1 Introduction

Exactly 200 years ago, in 1807 Francois Isaac de Rivaz from Switzerland applied the patent for the world's first vehicle powered by a hydrogen internal combustion engine. The progress achieved since then is outlined strikingly by the BMW H2R, which established the speed record for hydrogen cars at 302.4 km/h in 2004, and by the BMW Hydrogen 7, the first hydrogen vehicle provided to the customer in a small series since December 2006. But still the potential of hydrogen powered combustion engines is not fully exploited: The use of innovative development tools offers unexpected opportunities for further optimisation, as will be demonstrated in the course of this thesis.

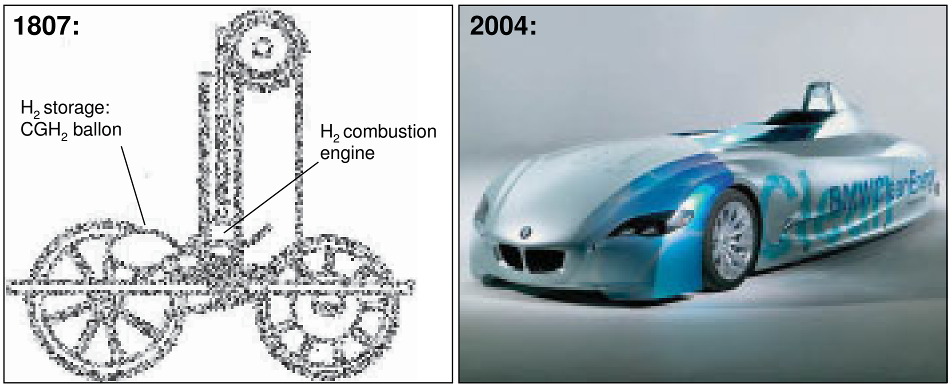


Figure 1.1: *De Rivaz' hydrogen vehicle (1807) and the BMW H2R (2004).*

1.1 Motivation

The motivation for the development of propulsion systems avoiding the emission of the greenhouse gas CO_2 is clear: The IPCC report "Climate Change 2007" [1], presented to the UN, clearly identifies the man-made emissions of CO_2 as the reason for the worldwide temperature rise and its well-known consequences. The depletion of the finite resources of fossil fuels certainly demands a transition to alternative energy sources. According to recent studies, the resources of oil will be exploited within the next two generations [2]. But due to the environmental impact it is doubtful whether it is affordable to fully exhaust the available reserves of fossil fuels. So the significant reduction of CO_2 emissions is the urgent reason to reduce the consumption of fossil fuels.

In search for alternative energy carriers, hydrogen is widely considered as fuel of the future for upcoming scenarios of a sustainable assured individual mobility. Generating hydrogen from regenerative energy sources, the discharge of climate-relevant CO_2 is prevented completely. While a broad consensus is already established on the fuel of the future, the question as to which form of energy conversion is most suitable for driving a car has not yet been answered. Today, the fuel cell (FC) and the internal combustion engine (ICE) running on hydrogen are both competing for this role in the future. Hydrogen internal combustion engines provide an opportunity to maintain or even outperform the performance level of current motor vehicle power trains.

Due to the physical properties of hydrogen, cryogenic liquid storage of the fuel provides the best basis to achieve currently customary cruising ranges. Consistent utilisation of the cold reservoir – on-board due to the liquid tank – opens new perspectives for the optimisation of internal combustion engines. By injecting cryogenic hydrogen into the intake port, the charge is cooled down and is thus densified. Especially in combination with an upstream densification by means of supercharging this process promises to provide highest level power density of spark-ignition engines and not only run such operating points stable, but also at optimum efficiency.

1.2 Applied methods

Future internal combustion engines will be developed using advanced methods. By using closely interlaced experimental measuring techniques and computational methods, a detailed investigation of the mixture formation as well as of the combustion process is possible. Based on ever increasing levels of computer performance, simulation tools gain more and more importance in the industrial development process. The numerical simulation of the in-cylinder flow and the combustion is an important component of the Computer Aided Engineering (CAE) of combustion engines. Similar to the experimental investigations there are different approaches at engine simulations depending on the issue: 1D thermo fluid dynamic simulations allow modelling of the gas dynamics of a complete engine system, while the simulation of the flow processes with 3D Computational Fluid Dynamic (CFD) tools allows the optimisation of the detailed geometry. CFD engine simulations are currently a field of research. For conventional fuels, successful industrial applications are reported, but many open questions remain, especially with regard to turbulence and combustion modelling. For the simulation of hydrogen engines, first attempts reported by previous authors are referred within this thesis. Providing reliable simulation tools ready for the optimisation of a cryogenic hydrogen ICE is the goal of this thesis.

While simulations of mechanical engine components are not affected by the chosen fuel, fluid dynamic simulations have to be adapted to the special properties of hydrogen. These advanced models have to be validated carefully to prove their ability to compute the in-cylinder flow during mixture formation and combustion. Since the cryogenic mixture formation is an innovative engine concept, the experimental measurement techniques consulted for the verification are also innovative. Laser - optical measurements are a popular example. Beyond the simulation of the in-cylinder flow, the simulation of frost formation inside the intake port, a phenomenon special to the cryogenic mixture formation, is coupled with the fluid dynamic simulation. Therefore, the development and also the validation of new computational methods is necessary.

The 1D thermo fluid dynamic simulations presented within this thesis are carried out using the commercial software GTPower and the in-house code of the Politecnico di Milano, Gasdyn. For the 3D CFD simulations, the commercial solver ANSYS CFX is applied using β-extensions for the simulation of hydrogen in-cylinder combustion. The frost formation model is embedded into 3D engine simulations with ANSYS CFX.

2 Fundamentals on Hydrogen Combustion Engines

Within this chapter, the general properties of hydrogen as a fuel for combustion engines and their influence on fluid dynamic simulations are presented. Different mixture formation strategies are introduced and the characteristics of the hydrogen research engines, consulted for validation of the simulation models, are listed.

2.1 Properties of hydrogen as an engine fuel

Hydrogen, being gaseous at environmental conditions, shows physical properties that differ in principle from the properties of the liquid fossil fuels which are primarily used in today's combustion engines. But not only the gaseous state and therefore the low density are characteristic for hydrogen: Also the properties relevant for the combustion differ significantly from conventional fuels, including gaseous fuels like methane. See Table 2.1 for a summary of the most relevant properties of chosen fuels. The consequences of the special properties of hydrogen with regard to the engine operation have been discussed extensively by previous authors, see for example [3, 4]. In the following the consequences with regard to the simulation of the engine processes are discussed.

Quantity	**Symbol**	**Unit**	**Diesel**	**Gasoline**	**Methane**	**Hydrogen**
lower heating value	H_l	[MJ/kg]	42.5	43.5	50.0	120
stoichiometric air req.	L_{st}	[kg_{air}/kg_{fuel}]	14.5	14.7	17.2	34.3
density at normal conditions [1]	ρ_{normal}	[g/l]	830	730 - 780	0.72	0.09
boiling temperature [2]	T_{boil}	[°C]	180 - 360	25 - 215	-162	-253
diffusivity	D	[m^2/s]	-	-	$1.9 \cdot 10^{-5}$	$8.5 \cdot 10^{-5}$
flammability limit		[λ]	0.5 - 1.3	0.4 - 1.4	0.7 - 2.1	0.2 - 10
laminar flame speed [3,4]	s_l	[m/s]	0.4 - 0.8	0.4 - 0.8	0.2 - 0.4	0.4 - 2.7
ignition energy [3,4,5]	E_{ign}	[mJ]	0.24	0.24	0.29	0.02
ignition temperature	T_{ign}	[°C]	~ 250	~ 350	645	585
carbon mass %	C	[% mass]	86	86	75	0

1) 1.013 bar, 0 °C 2) 1.013 bar 3) 1.013 bar, 20 °C 4) in air 5) $\lambda = 1.0$

Table 2.1: *Properties of hydrogen compared to fossil fuels (modified from [5]).*

Specialties when modelling hydrogen mixture formation: With regard to the simulation of the mixture formation process, the very low boiling temperature of hydrogen ensures that the hydrogen is always in the gaseous state, at least during regular engine operation[1]. The injection of liquid hydrogen is regarded to be technically not feasible [6]. For this reason, no phase transition of the fuel occurs – this holds also for cryogenic mixing.

The simulation of the injection of a gaseous fuel presents challenges that differ from those encountered when modelling liquid fuels: No spray modelling is necessary nor the simulation of evaporation or wall film formation, which are certainly crucial points of the simulation of conventional engines. On the other hand, gaseous fuels are preferably injected supersonically, depending on the injection pressure ratio. The simulation of supersonic flow requires an appropriate CFD solver scheme as well as adequate simulation settings.

Specialties when modelling hydrogen combustion: Due to the low molecular weight of hydrogen its molecular diffusivity is significantly higher than the diffusivity of any other fuel. The influence not only on the mixing but especially on the combustion has to be investigated: Wrinkling of the flame front is not only induced by turbulent eddies but, under lean conditions, also by the high molecular diffusivity of hydrogen, resulting in an increase of the effective flame speed [7]. This phenomenon should be taken into account by the combustion models.

The wide flammability limits of hydrogen offer the possibility to operate an engine mainly quality controlled, utilising the increased efficiency of lean operation. For this reason the laminar flame speed, required as input for the combustion models, has to be provided for variable mixture composition.

2.2 Mixture formation strategies for hydrogen engines

Eq. 2.1 and 2.2 show the computation of the volumetric mixture heating value H_M for port fuel injection and $\overline{H_M}$ for direct injection engines respectively:

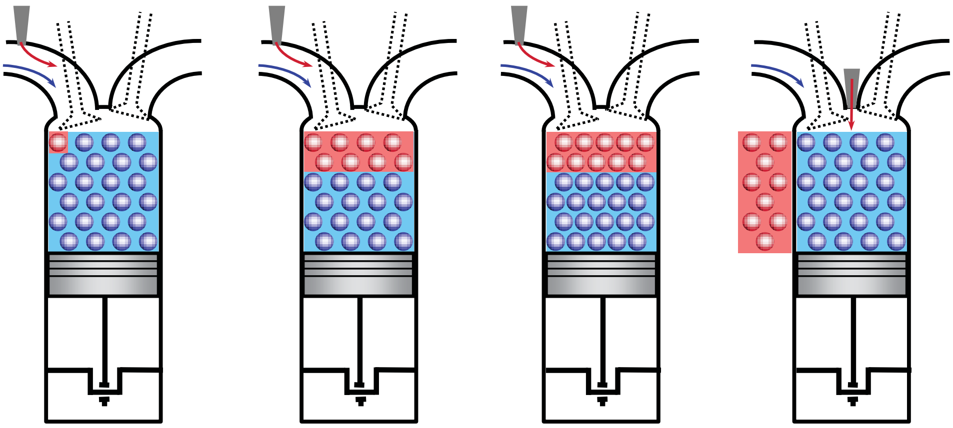
$$H_M = \frac{H_l \cdot \rho_{mixture}}{\lambda \cdot L_{st} + 1} \tag{2.1}$$

$$\overline{H_M} = \frac{H_l \cdot \rho_{air}}{\lambda \cdot L_{st}} \tag{2.2}$$

While for engines operated on liquid fuels H_M and $\overline{H_M}$ are nearly identical, H_M is significantly lower for engines operated on gaseous fuels due to the reduced density of the mixture. As a consequence, the theoretical power of a hydrogen engine with port fuel injection at ambient conditions is about 18 % lower than the power of a comparable gasoline engine. Besides conventional strategies to increase the mixture heating value like supercharging which apply for conventional engines as well as for hydrogen engines, the power deficiency of a hydrogen engine can be overcome by innovative mixture formation concepts: The cryogenic mixture formation and the hydrogen direct injection both exceed the power of a comparable gasoline engine theoretically. Figure 2.1 shows a

[1] At the injection of cryogenic hydrogen, liquid but boiling hydrogen might be available at the injector. But since the dosing of a boiling fluid is technically difficult due to density fluctuations, the injection of pure gaseous hydrogen is desirable.

Assumptions:
λ_a = const.
λ = 1
η_e = const.
p = 1 bar



Fuel	Gasoline	Hydrogen	Hydrogen	Hydrogen
MF strategy	PFI	PFI	PFI cryo	DI
T_M [K]	293	293	210	293
H_M [MJ/m^3]	3.9	3.2	4.5	4.6
P^* [%]	100	82	115	117

*) power related to gasoline

Figure 2.1: *Comparison of different mixture formation strategies (modified from [3]).*

comparison of the different mixture formation strategies. While the port fuel injection at ambient conditions is regarded to be state of the art, the cryogenic mixture formation as well as the direct injection of hydrogen are innovative technological concepts that are currently investigated within the EU project HyICE [8].

Hydrogen port fuel injection at ambient conditions: The external hydrogen mixture formation at ambient temperature offers the lowest theoretical potentials of the hydrogen mixture formation strategies presented. The injection of the hydrogen into the intake port displaces a significant amount of intake air, resulting in a power deficit. Due to the presence of hydrogen in the intake port, back firing might occur. Furthermore, pre-ignition and knocking are found to limit the performance of such engines [9]. If power deficiencies are accepted, this mixture formation strategy is certainly the simplest solution and therefore soonest technically feasible. For this reason this mixture formation concept has been applied for most vehicles powered by hydrogen combustion engines presented until now. Although this mixture formation concept is certainly not fully exploited yet, e.g. considering supercharged engines, it is not as promising as the other concepts presented in Figure 2.1. For this work external mixture formation at ambient conditions is only applied in optical validation experiments where no cryogenic hydrogen injection is feasible.

Port fuel injection of cold hydrogen: The focus of this work lies on the so called cryogenic mixture formation: If the hydrogen is stored in liquid form on board, the utilisation of the cold reservoir on board offers a promising mixture formation concept: The power deficiency of a hydrogen engine compared to a gasoline engine can be overcome by injecting the hydrogen at very low temperatures into the intake port. The cooling of the air results in a densification which nearly compensates the displacement of the intake air. Injection of liquid hydrogen, which would theoretically offer the highest potential[2], is regarded to be impractical. But if the temperature of the evaporated hydrogen is just above the boiling point, the power of a hydrogen engine with cryogenic mixture formation theoretically exceeds the power of a comparable gasoline engine by 15 %, which is close to the potential of a hydrogen DI engine. At the same time, the cooling of the mixture stabilises the combustion process: A clear reduction of back firing and pre-ignition could be demonstrated experimentally [9]. The reduction of knocking offers the possibility to run the engine at a higher compression ratio which in turn results in an increased efficiency.

The challenges of the cryogenic mixture formation are the stability of the injectors at very low hydrogen temperatures down to 30 K, and the very broad range of the volumetric injection rates[3]. Furthermore, at the start of the engine the hydrogen supply pipes have to cool down before cold hydrogen is available. During this period, the engine has to be operated on hydrogen at ambient temperatures. Temporary power deficits are currently regarded to be not acceptable to the customer. Several possible solutions like additional charging of the engine are in discussion, but a solution is not yet established. Finally, the formation of frost at the cold injector nozzle has been observed. Developing appropriate counter measures against the undesired frost formation is one of the main challenges of this thesis.

Hydrogen direct injection: If the hydrogen is injected directly into the cylinder after the valves are closed, no intake air is displaced by the gaseous fuel. Furthermore, no back firing can occur since no fuel is present in the intake port. Compared to port fuel injection, the injection timing offers an additional degree of freedom: The hydrogen may be injected at the beginning of the compression stroke, later during compression or even during the combustion by multiple injection pulses, depending on the injection pressure. Nearly homogeneous mixture distributions as well as stratification can be realised, each resulting in a different combustion process. So the combustion process can be controlled by an adequate injection strategy. Furthermore, pre-ignition can be suppressed if the hydrogen is injected shortly before ignition. From this point of view the hydrogen engine using direct injection, especially at high pressure, is a promising engine concept.

The realisation of this concept is demanding: For stratification, the hydrogen has to be

[2]Utilising the temperature difference between ambient air and cold hydrogen by a thermo dynamic process, the mixture temperature could be reduced further: The injection of cold hydrogen into ambient air is an irreversible process, i.e. the entropy of the resulting mixture is higher than the sum of the hydrogen's entropy and the air's entropy. Indeed the simple mixing of fluids at different temperatures maximises the entropy. As Carnot showed, the increase of the entropy is minimum (i.e. $dS = 0$) if temperature differences are leveled by a reversible process. The lower the resulting entropy of the mixture the lower its temperature. This means that the temperature of the hydrogen-air mixture could be reduced significantly compared to simple mixing if any thermo dynamic process, utilising the temperature difference between the warm air and the cold hydrogen, extracts mechanical power until both fluids have the same temperature. The mixture temperature drops depending on the amount of mechanical energy, extracted by the thermo dynamic process. A possible apparatus therefore was applied for patent [10] within this thesis.

[3]The injectors have to cover idle operation at hydrogen temperatures down to 30 K on the one hand and full load at ambient conditions, i.e. 300 K, on the other hand. The volume of hydrogen to be injected per cycle thus varies by two orders of magnitude.

injected within a short period. Due to the low density of hydrogen the volume of the fuel to inject is high, so the volumetric flow rate during injection has to be very high. This poses a challenge to the hydrogen injectors. Furthermore, a stable hydrogen rail pressure has to be ensured – up to 300 bar, required for supersonic injection during combustion. The on-board supply of high pressure hydrogen at affordable energy consumption is currently an open issue.

The realisation of a hydrogen engine with high pressure direct injection offers high potential and considerable technological risks at the same time, thus being a typical field for applied research. Several Ph.D. theses already cover different aspects of H_2 DI engines, see for example [4, 11], and intensive research on this field is carried out within the HyICE project. For this work, the direct injection of hydrogen is not investigated further.

2.3 Hydrogen research engines investigated

The ability of 3D CFD simulations to reproduce the injection of cryogenic hydrogen into air with good accuracy has been demonstrated earlier: Using different CFD solvers, Hallmannsegger computed the pulsed injection of cryogenic hydrogen into a continuous air flow and compared the results to optical PIV- and Schlieren-measurements [3]. Vogl, Zimmermann and Pfitzner verified the CFD predictions regarding jet shape and penetration depth for the supersonic injection of cryogenic hydrogen by comparison to high quality Schlieren-measurements [12]. So the CFD simulation of cryogenic injections is validated on a broad basis and is regarded to be reliable. The focus of this work is on the validation of engine simulations. Therefore, experimental results gained from optical and from thermodynamical hydrogen one-cylinder research engines are used as validation data. The geometry of both engines is quite similar, so the results gained at the optical engine should be portable to the thermodynamical engine. The main characteristics of the engines are listed in Table 2.2. For further details on the engines and the applied measurement techniques, the reader is directed to the literature [9, 13].

	thermodynamical engine	**optical engine**
engine type	single cylinder, 4-stroke SI	single cylinder, 4-stroke SI
valve train	4 valves, BI-VANOS	4 valves
displacement	499 cm^3	500 cm^3
bore	84 mm	86 mm
stroke	90 mm	86 mm
compression ratio	9.0 - 13.5	9.2
maximum speed	7000 rpm	3000 rpm
max. cylinder pressure	150 bar	60 bar

Table 2.2: *Characteristics of the hydrogen research engines modelled for validation.*