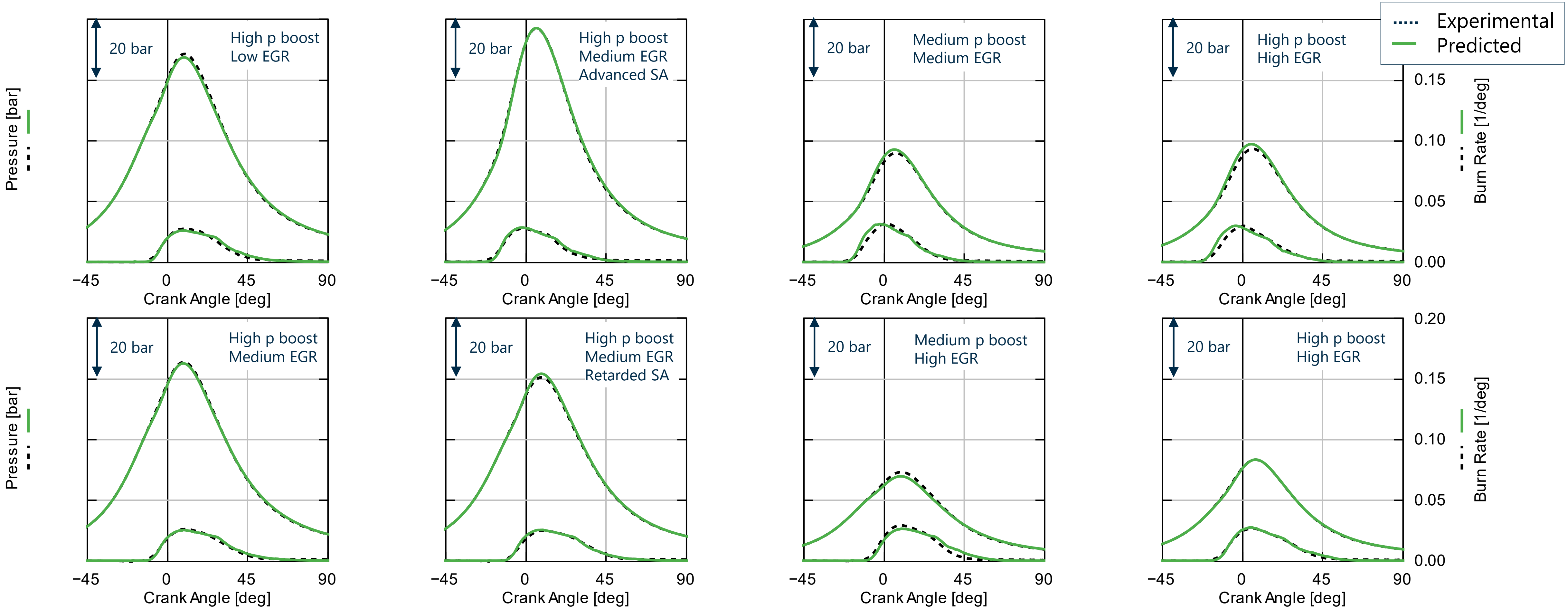
$$S_T = \boldsymbol{C_{TFS}} u' \left(1 - \frac{1}{1 + \boldsymbol{C_{FKG}} \left(\frac{R_f}{L_i} \right)^2} \right)$$

* Calibration constants are highlighted in red

1D-CFD predictive models for virtual calibration

Results: Predictive combustion model

An optimization base on a genetic algorithm has been performed with the aim of finding a single set of calibration parameters that has been maintained constant for all the engine operating conditions.



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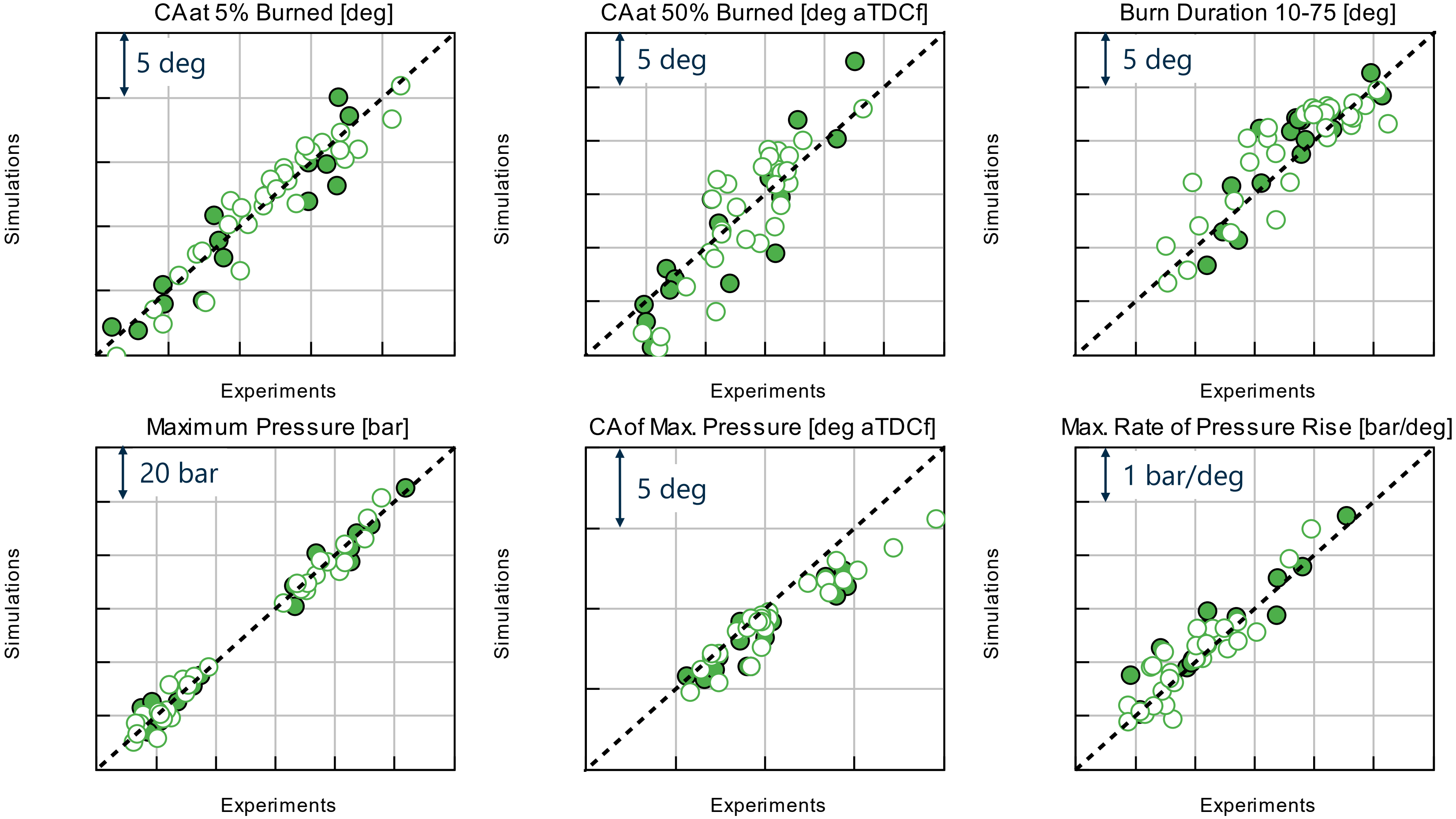


● Predicted – Calibration dataset
○ Predicted – Validation dataset

Combustion parameters are well predicted by the model using the tabulated approach both for full-load and part-load engine operating conditions.

RMSE	
MFB5	1.5 deg
MFB50	2.8 deg
MFB10-75	2.7 deg
Max Pressure	3.9 bar
CA @ Max Pressure	1.6 deg
Max Rate of Pressure Rise	0.3 bar/deg

1D-CFD predictive models for virtual calibration

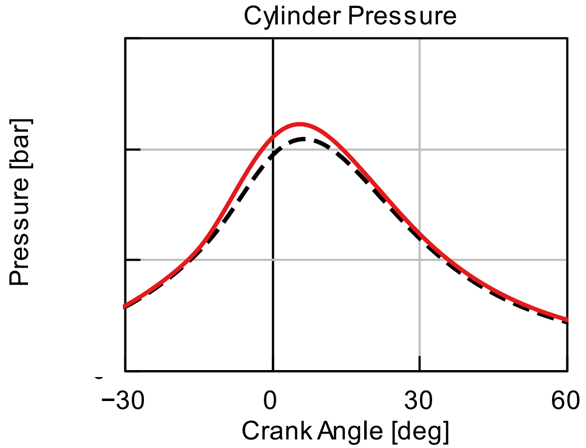
Cycle-by-cycle variability model

The CCV model, developed by Gamma Technologies, is a non-phenomenological model able to mimic the cycle-by-cycle variation of a SI engine.

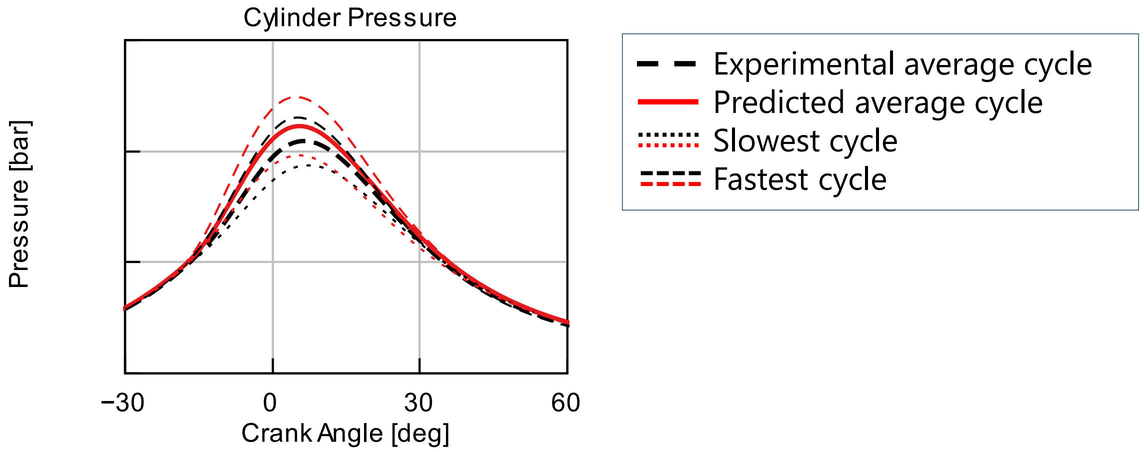
The variables Turbulent Flame Speed Multiplier $\boldsymbol{C_{TFS}}$ and the Taylor Length Scale Multiplier $\boldsymbol{C_{TLS}}$ of the combustion model are perturbed starting from a Gaussian distribution.
The standard deviations of the perturbations are the inputs of the CCV object, and have been optimized by means of genetic algorithm.

$$S_T = \boldsymbol{C_{TFS}} u' \left(1 - \frac{1}{1 + \boldsymbol{C_{FKG}} \left(\frac{R_f}{L_i} \right)^2} \right)$$

$$\tau = \frac{\boldsymbol{C_{TLS}} \lambda}{S_L} = \frac{\boldsymbol{C_{TLS}} \cdot L_i / Re_T}{S_L}$$



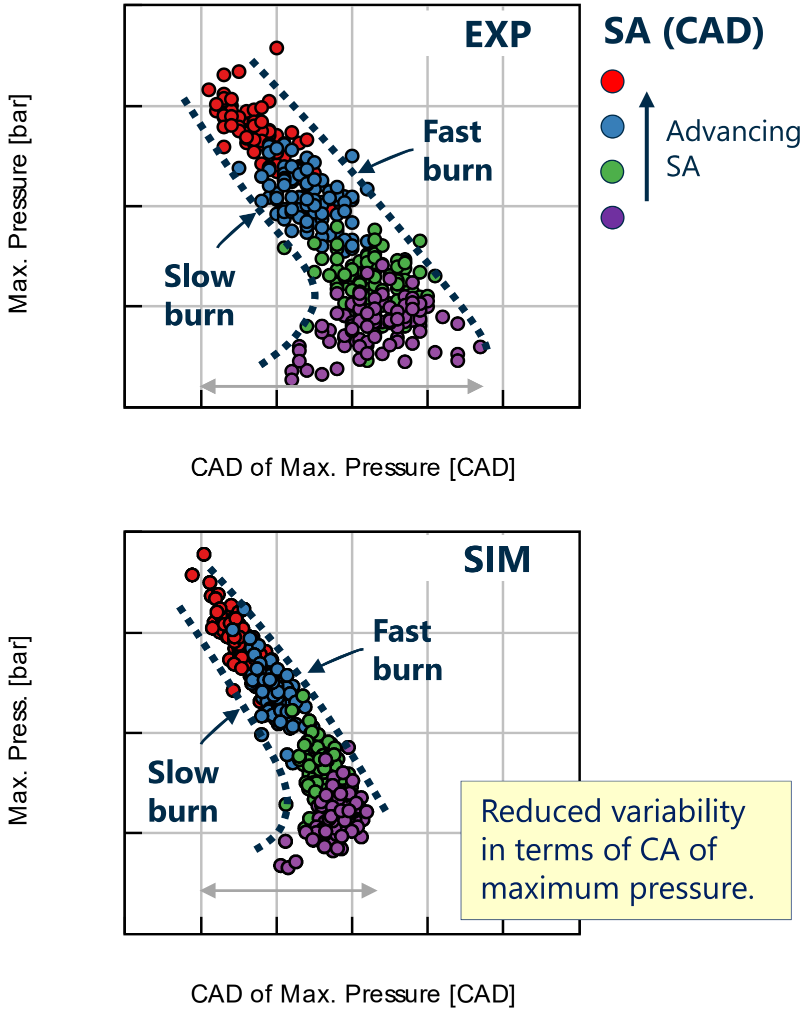
SITurb calibration parameters pertubation $\boldsymbol{\sigma_{TFSM}}, \boldsymbol{\sigma_{TLSM}}$



1D-CFD predictive models for virtual calibration

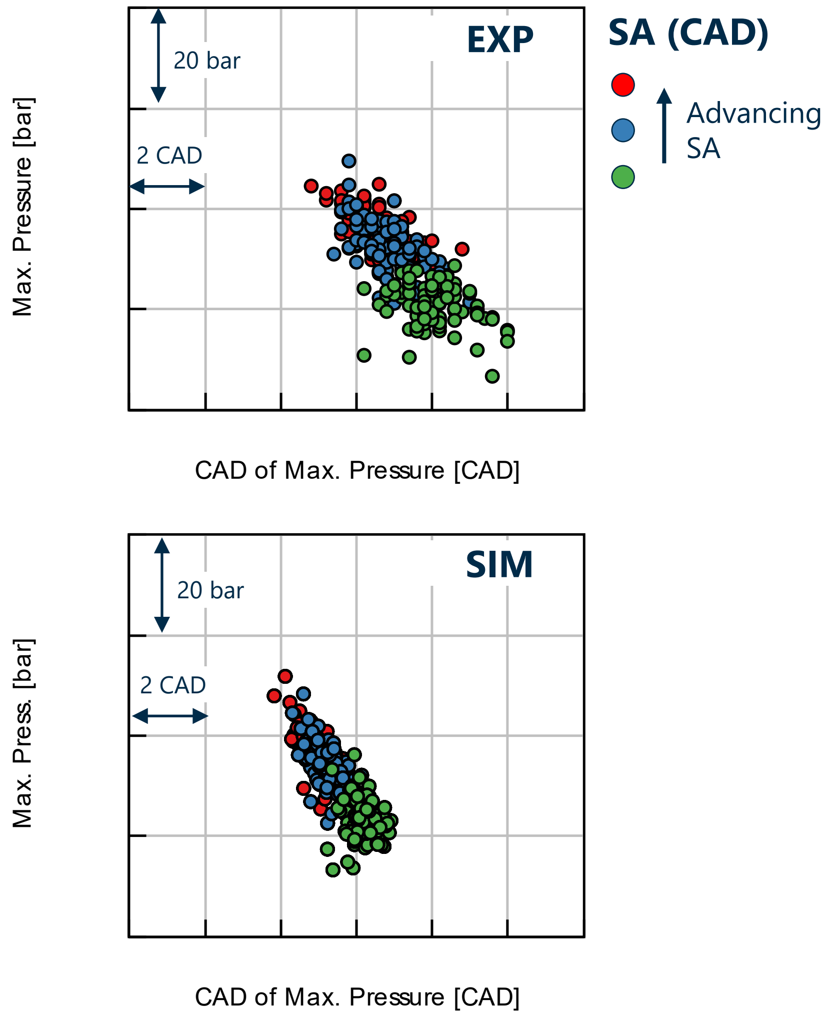
Cycle-by-cycle variability model | Results: Matekunas plot

High EGR



Reduced variability in terms of CA of maximum pressure.

No EGR



Experimental data:
At high dilution levels, the MaxPressure/CA@MaxPressure correlation show an almost flat trend: the retarded combustion phasing leads to a reduced rate of increase of pressure due to combustion, that is more than offset by the pressure decrease due to volume increase.

Simulation results:
Matekunas plot trends are predicted by the CCV model also for very retarded combustion phasing.
A slight underestimation of CoV of CA@PFP can be highlighted.

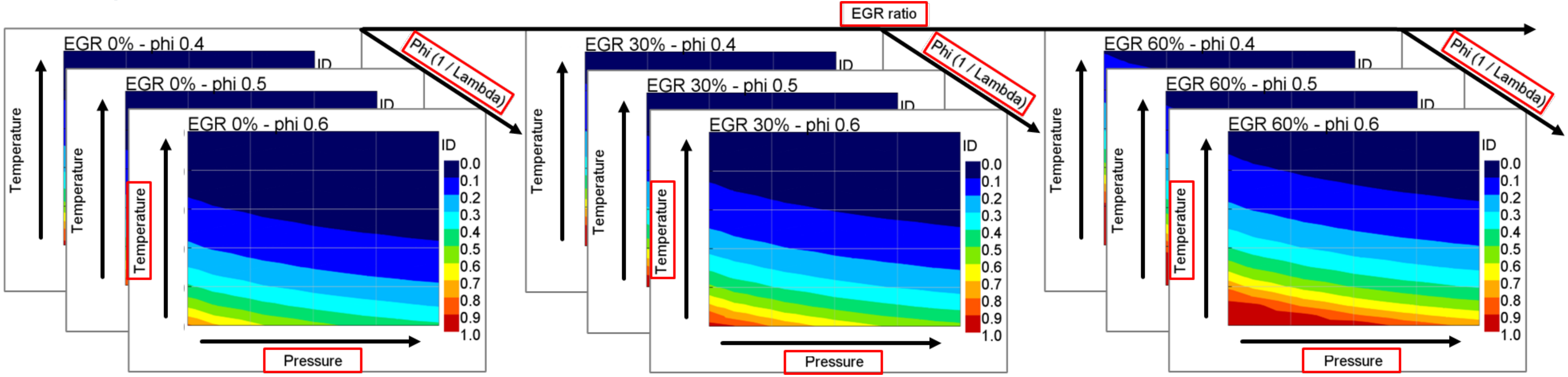
Comprehensive combustion model

Knock model

A knock model, based on the well-known Livengood-Wu approach, has been developed and implemented in GT-SUITE to quantify the knock tendency of the average cycle for a given operating condition.

The auto-ignition of the end gas occurs when: $\int_{t=0}^{t_{knock}} \frac{1}{\tau} dt = 1$

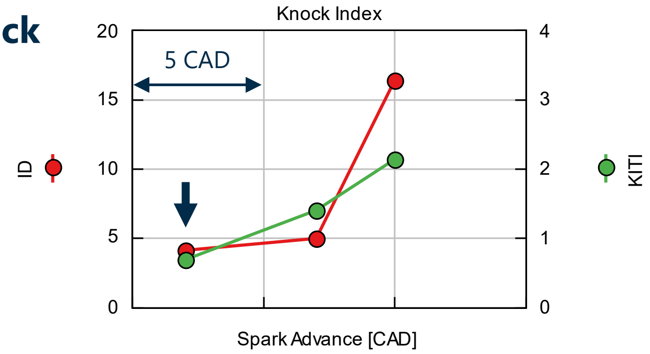
Starting from the detailed chemistry scheme developed by Zhang et al., 0D calculations have been performed to compute the value of the induction time for a wide range of pressure, temperature, mixture composition and dilution.



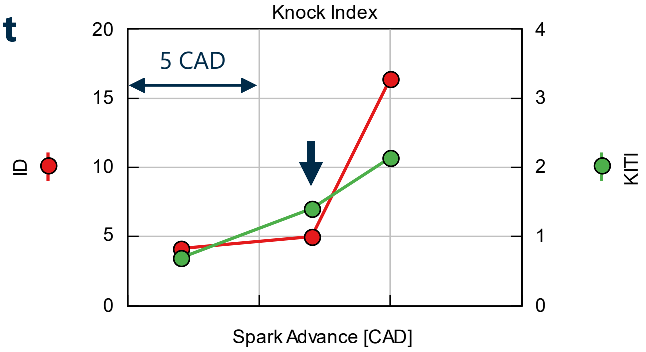
Comprehensive combustion model

Results: Knock model w/ predictive combustion

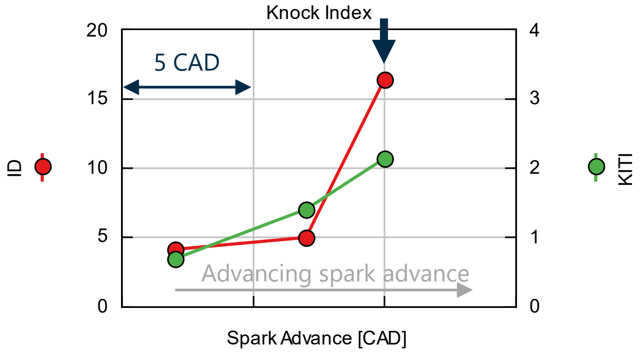
No-knock



Incipient knock



Heavy knock



🟥 Experimental
🟩 Predicted

Condition:

- Medium Boost pressure
- Low EGR
- High Lambda

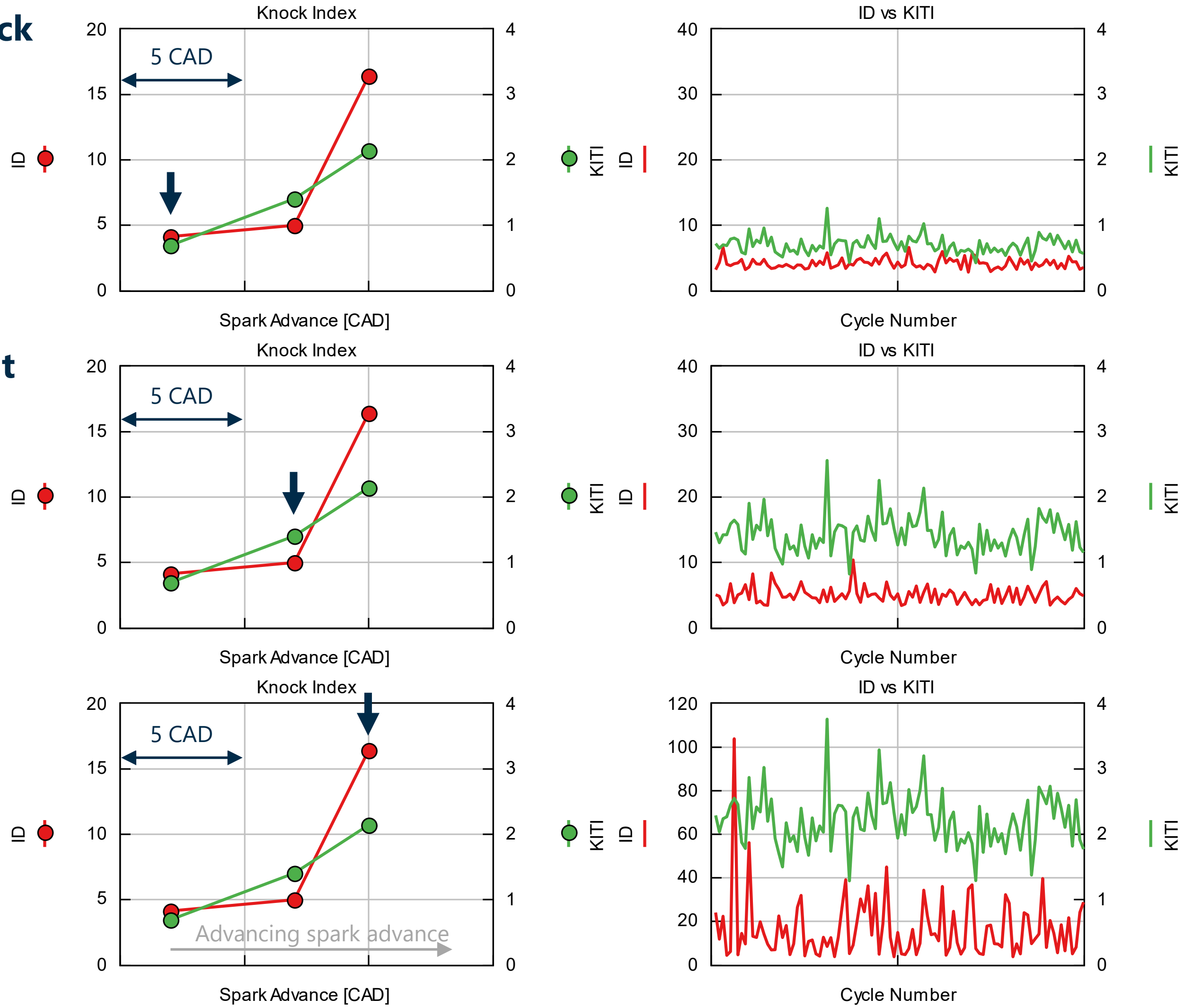
Comprehensive combustion model

Results: Knock model w/ predictive combustion

No-knock

Incipient knock

Heavy knock



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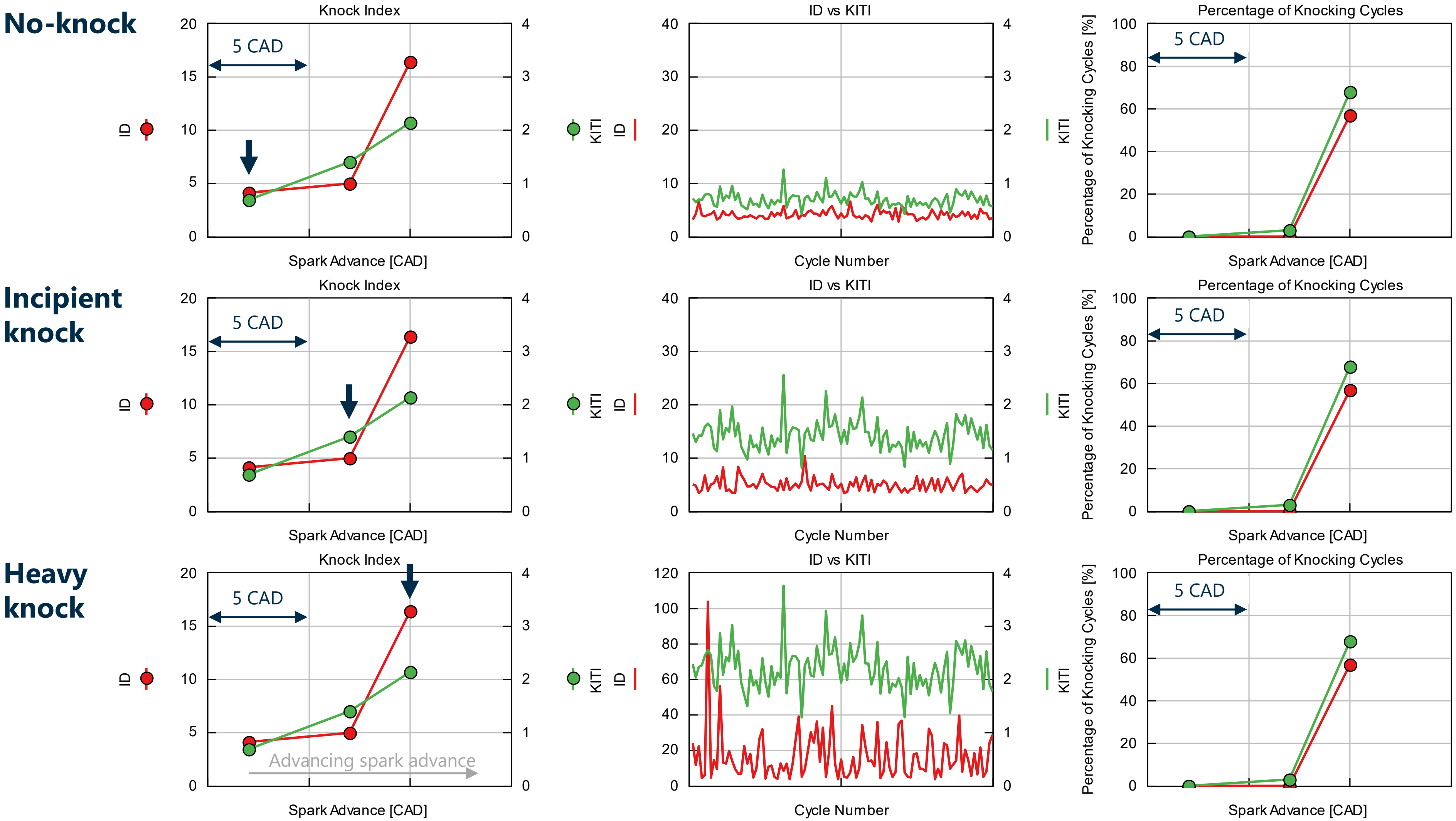

Condition:

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The combination of the combustion, CCV e knock models allows a cycle-to-cycle analysis of knock tendency also when the predictive combustion model is adopted.

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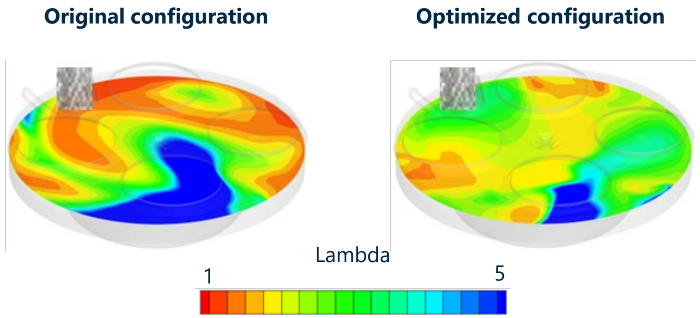
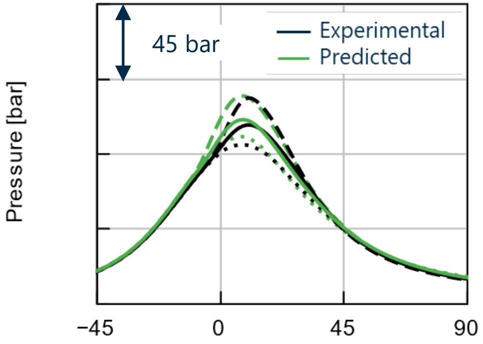
Conclusions

Comprehensive H2 simulation tool chain including 0/1/3D-CFD approaches (and their synergies) can help each phase of the engine development process reducing the overall lead time and cost consuming experimental activities.

Different simulation approaches can be adopted:

- ❑ 3D-CFD simulations
    - ❑ **Mixing simulations to optimize flow motion and its interaction with the H2 spray**
    - ❑ Combustion simulations to analyse performance, heat rejection, emissions, knock/pre-ignition
- ❑ 0/1D-CFD
    - ❑ Definition of the main requirements in terms of boost (e.g., valve timings, TC layout)
    - ❑ **Comprehensive model for the prediction of the H2 combustion process and its anomalies for reliable system-level analysis**
- ❑ Synergetic application of different simulation approaches





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Researching efficient uses of energy in automotive powertrains to minimize their CO2 and pollutants emissions.

Prof. Federico Millo

Politecnico di Torino
Energy Department "G. Ferraris"
C.so Duca degli Abruzzi, 24
10129, Torino – ITALY
@ federico.millo@polito.it
in federico-millo