

# 用于发动机虚拟开发的 3D-CFD-CHT 方法

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**摘要:** 为降低开发成本,需要在开发过程中明确几何结构、总成布置及不同燃料对内燃机性能的影响,这其中一种有效的创新性融和分析方法——三维计算流体动力学-热-结构耦合(3D-CFD-CHT)方法已然成为内燃机开发过程中必不可少的工具。该类工具正在被越来越多的制造商用于发动机开发方案筛选及样机原型确定。本文主要介绍一种由斯图加特汽车工程与车辆发动机研究所(FKFS)开发的针对内燃机虚拟开发的 3D-CFD 仿真工具—QuickSim。该工具通过将较为粗糙的计算网格与自行开发的内燃机模型有效结合,有效减少计算时间,能以较高精度模拟整个发动机的运行。本文以尽可能实现高燃烧效率及低污染排放为目标,展示该工具在不同替代燃料发动机方面的设计优化能力,探讨不同燃料如氢气、甲醇、各类合成燃料及生物燃料对不同发动机几何结构的影响,探讨燃油喷射系统以及点火系统(包括主动和被动预燃室)对发动机的影响。同时,针对甲烷和氢气发动机,讨论稀薄燃烧对减少节流和爆震的影响;总结如何根据任一选定燃料,通过合理的几何结构设计,提高发动机的指示功率。

**关键词:** 电子燃料; 甲烷; 甲醇; 氢气; 碳减排; 虚拟开发; 三维计算流体动力学(3D-CFD)

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## An Effective 3D-CFD Methodology for the Complementary Virtual Development of Alternative Fuels and Engine Concepts

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**Abstract:** With the aim of reducing the cost of developing internal combustion engines, while at the same time investigating different geometries, layouts and fuels, 3D-CFD-CHT simulations represent an indispensable part for the development of new technologies. These tools are increasingly used by manufacturers, as a screening process before building the first prototype. This paper presents an innovative methodology for virtual engine development. The 3D-CFD tool QuickSim, developed at FKFS, allows both a significant reduction in computation time and an extension of the simulated domain for complete engine systems. This is possible thanks to a combination of coarse meshes and self-developed internal combustion engine models, which simultaneously ensure high predictability. The present work demonstrates the capabilities of this innovative methodology for the design and optimization of different engines and fuels with the goal of achieving the highest possible combustion efficiencies and pollutant reductions. The analysis focuses on the influence of different fuels such as hydrogen, methanol, synthetic gasolines and methane on different engine geometries, in combination with suitable injection and ignition systems, including passive and active pre-chambers. Lean operations as well as knock reduction are discussed, particularly for methane and hydrogen injection. Finally, it is shown how depending on the chosen fuel, an appropriate ad-hoc engine layout can be designed to increase the indicated efficiency of the respective engines.

**Keywords:** eFuels; methane; methanol; hydrogen; CO<sub>2</sub> reduction; virtual development; 3D-CFD

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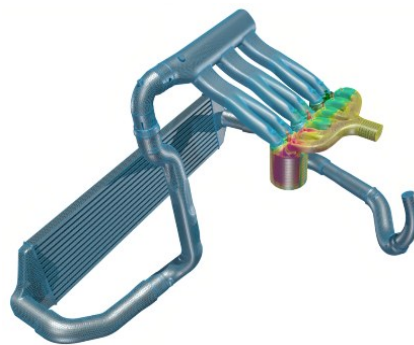
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## 1 Introduction

The reduction of Greenhouse gases (GHG) is the primary objective of the latest world energy policies, oriented towards carbon neutrality. As reported in several studies<sup>[1]</sup> a tank-to-wheel analysis is not the most accurate approach to assess the actual emissions and environmental impact of a vehicle. With the strong belief that ICEs will be one of the options alongside other mobility solutions, such as battery electric vehicles (BEVs), the design and optimization phase of ICEs becomes a crucial topic, especially with the introduction of synthetic fuels or alternative fuels that can make an ICE-powered vehicle carbon neutral. It is clear that the most efficient way to reach the climate goal of carbon neutrality is related to the diversification of the energy carriers employed, maximizing the benefits inherent to each solution while considering the ultimate field of application. The virtual development of new engine layouts and fuel formulations by means of 3D-CFD simulations is an indispensable resource to ensure a cost and time reduction within the development process. Additionally, it facilitates the investigation of various phenomena that are otherwise hard to be investigated through experiments.

The 3D-CFD simulations discussed in this work are carried out using QuickSim<sup>[2]</sup> a fast response 3D-CFD tool developed at the Forschungsinstitut für Kraftfahrwesen und Fahrzeugmotoren Stuttgart (FKFS). The fast response characteristics of QuickSim combined with its high flexibility allow the investigations of different fuels and different engine layouts, ensuring high reliability of the simulation results and the possibility to extend the computational domain to perform a full engine simulation (See Fig. 1).

This work focuses on the most promising concepts regarding alternative solutions to traditional ICEs, considering four different fuels and the subsequent geometry improvement required to maximize the efficiency of these solutions. The first analysis presented is a comparison between Methanol and a synthetic fuel called POSYN (Porsche



**Fig.1 Full engine mesh for QuickSim environment**

Synthetic fuel) used in a downsized engine with boost pressure up to 3 bar absolute, with the aim of demonstrating which are the necessary measures to be implemented to enhance the engine efficiency. Some hardware modifications are considered, such as the adoption of a pre-chamber spark plug (PCSP) to increase the engine indicated efficiency and initialize a faster combustion event. This work has been carried out in collaboration between FKFS and Porsche AG<sup>[3]</sup>. Different fuels can be considered to accomplish GHG reduction. Within this frame, Methane or in the future biogas can play a crucial role as an immediate solution to achieve CO<sub>2</sub> reduction [4], since it has long been employed in ICEs and can rely on an already existing partial infrastructure and distribution network. Therefore, the second case presented shows the virtual development of a Methane engine, the object of a research project carried out in collaboration with Ford-Werke GmbH, Fraunhofer-Institut für Chemische Technologie (ICT), FKFS, Rosswag GmbH and BRIGHT Testing GmbH. During the project many geometry modifications have been investigated, that have led to the adoption of an active PCSP and a completely redesigned combustion chamber. The final case reported in this work focuses on the usage of hydrogen fueling a single-cylinder engine with port fuel injection and pre-chamber ignition. Hydrogen fueled ICE are an interesting alternative to standard ICE or fuel cell (FC) electric vehicles and, even if the H<sub>2</sub>-ICE requires partial hardware adjustments compared to standard fossil-fuel ones, it is a promising and cost-effective technology. This third case, carried out together with the Fraunhofer ICT,

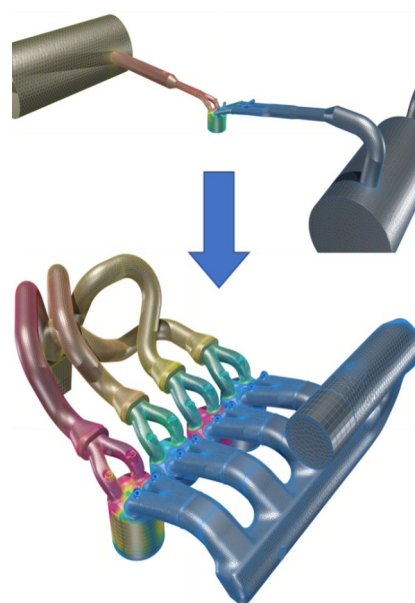
aimed to illustrate the behaviour of hydrogen combustion in combination with a passive pre-chamber system leading to the development of an optimized engine setup for hydrogen operation.

## 2 Simulation Methodology

Optimizing charge motion, mixture formation and combustion are key challenges in the development of ICEs. A detailed analysis of these complex phenomena is essential to fulfil current and future emission and efficiency standards. 3D-CFD Simulation can help to investigate operating strategies or engine configurations to understand different occurring phenomena at the test bench.

The 3D-CFD Tool QuickSim has been and still is continuously further developed for more than 20 years<sup>[2]</sup>. It is specifically designed to serve as a virtual ICE development environment to complete or even to replace time and cost-expensive test bench investigations. This tool is based on the commercial CFD-Solver Star-CD, but the scope of functions has been extensively enlarged by self-developed and validated models for ICEs. It offers the possibility to reduce the computational expense for a simulation drastically and has proven to deliver highly accurate results in various industrial and research projects. Specifically, for ICE applications optimized models such as injection, fuel and combustion models, combined with an innovative meshing and mesh motion methodology lead to a significant reduction in computational effort compared to traditional 3D-CFD approaches. For the combustion chamber high quality hexahedron meshes are used, which are fine enough to capture and resolve relevant flow effects. These meshes enable an efficient mesh motion strategy that does not require remeshing operations during the engine cycle and therefore avoid mapping errors and save computational time. With high quality cells in critical flow regions, numerical instabilities can be avoided and allow greater timesteps without sacrificing accuracy. By extending the simulation domain to the full test bench dimensions, the influence of boundary conditions can be minimized

and the real testbench's behaviour is reproduced, especially for multiple consecutive operating cycles, more accurately. Meshes can be prepared in a way that provides modularity to quickly change engine components and test different configurations or extrapolate a single cylinder engine to a multi cylinder full engine model, as shown in Fig. 2.



**Fig.2 Extrapolation of single cylinder test bench to a real full engine model**

In QuickSim every possible fuel can be modelled with the real surrogate composition and the real fuel properties. Fuel surrogates are selected considering all the main chemical species that are present in the real fuel. Combustion properties are evaluated in a preliminary phase by using a detailed reaction mechanism in Cantera<sup>[5]</sup>. Besides the necessary caloric properties, which are determined for all possible combinations of temperature, pressure and mixture compositions, also fuel-related combustion properties such as laminar flame speed and ignition delay time are calculated. All these values are stored as look-up tables so that there is no additional effort to calculate chemistry during the simulation. It allows the application of a 3D-auto-ignition model, which was specially developed for this chemistry calculation approach in order to predict abnormal combustion phenomena such as knocking, pre-ignition and back-firing. The auto-ignition model uses an adjusted integral of the ignition delay time in each cell to

describe the chemical process until the combustion event is triggered<sup>[5]</sup>. Especially for Hydrogen and other very knock-sensitive fuels reliable combustion and auto-ignition models are indispensable to ensure a fast and successful ICE development<sup>[6]</sup>.

Correct fuel properties are crucial for modelling the injection process, especially for liquid fuels. Particularly, mixture formation, spray propagation, penetration and evaporation need to be investigated. Optimized droplet break-up and evaporation models in QuickSim together with real temperature dependent fuel properties deliver a reliable base for spray simulations. Spray chamber optical measurements are used to calibrate the simulation and to consider specific injector behaviour and geometrical influences. For this task, a PDA (Phase Doppler Anemometry) laboratory is operated at FKFS to conduct measurements on liquid fuels.

The 3D-CFD injection simulation of hydrogen and other gaseous fuels holds many challenges regarding the numerical setup, stability and computational effort. To cover all detailed effects occurring inside the needle gap of an injector, an extremely high spatial and temporal resolution is required in the simulation to achieve good results and to fulfil all the convergence criteria<sup>[7]</sup>. To avoid these challenges a lagrangian approach similar to the conventional injection of liquid fuels is preferred<sup>[8]</sup>. Since this method is a simplified description of a complex injection event, an appropriate calibration is required to deliver accurate results.

By applying this methodology, the complementary virtual development of alternative fuels and engine concepts is represented in this paper in the following three projects: ① potential of synthetic fuels; ② active PCSP with lean methane operation; ③ thermodynamics of hydrogen combustion.

### 3 Potential of Synthetic Fuels

The adoption of synthetic, CO<sub>2</sub>-neutral fuels, so-called eFuels, is one of the most promising solutions for an immediate defossilization of the transport sector<sup>[9]</sup>. Furthermore, eFuel formulations can be

designed to obtain specific behaviours, such as a reduction in emissions of particulate matter (PM) and total hydrocarbons (THC)<sup>[10]</sup>, as well as an increase of engine efficiency. In a project between FKFS and Porsche AG the fuel POSYN is compared with a conventional RON98 fossil gasoline and with methanol to highlight the impact of the fuel choice for the engine development. POSYN mainly contains isoparaffins, cycloalkanes and others, that are all potentially renewable when produced via e. g. Methanol-to-Gasoline (MtG) synthetics. The POSYN composition deliberately lacks aromatics and olefins since the low volatility of these components leads to the formation of PM. In addition, thanks to this specific formulation, POSYN shows higher knock resistance than the conventional RON98 (Research octane number) fuel. Methanol is the second renewable fuel considered in this analysis and one of the most promising alternative fuels for large-bore stationary applications. Methanol has many favourable characteristics for ICE application, such as High Heat of Vaporization (HOV), High Laminar flame speed (LFS) and High hydrogen-to-carbon ratio. Particularly, high HOV of methanol (HOV<sub>methanol</sub> 1 160 kJ/kg at 25 °C) compared to gasoline (HOV<sub>gasoline</sub> ~ 380 kJ/kg at 25 °C) leads to high knock resistance and therefore permits to obtain high break thermal efficiency. Moreover, methanol shows advantages concerning the production process due to its high synthetization efficiency. On the other hand, the cold starting of alcohols is very challenging. Due to its lower energy density (LHV<sub>methanol</sub>=19.93 MJ/kg), the evaporation of more mass is required to run a certain operating point (OP). Additionally, the evaporation of Methanol requires higher energy, as a consequence of its very high HOV compared to gasoline. Furthermore, the low stoichiometric air-to-fuel ratio ( $\alpha_{st}$ =6.5 kg/kg) leads to the necessity of a higher vapour pressure to obtain a stoichiometric mixture. Finally, methanol is a single-component fuel and the lack of volatile components makes cold-start operations very difficult.

For the calibration and validation of the 3D-CFD



simulations a single cylinder engine (SCE) operated by Porsche AG is used (see Tab. 1).

**Tab.1 Engine specifications**

Displaced volume	Parameter
Displaced volume	468.3 cc
Stroke	81 mm
Bore	88.5 mm
Connecting rod	142 mm
Stroke/Bore ratio	0.92
Compression ratio	13.2:1
Number of valves	4

Some hardware modifications are considered to increase the engine indicated efficiency, such as adopting a PCSP, which permits initializing a faster combustion event and better control the mixture and turbulence conditions at the electrode. All comparisons are run at 7 000 r/min and 22 bar IMEP (indicated mean effective pressure), analyzing different engine configurations (conventional spark plug or PCSP) in combination with various valve profiles (including Millerization concepts) and different fuels. The indicated efficiency resulting from the tests is reported in Tab. 2. Injecting POSYN leads to an increase of the indicated efficiency of 0.5%-pt compared to the conventional fuel (RON98) in the case of spark plug (SP). The adoption of the PCSP increases indicated efficiency of 0.3%-pt for the conventional fuel (RON98) and 0.7%-pt for POSYN, due to the higher knock resistance of the synthetic fuel.

**Tab.2 Resume of the indicated efficiency values of each investigation.**

Test	Indicated efficiency/%
SP—RON98 conv. fuel	39.4
PCSP—RON98 conv. fuel	39.7
SP—POSYN	39.9
PCSP—POSYN	40.6
Methanol	38.8

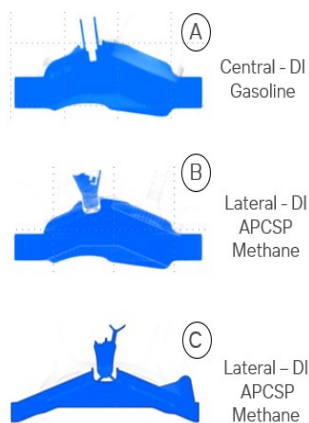
Considering a lower power density and stoichiometric ratio of Methanol, some hardware modifications are mandatory. The first direct injector is replaced with one having the same targeting, but twice the injection rate despite working at the same pressure of 350 bar. To operate the engine at the same torque the injected fuel mass has to be more than double compared to the gasoline case, and for

this reason, a low-pressure injector (10 bar) with 4 holes and a flow rate of 9 g/s is installed into the intake port, delivering the 75% of the total injected mass per cycle. The boost pressure can be raised due to methanol high heat of vaporization, cooling down the in-cylinder charge and reducing the knock tendency. Nevertheless, Methanol injection did not produce any rise of the engine indicated efficiency, because of limitations deriving from the hardware configuration (too low compression ratio for Methanol engine) and worse evaporation (injector not tailored for Methanol application). This analysis highlights the need of further work to better understand which design modification can improve a Methanol fueled engine. On the other hand, the combination of POSYN with a PCSP leads to an increase in indicated efficiency higher than 1 %, with 18% higher boost pressure compared to the conventional RON98 fuel with the standard SP.

## 4 Active PCSP with Lean Methane Operation

Methane has a higher hydrogen-to-carbon ratio and it exhibits superior knock resistance compared to gasoline, allowing the use of an increased compression ratio and, consequently, enhancing the combustion efficiency. Considering both these aspects, a reduction of 30% CO<sub>2</sub> can be achieved using methane<sup>[4,11]</sup> instead of gasoline (CO<sub>2</sub> reduction is potentially even higher considering bio-methane, once the fuel production is considered). In order to design an engine that can exploit the natural gas advantages, a consortium made by Ford-Werke GmbH and different partners run a 36 months project (No. 19I20014E) called MethMag (Methan Mager Motor). Considering a gasoline engine of comparable power targets as a benchmark (Fig. 3 A), the aim of the project is to develop a 3-cylinder natural gas engine (1.5 l displacement) that can operate with a very lean mixture and high compression ratio (reducing specific fuel consumption), which could be suitable for use in a light duty commercial vehicle.

Fig. 3 shows how the virtual development led to



**Fig.3 Steps of virtual engine development process**

the design of a new combustion chamber, high-tumble channels, new piston, new active pre-chamber (APCSP) and injector layout:

(1) 3-cylinder gasoline engine from Ford, called Ecoboost<sup>[12]</sup>, with central gasoline injector and spark plug. It has been used to calibrate the 3D-CFD model compared to experiments.

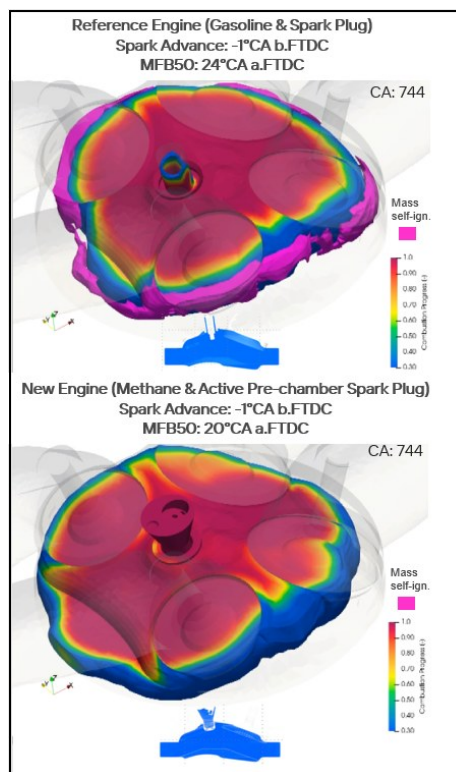
(2) First design of an active pre-chamber spark plug, which replaces the conventional spark plug of the gasoline application (same bore). The direct methane injector is placed laterally between the intake ports (first configuration tested with methane instead of gasoline).

(3) After more than 180 3D-CFD simulations with different loads, geometry combinations, valve profiles, injector positions, pre-chamber and cylinder head concepts, a new 1-cylinder engine geometry with methane direct injection and a central active pre-chamber spark plug has been designed.

The single-cylinder engine with the new geometry has been manufactured and installed at Fraunhofer ICT for validation and further investigations. As reported in Ref. [13], the simulated load points highlight a remarkable rise in indicated efficiency with respect to the reference engine, from 35.0% to 42.3 % for the engine operating point 2 000 r/min full load. As displayed in Fig. 1, the 3-cylinder engine has been also implemented in the 3D-CFD virtual environment for further optimization and refinement of the overall engine thermodynamics and efficiency.

Fig. 4 represents the combustion progression of

the reference gasoline engine (Fig. 3 ①) and the first pre-chamber design operated with methane (Fig. 3 ②), at the same ignition point for the engine operating point 2 000 r/min full load. It is clear that the pre-chamber combustion is faster, moving the MFB50 (50% mass fraction burned) almost 4° CA earlier. Purple regions identify the areas where the mass in self-ignition is located (knock onset). The engine operated with APCSP and methane has a lower tendency to knock. For further details about the combustion process and the geometry investigation refer to Ref. [3, 13, 14].

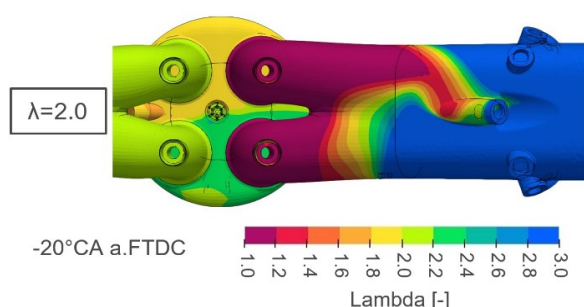


**Fig.4 Comparison of the combustion progress of the reference engine operated with gasoline (top) and the first pre-chamber design operated with methane (bottom)**

## 5 Thermodynamics of Hydrogen Combustion

Hydrogen combustion and its effect on the engine thermodynamics have been investigated through 3D-CFD simulations by analyzing different concepts of injection and ignition systems. In the presented investigation, a single-cylinder engine was

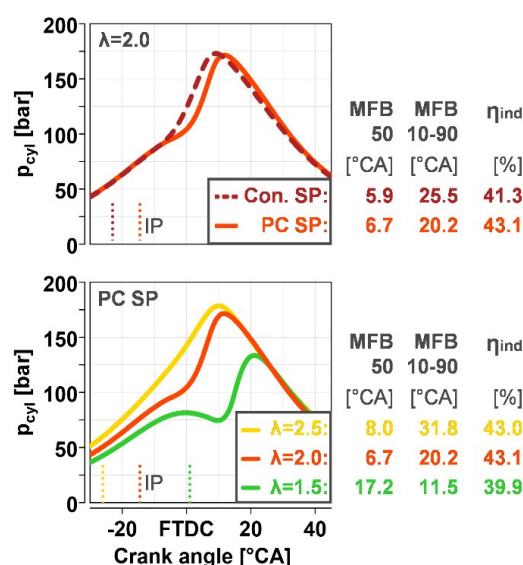
tested at Fraunhofer ICT. for various strategies of port fuel injection (PFI), as well as for different ignition systems. Due to hydrogens low ignition energy, a sophisticated injection strategy is crucial in combination with a PFI system to prevent dangerous back-fire events. By carrying out a virtual analysis of the injection and mixture formation, it was possible to optimize the injection timing<sup>[15]</sup>. The investigations show that if the injection is too late, the mixture cannot reach the cylinder and the intake manifold is pre-charged for the next cycle, as shown in Fig. 5.



**Fig.5 Lambda distribution inside the intake channel and cylinder at lambda 2 operation<sup>[6]</sup>**

Besides back-fire events during the gas exchange, also the knocking tendency of the hydrogen-air mixture during the combustion is of high importance, especially for nearly stoichiometric operation. For this matter, the ignition system and the mixtures stoichiometry are important factors to have a detailed look at. The simulation results of the project, including a comparison of a conventional spark plug with pre-chamber (PC) ignition, as well as three different lambda operations, are shown in Fig. 6.

The displayed pressure curves highlight the various possibilities of hydrogen combustion at similar engine load. By using two different ignition systems and applying various boundary conditions it was possible to optimize the center of combustion (MFB<sub>50</sub>) and also affect the combustion duration (MFB<sub>10-90</sub>) tremendously. Through efficient and fast examinations of the virtual environment, it was possible to achieve an indicated efficiency ( $\eta_{ind}$ ) of up to 43.1% with this particular concept of a hydrogen combustion engine.



**Fig.6 Comparison of spark plugs (SP) and different lambda operations at 3 000 r/min and 23 bar IMEP<sup>[6, 15]</sup>**

## 6 Conclusion

The utilization of 3D-CFD simulation in the ICE development process is nowadays absolute essential. The virtual engine development tool QuickSim is adapted for the needs of this complex task and represents a significant step forward in the field of internal combustion engine analysis and design. Through the interaction of well-calibrated phenomenological models, a special meshing approach and over 20 years of experience, a reliable and fast development of engine configurations, operating strategies and fuel compositions can be achieved. The reliability of the results has been proven in plenty of research and industrial projects of which three projects are presented in this paper more detailed. The above discussed methodology has been used to develop synthetic fuel composition and tailored engine geometry, by testing different configuration (injectors, pre-chamber, millerization). Gaseous fuels like methane and hydrogen could also be investigated for successfully increase engine efficiency and operability. Methane engines with dedicated combustion chamber design and operating lean represent an interesting technology for immediate CO<sub>2</sub> reduction and from the costs point

of view. The optimization of hydrogen powered ICE has just begun. Injectors and combustion control are complex thermodynamic topics to be investigated and understood. For all these reasons, time-effective 3D-CFD simulation becomes essential for the reciprocal development of fuels and the ICE in the nowadays complex scenario of possible mobility solutions. If the road to GHG reduction is to be pursued, diversification of solutions to the mobility problem is the key, and for the full exploitation of all these technologies, virtual development is indispensable.

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