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Master of Science in Automotive Engineering

Master Thesis

STUDY OF WATER INJECTION STRATEGIES TO ENHANCE EVAPORATION IN SI-ENGINES THROUGH 3D-CFD SIMULATIONS



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Sommario

Le restrizioni sempre più severe in termini di emissioni di CO₂ da soddisfare entro il 2020 e le ulteriori riduzioni di tali emissioni previste per gli anni successivi hanno innescato un periodo di intenso sviluppo e trasformazione tecnologica del settore automobilistico. Nella presente dissertazione viene analizzato il concetto di iniezione d'acqua nei motori ad accensione comandata. Questo metodo sarebbe in grado di migliorare l'efficienza del motore in modo da ridurre la produzione di gas a effetto serra. L'iniezione d'acqua è già stata adottata in passato principalmente su velivoli e auto da corsa per aumentarne la potenza, ma ora viene rivisitata per essere applicata alla produzione di veicoli su larga scala. Il primo passo di questo lavoro riguarda l'acquisizione di una solida conoscenza delle caratteristiche dell'acqua, evidenziandone le principali differenze rispetto alla benzina. Questa analisi è stata necessaria per comprendere e prevedere il comportamento dell'acqua, durante gli eventi di iniezione e i fenomeni post-iniezione (atomizzazione, evaporazione, miscelazione), a partire da quello della benzina. Successivamente, grazie allo strumento 3D-CFD QuickSim sviluppato da Dr.-Ing. Marco Chiodi durante il suo dottorato di ricerca presso il Forschungsinstitut für Kraftfahrwesen und Fahrzeugmotoren Stuttgart (FKFS) / Institut für Verbrennungsmotoren und Kraftfahrwesen (IVK) dell'Università di Stoccarda, è stata effettuata un'analisi numerica sui parametri più rilevanti che influiscono sull'evaporazione dell'acqua. La ragione del grande interesse per l'evaporazione dell'acqua dipende dalla sua capacità di ridurre fortemente la temperatura della miscela (acqua-aria/acqua-aria-carburante) grazie al suo maggiore calore latente di vaporizzazione rispetto alla benzina. Questa caratteristica verrà in seguito spiegata come uno dei principali vantaggi della strategia di iniezione dell'acqua. Un'altra considerazione importante quando si ha a che fare con questo liquido è che l'acqua viene iniettata in una corrente d'aria la cui composizione comprende anche una minore quantità di vapore acqueo. Se l'umidità relativa ha effetti trascurabili sull'iniezione di benzina, per l'iniezione d'acqua risulta essere un fattore limitante. Pertanto, uno studio analitico di tale comportamento ha reso possibile non solo di capire quanto l'umidità relativa iniziale dell'aria esterna influisca sulla quantità massima di acqua iniettabile, ma anche di implementare questa conoscenza nel software 3D-CFD, in modo da ottenere una valutazione più affidabile e realistica del fenomeno. L'obbiettivo finale del lavoro ha riguardato la possibilità di implementare in QuickSim un modello per valutare il contatto dell'acqua con le pareti. Ancora una volta, a causa della differenza tra le proprietà dell'acqua e della benzina, è necessario eseguire un'analisi più dettagliata su tale aspetto. Con l'aiuto del software commerciale 3D-CFD STAR-CD è stato possibile effettuare una prima valutazione del fenomeno. Successivamente, i sotto-modelli caratterizzanti il comportamento dell'acqua a contatto con le pareti sono stati analizzati per essere implementati in QuickSim in modo da ottenere tutti gli strumenti necessari a descrivere ed esaminare correttamente la strategia di iniezione dell'acqua.

Abstract

The increasingly severe restrictions in terms of CO₂ emissions to be fulfilled within 2020 and the further reductions of such emissions set for the following years are causing the Automotive field to face a period of intensive technological development and transformation. In the present dissertation the focus is on the water injection concept in SI-engines (spark ignition engines). This method would be able to improve the engine efficiency in order to reduce the production of Greenhouse gases. Water injection has already been adopted in the past mainly on aircrafts and race cars for power improvement purposes, but now it is revisited to be applied on largescale vehicle production. As a first step of this work, a solid knowledge of water characteristics has been obtained, highlighting the main differences compared to gasoline. The analysis was required to understand and predict the water behaviour, during both injection events and postinjection phenomena (atomization, evaporation, mixing), starting from the gasoline one. After that, using the 3D-CFD tool QuickSim developed by Dr.-Ing. Marco Chiodi during his PhD at Forschungsinstitut für Kraftfahrwesen und Fahrzeugmotoren Stuttgart (FKFS)/ Institut für Verbrennungsmotoren und Kraftfahrwesen (IVK) of University of Stuttgart, the numerical investigation of the most relevant parameters affecting water evaporation has been performed. The reason behind the great interest in water evaporation depends on its ability to highly reduce the mixture temperature (water-air/water-air-fuel) through to the greater HOV (heat of vaporisation) compared to gasoline. Such characteristic will be later explained as one of the major advantages of water injection strategy. Another important consideration when dealing with this liquid is that water is injected into an airstream which composition consists also of a smaller quantity of water vapour. Even though a relative humidity does not significantly affect injection events involving gasoline, for water injection it represents a limiting factor. Therefore, an analytical study of this behaviour has made possible not only to understand how much the initial relative humidity of the external air affects the maximum amount of water to be injected, but also to implement this knowledge in the 3D-CFD tool, so that to obtain a more reliable and realistic evaluation of the concept. The final task involved the possibility to implement in QuickSim a model to evaluate water wall impingement. Again, because of the difference between water and gasoline properties, a more detailed analysis must be performed on this last aspect. With the 3D-CFD commercial software STAR-CD a first evaluation of the phenomenon has been possible. Subsequently, the wall impingement sub-models were analyzed to be

implemented in QuickSim in order to obtain all the tools necessary to correctly describe and examine the water injection strategy.

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1. Introduction

1.1. Modern Automotive Trend

Nowadays most OEMs have already added to their vehicle fleet at least one Hybrid or fully Electric model. This common strategy comes from the favourable current legislative treatment to which all these vehicles are subjected (1). In fact, for the standard, just the so called "Tank-to-Wheel" (TTW) emissions, very low for hybrid electric vehicles (HEVs) and equal to zero for battery electric vehicles (BEVs), are considered, while no restrictions are applied to the amount of CO₂ produced in all the processes meant as "Well-to-Tank" (WTT), where internal combustion engines vehicles (ICEs) and HEVs are comparable and BEVs emissions are no more negligible. A picture of the passages contained in WTT and TTW is given by Figure 1 (2):



Figure 1: "Well-to-Wheels" processes definition.

Governments and car makers continue to propose new commitments for electric vehicle sales, while manufacturing cost continues to fall, making HEVs and BEVs more competitive with internal combustion engine vehicles. Additionally, new lithium-ion battery technologies and fast charging structures are making the range problem, main constraint of these vehicles, more acceptable for customers that are following this trend (3). Despite all such considerations would seem to enhance a fast conversion towards these new technologies, this conception is slowed down by several factors such as the limited presence of fast charging stations (4), the need of new safety policies and the introduction of additional production lines in the already solid and

efficient structure dedicated to large-scale ICEs realisation. In the short-term period, even though an increasingly higher number of electric vehicles could be noticed, ICEs will remain the main transport method, also considering their combination together with electric machines in hybrid solutions. The major effort is given to develop innovations for spark ignition (SI) engines since they have less problems to manage noxious emissions relative to compression ignition (CI) engines, thanks to the use of the Three-Way Catalyst (TWC). For the same reason today, in almost all hybrid powertrains a SI-engine can be found.

SI-engines pollutant emission targets have been already reached with the TWC technology, so now the main focus is on CO_2 emissions and since they are chemically related to the amount of fuel burnt to provide vehicle motion, there are two main solutions to limit this problem:

- Adopting fuels with low carbon content;
- Improving the engine fuel conversion efficiency η_f .

Due to this, the automotive research field is currently split in two big sections: on one side new blends of fuels with same potentialities of the conventional ones, but with both a lower carbon concentration and cost, are investigated; on the other one a frequent implementation of new technologies in ICEs to improve their efficiency is preferred (5).

An overview of some important strategies already implemented on SI-engines is shown in the next section.

1.2. SI Engines Development

1.2.1. Downsizing and Turbocharging

Most of the time, engines work in their low-efficiency region as is shown in Figure 2.



Figure 2: Break Specific Fuel Consumption Map of two low-segment vehicles over the WLTP driving cycle.

Here two low-segment vehicles have been tested over the new European type approval driving cycle: Worldwide Harmonised Light Vehicle Test Procedure (WLTP). What stands out from the graph is that a great concentration of engine working points lies in the region of both low engine speed (n) and load (bmep) that is in turn characterized by low values of engine fuel conversion efficiency. To reduce in part this problem engine downsizing and turbocharging solutions are exploited.

$$P = bmep \cdot iV \cdot \frac{n}{m} \tag{1}$$

Considering equation [1], with a smaller displacement volume (V) and both the same power (P) guaranteed by the turbo-compressor system and the same engine speed obtained maintaining the gearbox unchanged, a load increase is perceived, leading to engine points movement toward higher efficiency regions.

1.2.2. Variable Valve Actuation (VVA)

This technology allows to completely control either the intake valve or both intake and exhaust valves, for instance to perform cylinder deactivation. Different solutions have been developed but goals to be achieved are the same. The first target is to adapt valve timing, and in particular the intake valve closure (IVC) delay, to different engine speed conditions, so that to prevent *backflow* at low engine speeds and exploiting flow *inertia* at high speeds. Thanks to that the engine volumetric efficiency, eq. [2], is maximized and η_f increases as well.

$$\lambda_{\nu} = \frac{m_a}{\rho_a V}$$
[2]

Term m_a is the air mass introduced in the cylinder per cycle while ρ_a is the ambient air density. Varying the IVC is also exploited to throttle the airflow directly at the intake port instead of using the throttle valve leading to a pumping work reduction. Finally, since this solution is mainly adopted with gasoline direct injection engines, that require a great amount of turbulences to guarantee the homogeneity and fast mixing of the charge, a valve lift variation can allow to reach this goal.

1.2.3. Gasoline Direct Injection (GDI)

Main advantages of this application relative to port fuel injection (PFI) are:

- Improved warmup and transient conditions due to the absence of wall wetting phenomena, main cause of fuel enrichment in these conditions;
- Higher compression ratios (ε) may be employed due to the charge cooling effect obtained by injecting fuel in the induction stroke;

- For the same reason λ_v increases leading to higher fuel conversion efficiency.

1.2.4. Full-load Limitations and Solutions

Implementing all these technologies together can even enable further advantages such as *Scaveging Effect* (6) and *Miller Cycle* (7). However, due to several constraints typical of SI-engines (see Figure 3), downsizing and turbocharging rates are limited.



Figure 3: Full-load Limitations for SI-engines: the red line in the T-n graph represents the full-load curve.

These limits are:

- 1. Turbo-compressor surge line;
- 2. Engine knock;
- 3. Torque max;
- 4. Components structural resistance, especially for the turbine, fix a limit on the maximum exhaust temperature (T_{exh} , or T_3 in the graph above);
- 5. Mass choking in the turbocharger, and gearbox structural reliability.

To guarantee the engine structural integrity by containing the effects caused by (2) and (4), the following solutions are adopted:

- a) Limiting $\varepsilon = 10 12$ to reduce pressures and temperatures at the end of compression to avoid charge autoignition;
- b) Spark timing retarding to move the centre of gravity of combustion (MFB50%) toward the expansion stroke so that to reduce the pressure peak experienced in combustion chamber;
- c) Mixture enrichment to decrease T_{exh} , furtherly increased because of (b).

1.2.5. Problems

Downsizing and turbocharging, VVA and GDI have been implemented to improve SI-engine efficiency and reduce both fuel consumption and CO₂ emissions. However, to protect the engine structure, the opposite behaviour is obtained. In fact, from the definition of ideal efficiency (equation [3]), limiting ε means reducing the maximum efficiency value reachable by the engine:

$$\eta_{SI,id} = 1 - \frac{1}{\varepsilon^k - 1} \tag{3}$$

Shifting the MFB50%, so decreasing the pressure peak, does not allow to reach the maximum power available, therefore the fuel conversion efficiency worsens (equation [4]):

$$\eta_f = \frac{P}{\dot{m}_f L H V} \tag{4}$$

Where *LHV* is the lower heating value while \dot{m}_f is the fuel flow rate.

Finally, TWC properly works just in a relative air fuel ratio range between $0.9 < \lambda < 1.1$. Therefore, once $\lambda < 0.9$ because of fuel enrichment, pollutant emissions increase. All such problems are summarized in Figure 4:



Figure 4: Consequences of downsizing and turbocharging, VVA and GDI implementation in SI-engines.

Among the solutions proposed to solve these negative effects, well treated in (8), (9), (10), (11), (12), (13), (14), another strategy is currently under deep investigation due to its great amount of potentialities which could completely overcome all such problems. It consists in performing an engine Water Injection. Its characteristics will be treated in the next chapter.

2. Water Injection Features

2.1. Motivation

The first application of water injection dates back to the first half of the 20th century when it was used to temporary increase aircraft engines power. In 1945 the National Advisory Committee for Aeronautics (NACA) has investigated its utilisation from an efficiency perspective. Again, water injection implementation as power enhancer has been employed in Formula 1 during '80s and was proposed as an option on the SAAB 99 first turbo serial application (15). BMW has currently produced a limited serial application of the M4 GTS model fitted with an indirect water injection system that allows this vehicle to reduce fuel consumption up to 13% and to gain almost 5% of power more respect to the base model (16), (17). However, due to both high costs and application efforts a serial introduction of this technology is, up to now, still not possible.

The main reasons why this solution is being largely analysed these days, are shown in either Table 1 and Figure 5:

$T_{ref} = 300 K$	Water	Gasoline	W/G
HOV [kJ/kg]	2431	346	7
c _p [kJ/kgK]	4196	2144	≈2

Table 1: Water & Gasoline Properties Comparison, Heat of Vaporisation and Specific Heat.



Figure 5: Water & Gasoline Properties Comparison, Heat of Vaporisation (rvap) on the left and Specific Heaton the right.

Depending on the type of injection performed, indirect (IWI) or direct (DWI), water can be either injected directly in the airstream or in a mixture of gasoline and air respectively. Comparing gasoline and water evaporation processes, the 7 times higher HOV of water causes a much greater mixture temperature (T_{mix}) reduction than gasoline. It has been proved by (1) that also the higher c_p value of water has a minor but positive effect on the T_{mix} reduction. Having a lower mixture temperature at the end of the compression stroke means that lower temperatures will be then experienced during combustion and at the exhaust. Therefore, a dual advantage is obtained:

- Knock tendency decreases (lower flame temperature);
- Less restrictions due to the turbine structural strength (lower T_{exh}).

Since knock and high T_{exh} are the two main constraints of spark ignition engines, relaxing such limits would open the way for many different possibilities to improve power or fuel consumption as well as engine emissions.

A deep analysis of all the advantages coming from a T_{mix} reduction is largely available in literature (1), (18), (19), (20), (21), however, a list of the main ones is shown to better understand why this strategy could be essential to achieve future emissions targets.

In terms of performance, the temperature reduction leads to an increase of λ_v that causes in turn the *bmep* to rise. This is the solution adopted by BMW on its M4 GTS model.

On the other hand, several actions can be done to improve η_f reducing in turn fuel consumption (bsfc) and CO₂ emissions, that is the major goal of this analysis:

- Due to better knock resistance the compression ratio can be increased. In this way the same temperature conditions can be obtained at the end of compression but with a higher efficiency (see equations [3], [5]):

$$T_2 = T_1 \cdot \varepsilon^{\gamma - 1} \tag{5}$$

Where T_1 and T_2 are the temperatures at the beginning and at the end of compression respectively, γ is the specific heat ratio;

- Instead of modifying ε , the same result can be obtained by advancing the spark timing, so the MFB50% can shift as close as possible to the top dead centre (TDC) optimizing the combustion work;
- Since the closer the centre of combustion is to the TDC the lower will be the T_{exh}, the previous point causes this temperature to decrease enabling the use of a stoichiometric mixture (λ ≈ 1) also in full load conditions;
- When the engine runs in stoichiometric conditions the TWC can effectively work in its high efficiency window, meaning that no more problems of pollutant emissions at high loads have to be managed.

Figure 6 schematically highlights such advantages:



Figure 6: Consequences of Water Injection on Engine Management.

2.2. Water vs Gasoline

Despite benefits shown in Figure 6 could partly or completely solve the major SI-engines weak points, this is only possible if water vaporises. It is well known that gasoline is a highly volatile compound and is characterized by a good atomization behaviour. Additionally, a wide knowhow of its injection characteristics can be easily found in literature. Unfortunately, water properties are quite different from the gasoline ones, meaning that the same considerations deeply experimented for the latter cannot be applied on the former. Furthermore, since water implementation in passenger cars is being considered just since few years, a very poor background showing its behaviours is available.

A comparison between these two fluids has been made to predict water injection phenomena. The main properties describing spray break-up and evaporation are shown in Table 2 at the same temperature, and in Figure 7 for a wider temperature range:

$T_{ref} = 300 K$	Water	Gasoline	W/G
psat [Pa]	3543	53951	≈1/15
σ [N/m]	0.072	0.025	≈3
ρ [kg/m ³]	1000	745	1.3
μ [Pa s]	0.00087	0.00045	≈2

Table 2: Water & Gasoline Properties Comparison, Saturation Pressure, Surface Tension, Density, Dynamic Viscosity.



Figure 7: Water & Gasoline Properties Comparison, Saturation Pressure, Surface Tension, Density, Dynamic Viscosity.

2.2.1. Volatility

Due to its 15 times lower saturation pressure, water evaporation tendency is much worse than gasoline one. From Figure 8 it can be easily seen why this happens:



Figure 8: p-v Diagram.

However, Figure 7 shows that this trend is maintained up to a temperature of about T=370 K, after that gasoline and water volatility behaviours switch. Considerations about this change will be treated in section **Errore. L'origine riferimento non è stata trovata.**

2.2.2. Atomization

Atomization represents the first phase of an injection event. It will build the correct environment to let the liquid injected vaporise. Of course, the finer are the droplets produced, the higher will be the evaporation tendency. This phenomenon is affected by the following parameters:

$$Re = \frac{\rho v d}{\mu} \tag{6}$$

$$We = \frac{\rho v^2 d}{\sigma}$$
[7]

$$Oh = \frac{\sqrt{We}}{Re} = \frac{\mu}{\sqrt{d\rho\sigma}}$$
[8]

Where in each equation *d* represents the injector hole diameter and *v* the liquid velocity. The Reynolds number (equation [6]) is proportional to the inertial and viscous forces depending on *v* and μ respectively. It gives a measure of both the quality and the intensity of the liquid jet turbulence, so at high Re values the spray break-up is improved by a more turbulent jet. The Weber number (equation [7]) correlates inertial forces and surface tension forces, that depend on σ . Finally, the Ohnesorge number (equation [8]) links all such forces together. Considering the same pressure conditions across the nozzle (Δp), by including properties values of Table 2 in equations [6], [7], [8], and considering that from the *Bernoulli* relation $\nu \propto \sqrt{\Delta p/\rho}$, water shows relative to gasoline:

- Higher resistance against break-up forces due to the almost 3 times higher surface tension;
- Approximately 15% lower speed across the nozzle due to the 1.3 times higher density;
- Around 67% lower Re, meaning that the jet kinetic energy of the former has a lower intensity than the latter one. For T>370 K the situation is reversed (see μ-T graph in Figure 7).

Since water not only shows a worse volatility, (at least for T<370 K), but also a lower breakup tendency compared to gasoline, a largely different amount of vaporised mass between the two is expected if they are injected starting from the same initial conditions. Atomization characteristics of the two compounds are highlighted in Figure 9:



Figure 9: Primary fragmentation modes of a liquid jet in pressurized atomization with $p_{inj}=200$ bar for both Water (cyan) and Gasoline (orange). References values have been taken from (1).

What can be predicted considering Figure 9 is that water droplets will be bigger than gasoline ones, so comparing their Sauter Mean Diameters (*SMD*), $SMD_{water} > SMD_{gsoline}$. Therefore, since the liquid mass is proportional to $m \propto SMD^3$, then the water mass will be much greater than the gasoline one. Higher liquid mass not only penalizes furtherly vaporisation and mixing phenomena but causes water to easily remain stuck on surfaces. The liquid film that forms could cause more severe problems of oil dilution and the formation of a thick water layer next to the walls that can compromise the combustion process. Analysis on this behaviour will be treated in chapter 5.

2.2.3. Additional Drawbacks

In this section further drawbacks related to water injection implementation are considered. Water has very poor mixing capability that makes difficult to obtain homogeneous mixture and could cause an increase of pollutant emissions. In literature some applications involving DWI of water-gasoline emulsions have been analysed (15), (22). Considering the combustion process, high instabilities occur as the water-to-fuel ratio increases (WFR). Additionally, an extreme temperature reduction due to water evaporation could excessively slow down the flame speed with a consequent increase of the combustion duration.

In the end, other problems, not correlated to the thermodynamics but still important, are: water consumption due to wall impingement; corrosion and freezing problems due to having water flowing in systems of ducts; need to refill an additional tank; increase of the packaging complexity due to all the additional components needed; high increase of the overall vehicle price.

2.3. Injector Configurations

2.3.1. Indirect Water Injection (IWI)

Since water is here injected in the intake manifold, low injection pressures are exploited (between 5-10 bar). For this reason the overall injection system is less expensive than the DWI one. On the other hand, low injection pressures mean both low injection velocity and Re and it has been already shown in section 2.2.2 that the lower these parameters are, the worse will be the atomization of the spray, so a worse evaporation tendency of water should be expected. Two different configurations of the injector are illustrated for IWI:

a. Plenum Injection:



Figure 10: Plenum Injection Layout.

Water injection takes place in the air intake pipe, across the throttle valve, or within the intake manifold (in this case one injector per cylinder is required). The water injector is located downstream of the intercooler Figure 10, so that water droplets should have long time to vaporise.

b. Port Injection:



Figure 11: Port Injection Layout.

In this case, water injection takes place upstream of each cylinder's inlet channels. There is one water injector per cylinder differently from the previous layout, so a more homogeneous mixture will form.

In some solutions also a combination of plenum and port injection can be adopted.

2.3.2. Direct Water injection (DWI)

In this case the following configurations can be adopted:

c. Direct Injection of Water-Fuel Emulsion:



Figure 12: Direct Injection of Water-Fuel Emulsion.

The water-fuel emulsion is prepared just before reaching the injector in a proper mixing chamber. Since water and fuel are not soluble in each other (15), additional devices are required to correctly mix them. The main problem of this solution is that water and fuel are sent to a common rail before being injected, so feeding the rail for each working condition with the proper WFR is hard. Furthermore, in the period between two following injection events, the water in the rail could start to separate more and more from the fuel leading to a not homogeneous mixture among different cylinders. In the worst case the complete separation of water and fuel can be experienced. To manage this issue an accurate design procedure of the overall injection system is required with a high increase of the cost.

d. Direct Water Injection:



Figure 13: Direct Water Injection with Separated Injectors for Water and Gasoline.

Finally, there is the direct injection configuration in which two separated injectors are used for water and fuel respectively. A problem of this solution is that within the cylinder roof, the water injector tip must be cooled to avoid damage. In fact, with separate injector, the water one would be cooled just at high loads when water is essential. For this reason a minimum amount of water must be injected during each cycle, even when it would not be thermodynamically needed for the engine. This will reduce the water tank fill and in the extreme case, when the water tank is empty, a power reduction of the engine is required to avoid thermal overload of the injectors. Also in this case costs and packaging problems highly increase.

In Table 3 a comparison of all these solutions is shown:

		Indirect Injection	Direct I	njection	
INJECTOR POSITION		INTAKE MANIFOLD	INTAKE PORT	CYLINDI	ER HEAD
FEATURES	PIPE	(1 inj. X cyl)		Emulsion	Double-Injector
Cooling of m_{mix}	+	++	+++	+++++	+++++
Equal in- cylinder Distribution	++	++	++++	+++++	+++++

Homogenization	+	+	++	+++++	++++
Water Consumption	+	+	++	++++	++++
Knock Mitigation	+	+	+++	+++++	+++++
Break-up	++	++	+++	++++	++++
Packaging	+++++	+++	+++	++	+
Pump (p _{inj})	+++	+++	+++	+	+
Calibration	++++	+++	++	++	+
Complexity	+++++	+++	+++	++	+
Cost	+++++	+++	+++	+	+
Transients	+++++	+++++	+++++	+	+++++
Tot	34	29	36	37	37

Table 3: Comparison of IWI and DWI Layout Solutions.

2.4. Water Sources Overview

After the analysis of main pros and cons of this strategy and the representation of the different layout possible for its implementation, now the last topic to treat concern all types of sources from which water could be taken.

The first source considered is a proper tank of distilled water. Since and additional tank is required, with the correspondent system of pipes and pumps, this solution negatively affect the overall cost of the vehicle. Special solutions must be adopted to avoid freezing and corrosion problems. Major issues are the higher cost of distilled water compared to tap one, and the need to refill the tank just with the former to avoid damages of the overall system. An alternative could be to use tap water in place of the distilled one so that to reduce the refilling cost. However in this case special filters should be employed to clean different types of this water from every impurity that could compromise the system. A completely different approach could be storing the water obtained from the condensation of the water vapour fraction contained in the air passing through the air conditioning system of the vehicle. The resulting liquid would have better quality compared to tap water but unfortunately it would be available just in special

temperature conditions in which the air passing through the A/C module reaches its dew point. Also the collection and storage of rain could be taken into account. However, several sensors and an additional water aftertreatment system should be used to control the contamination level of this water. Finally considering that one of the main combustion products is H_2O , a further solution could be to condense water directly from the exhaust stream. For this application both the amount of water available in different working conditions and its quality have still to be understood. More details about this last solution are shown in (23).

A schematic representation of these alternatives with the corresponding issues connected, is shown in Figure 14:



Figure 14: Water Supply Systems and main Problems affecting them.

3. Water Evaporation Analysis Through 3D-CFD Simulations

3.1. Numerical Analysis Introduction

In section 2.1 the great amount of water injection potentialities to mitigate knock and manage high exhaust temperatures that could damage the turbo-group, has been treated. From section 2.2 it has been understood that, only if water vaporises all these advantages can be actually exploited. However, due to the worse atomization and volatility properties of water respect to gasoline, the evaporation tendency of the first is very low.

The main goal of this chapter is to deeply analyse water thermodynamic behaviours to find out the best injection conditions to maximize the amount of water vaporised. To do that, numerical analyses with the 3D-CFD tool QuickSim have been performed with different boundary conditions of both the injection event and the tube.

3.2. Tool Features

Computational fluid dynamics is a part of fluid mechanics that allows to numerically analyse fluids behaviour and their interaction with other fluids (liquids or gases) and/or surfaces, starting from user defined boundary conditions. The model to be studied is divided in discrete cells (mesh) to which all thermodynamic equations, needed to completely describe the considered fluid, are applied. Once the simulation has converged a post-processing evaluation of the results can be performed thanks to coloured plots, droplets representation and other features that allow to easily compare different outcomes. However, one of the main limits of this approach is the huge computational time required to calculate numerical 3D flow field solutions, in addition to the one needed to set-up the simulation (pre-processing) and to analyse the results.

QuickSim has been developed and continuously updated with the purpose to reduce as much as possible the CPU-time, to guarantee outcomes reliability and allow for a clear results representation. 3D-CFD simulations are more commonly used for research purposes or isolated (pre-) development tasks, so a huge number of variables should be constantly changed to obtain a detailed picture of the fluid behaviour in different conditions. With conventional software every simulation would last from at least days, up to months, meaning that only a limited amount of variables can be effectively analysed. Thanks to both specific ICE models

implemented and the always manually defined meshes for each model considered, characterized by a proper cell discretization length slightly bigger than commercial software, QuickSim allows to drastically reduce the simulation time. This feature can be seen in Figure 15 and Figure 16:



Figure 15: CPU-time of one engine operating cycle in dependence of the cell discretization (24).

CPU time [s]				8 h					
					2	0 min		1 day]
10-3	10-2	10-1	1	101	102	10 ³	10 ⁴	10 ⁵ ↓	106
Mode contr (real	l-based ol unit time)	l	Real working process analysis and 1D-CFD simulation				3D simu (1 cy	-CFD 1lation vlinder)	
				ĺ	3D-CF Quick	D simu Sim (f	ilation ull eng	with ine)	

Figure 16: CPU time comparison of different calculation/simulation tools with QuickSim classification (24).

QuickSim allows not only to perform faster simulations compared to other commercial software, but these simulations can also involve the whole engine, meaning that all components (intake manifold, plenum, exhaust manifold ...) affecting the fluid behaviour are taken into account to produce more accurate results. Since even with the full engine analysis the CPU-time remains very low, a wide number of parameters can be varied and studied during the development process of new engine strategies, such as for instance the water injection discussed in the present dissertation.

To greatly reduce computational time maintain high levels of simulations reliability, QuickSim exploits some assumptions and setting characteristics. Solving thermodynamic equations for each single droplet injected during an injection event would require high computational time. To accelerate the analysis groups of droplets are considered instead. These groups are called

Parcels. The $\frac{droplets}{parcel}$ ratio represents one of the main QuickSim settings to obtain fast results

(see Figure 17).

Droplets/parcel	Number of parcels	CPU-time	Run time
50	541,085	30 min 19 s	33 min 02 s
100	270,535	19 min 48 s	22 min 05 s
500	53,763	9 min 44 s	11 min 37 s
1000	26,929	8 min 40 s	10 min 35 s
2000	13,225	7 min 59 s	9 min 48 s
4000	6,515	7 min 44 s	9 min 37 s
6000	4,257	7 min 36 s	9 min 28 s

CPU-time comparison for different droplet per parcel definitions (1.0 ms a. SOI; m_B =32.95 mg; processor: Intel® Xeon® E3-1245 v3 @ 3.4 GHz)

Figure 17: Simulation time variation with droplets/parcel.

Another tool characteristic concerns the boundary conditions definition for the fluid to be injected. These initial properties are set in a conical region within two planes perpendicular to the injector axis at distances L_{min} and L_{max} from the injector tip, as shown in Figure 18. With this simplification the secondary break-up phenomenon is taken into account while the primary one and all what happens inside the injector are neglected. The jet then develops along the injection duration following the main thermodynamic relations starting from the conditions fixed in that region at the instant considered.



Figure 18: Jet Boundary Conditions definition region.

Among the initial parameters to be set in this boundary region, also the *SMD* value can be decided. To initialize the droplets population at each injection instant QuickSim computes a Rosin-Rammler distribution $(f(x) \propto SMD)$ that depends on the *SMD* value chosen at the considered instant of time. Two options are considered:

- *SMD* = *const* for the whole injection duration. It means that the same statistical distribution is adopted for the whole injection

- $SMD \neq const$. Here in each injection instant a new statistical distribution is created. Figure 19 shows this difference:



Figure 19: Different inputs for SMD.

3.3. Model Description

To study the water evaporation phenomenon an IWI analysis has been performed. The experimental system, specifically realized for this purpose, is shown in Figure 20:



Figure 20: Experimental System Realized to Perform an Indirect Water Injection Event.

It consists of a water optimized injector (a), specifically tested with water to take into account its different properties (density, viscosity ...) respect to gasoline. In that way real flow rate and injected quantity have been computed. Water is injected within a tube (b) representing a scaled intake manifold. This tube is made of a transparent material so that the whole injection event can be monitored and recorded by a high-resolution camera (d). Photos were taken to compare experimental results with the ones coming from the simulation in order to calibrate the model used for the numerical analysis. Finally a pump (c), put directly at the end of the tube, is needed to attract air in it so that to build the same flow conditions experienced in the real intake manifold at different loads.

To reproduce the system adopted in laboratory the model illustrated in Figure 21 has been created in QuickSim:



Figure 21: Model used for IWI analyses with QuickSim.

The big volume just before the tube is needed to simulate the real air behaviour at the inlet and to avoid undesired pressure waves in the tube that could compromise the results reliability.

3.4. Calibration

The set of simulations described in this section were required to calibrate the model in order to efficiently analyse the main thermodynamic parameters affecting water injection. The goal is to understand to what extent different calibration parameters affect the amount of water vaporised so that to simplify the following analyses, saving additional time.

3.4.1. Droplets/Parcel Sensibility

In Figure 17 a d/p sensibility for gasoline direct injection has already been done. This ratio is now adapted to the lower injection pressure, so the higher *SMD*, of the indirect injection. Simulation inputs are shown in Table 4:

Tube inputs					Injectio	n inputs		
T _{int}	<i>p</i> _{int}	T _{wall}	m _w	t _{inj}	<i>T_{H20}</i>	<i>p</i> _{inj}	SMD	N _d
305	1.5	330	26	5	333	7	79	101236
[K]	[bar]	[K]	[mg]	[ms]	[K]	[bar]	[µm]	[#]

Table 4: d/p Sensibility inputs.

 N_d was obtained from the knowledge of the total amount of water injected m_w , its density and the *SMD*. The d/p sensibility has been performed considering the values reported in Table 5:

<i>d/p</i> [-]	1	15	25	27
N _p [#]	101236	6749	4049	3749

Table 5: d/p variation.

The d/p variation has been chosen in order to remain within a range of N_p values close to the GDI one (Figure 17). The output of the analysis can be seen in Figure 22:



Figure 22: Evaporated Water Mass trend for different d/p.

The error obtained considering d/p = 27 respect to d/p = 1 is negligible, so the former value is preferred to reduce computational time without affecting the final result.

3.4.2. Injector Ballistic Effect

Due to their mechanical and hydrodynamic characteristics, injectors show delays either in the nozzle opening or closing. In these transients the injector is said to work in its ballistic region, where the correlation between energizing time (tcmd [μs]) and injected fuel amount (Q [mg/shot]), becomes highly non-linear (red circle in Figure 23).



Figure 23: Injector Ballistic Effect.

Jet characteristics (spray cone angle, spray velocity, *SMD*...) are highly affected by this nonlinearity and their values are far from the ones obtained for the full developed jet. This effect can be taken into account with QuickSim by defining a variable trend for either *SMD* or droplet velocity initialization instead of considering the same value for the whole injection. Here the *SMD* has been modified.

Tube Inputs			Injection Inputs			
T _{int}	p _{int}	T _{wall}	m_w	t _{inj}	<i>T_{H20}</i>	p _{inj}
305	1.5	330	26	4	453	10
[K]	[bar]	[K]	[mg]	[ms]	[K]	[bar]

To simulate this effect the input parameters listed in Table 6 were used:

Table 6: Injector Ballistic Effect Inputs.

Taking into account Figure 19 two input values for the SMD have been set:

- $SMD = 62\mu m$
- SMD = ramp

For the second simulation the trend shown in Figure 24 was used. Such trend is an approximation of the actual *SMD* variation measured along the whole injection duration.





Simulation results are illustrated in Figure 25:



Figure 25: Injector Ballistic Effect Sensibility.

The two curves perfectly overlap, so a constant *SMD* can be adopted to simplify the simulation settings without relevant discrepancies from the actual result.

It is now possible to focus the analysis on thermodynamic aspects to maximize water evaporation.
3.5. Influence of Injection Parameters

3.5.1. Introduction

In section 2.2.1 it has already been shown the effect of water saturation pressure on its volatility tendency in comparison with gasoline at the same reference temperature. Additionally, looking at Figure 7 (page 9), it can be noticed that p_{sat} increases as the liquid temperature rises, meaning that by injecting water at high temperatures evaporation is more likely to occur. This has been considered as the starting point for the research of the optimal injection condition to maximize the amount of vaporised water.

Considering Figure 26 and Figure 27 can help to understand why water is less likely to vaporise when the injection is performed in the intake manifold:



Figure 26: p_{sat} vs T diagram with two reference temperature conditions that can be easily experienced in the intake manifold (T_{int}) and in combustion chamber (T_{cc}) .



Figure 27: p-V Diagram Characteristics.

Evaporation occurs as soon as the liquid partial pressure is lower than its saturation pressure p_{sat} (Figure 27). What comes out from Figure 26 is that, considering different engine load conditions, generally characterized by $p_{int} \approx 1 - 2.5 \text{ bar}$, the water saturation pressure at the

intake temperature (T_{int}) could be much lower than its partial pressure (p_w). On the other hand, when the compression stroke starts, the mixture temperature increases much faster than the water partial pressure does, so, sooner or later, the condition for which $p_{sat,w} > p_w$ is reached and water will start to vaporise.

Since the intake temperature depends on the boundary conditions and cannot be completely controlled, to improve water vaporisation tendency the liquid injection temperature (T_w) will be progressively increased until the optimal condition is achieved.

A first simulation has been performed to prove what has been said in this section, so concerning the difficulty of water to vaporise in the intake manifold due to low temperature conditions experienced. Main inputs for this simulation are shown in Table 7 and Table 8:

Tint	Pint	T _{wall}	m _w
[K]	[bar]	[K]	[mg]
305	1.5	330	26

Table 7: Simulation Boundary Conditions.

Sim n°	pinj [bar]	T _w [K]	t _{inj} [ms]
Sim 1	7	333	5

Table 8: Injection Initial Conditions for Sim 1.

As expected, the amount of vaporised water over the total mass injected (m_w) obtained during the induction stroke is almost negligible ($\approx 1.5\%$). This simulation will be used as reference for the injection temperature sensibility analysis treated in the next section.

3.5.2. Injection Strategy Explanation

The reason why the vaporised mass obtained in Sim 1 is so low, not only depends on the volatility behaviour, but also on the other properties shown in Figure 7 page 9. In fact, for the liquid temperature of T_w =333 K water still shows worse characteristics relative to gasoline. However it has been highlighted (sections 2.2.1 and 2.2.2) that after a certain temperature value (T \approx 370 K) both p_{sat} and μ reverse their behaviour and become more favourable for the former. For this reason, to increase both evaporation and break-up tendencies, water should be injected at the highest temperature as possible and at least at T_w>370 K.

When a compound enters its two-phase region (see saturated liquid-vapour region in Figure 27) temperature and pressure are no longer independent, meaning that for each saturation pressure there is a unique saturation temperature and vice versa (25). Since injection events are performed at high pressures, the highest injection temperature to adopt should be as close as

possible to the saturation temperature corresponding to the pressure at which the liquid is injected ($T_w \approx T_{sat}(p_{inj})$). This strategy can be better understood looking at Figure 28:



Figure 28: p-v Diagram with different T_w .

In Figure 28, point (a) represents the water saturation condition with a quality value of x = 0, (where $x = \frac{m_v}{m_v + m_l}$). The injection temperature at this point is $T_w = T_{sat}(p_{inj})$ and is the highest value that can be used. All values of x > 0 and $T_w > T_{sat}(p_{inj})$, point (b), are not considered to avoid the occurrence of boiling phenomena inside the nozzle that could affect the injection event. Finally, point (c) shows injection conditions simulated in Sim 1 (see Table 8 page 24), since $T_w < T_{sat}(p_{inj}=7 \text{ bar})=438 \text{ K}$.

In the ideal case in which water is injected exactly in the condition illustrated by point (a) without any problem due to boiling phenomena, huge advantages in terms of vaporised mass are expected. However, since T_w is quite high and the main goal of water injection is to reduce the mixture temperature before combustion starts, it should be analysed either if the effect of HOV_w can still lead to an effective T_{mix} reduction or the high injection temperature of water prevails on the former effect. In the latter case IWI would be useless in such conditions.

3.5.3. Simulation Inputs

As stated in section 3.5.1, Sim 1 has been used as reference point for next simulations. For these analyses an injection temperature variation was performed. The temperature range considered went from the temperature adopted in Sim 1 up to the saturation temperature at the injection pressure (point (a) in Figure 28). A further temperature increase has been possible, avoiding bubble formation (point (b)), by increasing the injection pressure from 7 bar to 10 bar. The same boundary conditions of Sim 1 have been used (see Table 7 page 24), while in Table 9 the injection characteristics are shown:

Sim n°	p _{inj} [bar]	T _w [K]	t _{inj} [ms]
Sim 2	7	418 ^(c)	5
Sim 3	7	438 ^(a)	5
Sim 4	10	438 ^(c)	4
Sim 5	10	453 ^(a)	4

Table 9: Injection Initial Conditions for Sim 2, 3, 4, 5. Apices (a) and (c) correspond to point (a) and (c) in Figure 28 respectively.

First of all it should be noticed that the injection duration (t_{inj}) for Sim 4 and 5 is lower as a consequence of the injection pressure increase. For what concerns the injection temperature two different conditions have been chosen: $T_w < T_{sat}(p_{inj})$ for Sim 1, 2 and 4; $T_w = T_{sat}(p_{inj})$ for Sim 3 and 5. Considering water properties trends (see Figure 7 page 9), the results expected from such analyses are values of vaporised water mass much higher than the one obtained in Sim 1 (>>1.5%). This prediction is supported by data shown in Figure 29:



Figure 29: Water properties improvements obtained by increasing T_w .

Figure 29 illustrates that a higher T_w leads to an improvement of all water properties in terms of evaporation tendency. In fact, the 20 times higher saturation pressure of Sim 2 relative to Sim 1 means that the volatility should increase of a comparable amount. Even if the other properties do not improve as much as the first one, the sum of all these effects (higher injection velocity due to lower density, better atomization quality due to the Re increase and lower break-up resistance due to a lower surface tension) translates in a more effective atomization.

3.5.4. Post-Processing Results

In the present section two different simulation outputs will be shown: the first represents the water evaporation rate during the whole injection duration; the second is a graphical depiction of the tube mid-section to illustrate both temperature and evaporated water trends at a chosen time instant during the injection. The first result is plotted in Figure 30 and the main outcomes from every simulation are listed in Table 10 to be easily compared:



Figure 30: Evaporated Water Mass Trend for different Tw and pinj.

Sim n°	p _{inj} [bar]	T _w [K]	t _{inj} [ms]	m _{w,vap} [mg]	m _{w,vap} /m _w [%]
Sim 1	7	333	5	0.4	1.5
Sim 2	7	418	5	4	17
Sim 3	7	438	5	4.5	19
Sim 4	10	438	4	5	20
Sim 5	10	453	4	6	22

Table 10: Simulation results: total vaporised water mass $(m_{w,vap})$ and vaporised water mass over the total amount injected $(m_{w,vap}/m_w)$.

The first thing that comes out from Figure 30 is the bi-linear trend of each curve (for the one at T_w =333 K the trend cannot be perceived just because the vaporised mass is much lower than the other cases). This can be explained by the fact that as soon as the injection event terminates no more turbulences are created and the intensity of the ones still ongoing drops. Since turbulences highly affect the spray atomization, the less intense they are, the less effective will be the spray break-up, so bigger droplets will be produced and the vaporisation rate will slow down. Another difference can be seen comparing Figure 30 with Figure 31 in which only the trend of Sim 1 is represented:



Figure 31: Evaporate Water Mass Trend: Sim 1.

Sim 1 shows a completely different trend relative to the others. In the former case the curve showing the vaporised mass can be divided in three parts: in the first one the water mass vaporises very slowly; after that the evaporation rate increases linearly with the injection time and finally it slows down again once the injection stops. In the latter case (see Figure 30), the water mass starts to vaporise immediately after the start of the injection. This behaviour can be understood introducing the concept of *flash-boiling* (analysed for gasoline injection in (26) and (27)). Flash-boiling is the rapid phase change from liquid to vapour that is experienced when the former is injected into an environment which pressure is lower than the liquid saturation pressure. In Sim 1 water is injected at T_w=333 K that corresponds to a saturation pressure of $p_{sat}=0.2$ bar. Since the pressure inside the tube is $p_{int}=1.5$ bar (from Table 7 page 24), in this case a normal evaporation occurs. On the other hand, in the case of Sim 2 where T_w=418 K and the p_{sat}=4 bar, the flash-boiling condition is obtained and water vaporises immediately after leaving the injector. In the end, thanks not only to the advantages already mentioned (see Figure 29) in terms of vaporisation and atomization of Sim 2 respect to Sim 1, but also to the flashboiling effect, an increase of about 15% of the vaporised water mass is perceived from the latter to the former, so that confirming the previously made assumptions. Further advantages were obtained injecting water at the saturation temperature corresponding to the injection pressure (Sim 3), where the 19% of the total mass injected has vaporised. Between Sim 3 and Sim 4 a comparison in terms of injection pressure can be done since water was here injected at the same T_w. In this case just a $\Delta m_{w,vap} \approx +1\%$ was obtained by increasing the injection pressure from 7 bar to 10 bar.

Now the second part of results is shown to better understand what happens inside the tube depending on the injection condition chosen. All the following plots have been obtained at $t_{inj}=3.5$ ms, so for every simulation the injection event is still ongoing.



Figure 32: Local Air Temperature (left) and Evaporated Water Mass Concentration (right) Trends for Sim 1 (t_{inj}=3.5 ms).



Figure 33: Local Air Temperature (left) and Evaporated Water Mass Concentration (right) Trends for Sim 2 (tinj=3.5).

In the plots on the left the temperature of the air flowing in the tube is represented, while in the right ones the ratio between the vaporised water mass over the total mass contained in the single

cell is considered. t_{inj} refers to the time after the start of the injection (aSOI). For both cases the injection duration is 5 ms, meaning that more than half of the liquid has already been injected. However, is evident that in the case of Sim 1 (Figure 32) no water is vaporising, or at least a negligible part just around the injector tip. In Sim 2 can be immediately perceived that a greater amount of water is vaporising since a huge temperature reduction of the airstream around the injector tip is shown and a much higher water concentration is visible all around the spray, compared to the previous case. In the left plot of Figure 33 the great ability of water to reduce the mixture temperature due to its significant HOV (see Table 1 page 6) can be finally seen. For Sim 3, 4, 5 almost the same results obtained from Sim 2 can be seen:



Figure 34: Local Air Temperature Trend for Sim 3 (left), Sim 4 (centre), Sim 5 (right) (t_{inj}=3.5 ms).



Figure 35: Evaporated Water Mass Concentration Trend for Sim 3 (left), Sim 4 (centre), Sim 5 (right) (tinj=3.5 ms).

The only difference that can be noticed in Figure 34 and Figure 35 is that comparing Sim 3 with Sim 4 and 5, the spray penetration in the second two simulations is longer, as a consequence of

an higher injection pressure employed. For this reason, the vaporisation affects a wider region of the airflow.

3.6. Influence of Tube Parameters

Tube parameters, such as intake temperatures and pressures, highly depend on both environmental and load conditions. Therefore, the control of these variables is much limited compared to the injection ones.

General values of intake pressures for a turbocharged SI-engine can go from $p_{int} \approx 1.5 - 2.8 \text{ bar}$, while for temperatures this range is limited between $T_{int} \approx 305 - 360K$. In this section, environmental and load conditions variation are simulated to see to what extent they affect water evaporation tendency.

3.6.1. Intake Pressure Variation

The injection inputs are the ones of Sim 5 (Table 9) that has shown the highest amount of vaporised water. They can be summarized in

	Injection	n Inputs		Tube	Inputs
p _{inj}	T _{water}	t _{inj}	m _{w,tot}	T _{int}	T _{wall}
10	453	4	26	305	330
[bar]	[K]	[ms]	[mg]	[K]	[K]

Table 11: Tube Pressure Variation Inputs.

The tube pressure was then varied from $p_{tube} = 1.5 - 2.8 \text{ bar}$. The numerical results can be seen in Figure 36:



Figure 36: Tube Pressure Sensibility Outputs.

In first approximation a load variation causes a negligible effect on the amount of vaporised water mass, with a difference of about $\approx 1\%$ between the trend at $p_{tube} = 1.5$ bar and $p_{tube} =$

2.8 *bar*. In second approximation a reduction of the vaporised water mass is perceived in Figure 36 with a load increase (so tube pressure increases). This behaviour could be explained considering that the higher the p_{tube} the smaller will be the Δp across the injector, so the flashboiling effect is reduced, as shown in Figure 37. Term Δp represents the pressure drop across the injector holes.



Figure 37: Flashboiling Reduction Effect with tube pressure increase.

The conclusion is that once the flashboiling condition has been reached, a small variation in the Δp does not affect the water evaporation phenomenon.

3.6.2. Intake Temperature Variation

For this evaluation a $p_{tube} = 2.8 \ bar$ was used, while the other input parameters were the same already listed in Table 11. The tube temperature has been changed from $T_{tube} = 305 - 363 \ K$. Simulations outputs are reported in



Figure 38: Tube Temperature Sensibility Outputs.

Tube temperature variation does not significantly affect the water vaporisation tendency, $\Delta m_{w,vap} < 0.5\%$ between the two extreme cases.

3.7. Considerations

In the last part of this chapter a load variation from low- to high-load conditions was simulated. In fact, intake manifold pressures and temperatures rise as the load increase. The result of this analysis is that load variation does not affect water evaporation tendency. Therefore, the only way to improve the water vaporisation behaviour is to manipulate injection parameters and particularly the water injection temperature. It has been found out that to vaporise high quantities of water, this liquid must be injected at very high temperatures, close to the saturation temperature corresponding to the injection pressure adopted. In case this strategy would be actually applied the problem could be how to warm water up to these temperatures. Fortunately, one of the main weak points of internal combustion engines is the huge amount of heat produced by the combustion process, so this heat can be directly exploited to rise the water temperature before the injection occurs.

4. Humidity

4.1. Psychrometrics Applied to Water Injection Concept

Humidity does not significantly affect engine performance. Therefore, in the past, there has been no need to implement models to control this phenomenon in SI-engines when performing 3D-CFD simulations. At most, proper correction factors are applied to tune NO_x emissions that are highly affected by the water content in the air (28), (29). For the same reason, up to now, the effect of humidity has been neglected in QuickSim and only dry air was considered. Nevertheless, whit the introduction of the water injection concept the interest for a better understanding of the humidity effect on this strategy is becoming increasingly widespread. ICEs exploit a mixture of external air and fuel to trigger the combustion process. Considering a moist airflow entering the engine, if additional water would be injected, the combustion process could change depending on the initial value of the air relative humidity.

The goal of this chapter is to evaluate to what extent the maximum injectable water mass is affected by different humidity values of the air for both IWI and DWI applications. In fact, the water vapour amount that can be contained in the air is limited, and once this limit is reached (see Figure 39), two situations can occur:

- water vapour and air cannot mix anymore;
- not mixed water may condense wasting all water injection strategy advantages.



Figure 39: T-v Diagram for Moist Air (25).

At the state of water vapour shown in Figure 39, fixed by the partial pressure p_v and the mixture temperature T, the vapour is superheated. When the partial pressure of the water vapor corresponds to the saturation pressure of water at the mixture temperature (p_{sat}) the mixture is said to be saturated. Therefore, saturated air is a mixture of dry air and saturated water vapor.

4.2. Major Assumptions and Fundamental Relations

Psychrometrics is the study of systems involving mixtures of dry air and water. Since moist air is a mixture of two compounds, to completely define its state at least three properties are needed. In most cases the independent intensive properties of the mixture of total pressure (p) and temperature (T) are known, additionally, one information about the composition is required. In the following such properties will be listed.

The main assumption concerning moist air compositions is that both water vapour and air itself can be treated as *ideal gases*, therefore the *ideal gas law* (equation [9]) can be used to relate p, V, T properties:

$$p_i V = m_i R_i T \tag{9}$$

Where p_i represents the partial pressure of the i-th component, V is the total volume occupied by the mixture, m_i and R_i are the mass and the gas constant of the i-th component respectively and T is the mixture temperature. For what concerns the water content contained in moist air, several indices are employed to describe it. One of them is the *humidity ratio* defined by equation [10]:

$$\omega = \frac{m_v}{m_a} \tag{10}$$

Where m_v and m_a are the water vapour and dry air masses respectively. Considering the *Dalton's Law*, for which the mixture total pressure corresponds to the sum of every component partial pressure ($p = p_a + p_v$), and substituting it, together with the ideal gas law (equation [9]), in equation [10], another form of the humidity ratio as a function of p and p_v is obtained:

$$\omega = 0.622 \cdot \frac{p_v}{p - p_v} \tag{[11]}$$

Another way to define the amount of water vapour in the air is through the *relative humidity*:

$$\phi = \left(\frac{p_v}{p_{sat}}\right)_{T,p} = \frac{m_v}{m_{sat}}$$
[12]

Where p_v and p_{sat} are the same pressures already shown in Figure 39. This parameter depends on both mixture temperature (T) and total pressure (p).

The last important parameter to be introduced is the *specific enthalpy* of the mixture. It is computed over the dry air mass:

$$h = \frac{H}{m_a} = c_{p,a}T + \omega(c_{p,v}T + HOV_0)$$
^[13]

Where c_p is the specific heat of dry air (a) and water vapour (v), T is the mixture temperature at the considered state, while HOV_0 heat of vaporization considering as reference point T₀=0 °C and h₀=0 J/kg.

For next analytical analyses (see sections 4.3 and 4.4) the reference system shown in Figure 40 will be used:



Figure 40: Reference System for Moist Air Analysis in combination with Water Injection.

Finally, to solve such system, mass (equations [14] and [15]) and energy (equation [16]) balances in steady state conditions will be applied:

$$\dot{m}_{a1} = \dot{m}_{a2} = \dot{m}_a \tag{[14]}$$

$$\omega_1 \dot{m}_a + \dot{m}_w = \omega_2 \dot{m}_a \tag{15}$$

$$\dot{Q} - \dot{L} + \dot{m}_a(h_1 - h_2) + \dot{m}_w h_w(T_w) = 0$$
[16]

Where \dot{Q} and \dot{L} represent the energy transfer by heat and work respectively, h_w and T_w are the enthalpy and the injection temperature of the water respectively and \dot{m}_w is the water flow rate.

4.3. Computation of the Max Injectable Water Mass

4.3.1. Analysis Description

To understand how much water injection is affected by moist air, the maximum injectable water mass ($m_{w,max}$) has been computed for different values of initial relative humidity. To do that, experimental pressure and temperature data collected from an engine running at fixed working point, have been used. Such trends vary as a function of the engine crank angle (θ), each of which represents a possible state 2 in the system of Figure 40. In fact, this analysis consists of fixing the ambient conditions (p_1 and T_1) with a proper value of $\phi_1 \neq 0$ and varying $p_2(\theta)$ and $T_2(\theta)$ in order to find $m_{w,max}(\theta)$ for every crank angle of the engine cycle. The result has been then exploited not only to quantify the influence of different ϕ_1 on the total amount of water injected but also to decide the optimal injection strategy to avoid water condensation. For IWI, every state 2 will be characterized by a couple $p_2(\theta)$, $T_2(\theta)$ experienced in the intake manifold (Figure 41) at a chosen θ :



Figure 41: Intake Pressure and Temperature Trends representing the State 2 for IWI.





Figure 42: Combustion Chamber Pressure and Temperature Trends representing the State 2 for DWI.

The working point at which such trends have been measured and other important engine parameters are listed in Table 12:

n	imep	dm _{tot} /dt	dm _f /dt	m _f
[rpm]	[bar]	[kg/h]	[kg/h]	[mg]
2500	15	32	2	31

Table 12: Engine Main Parameters.

Where dm_{tot}/dt is the moist air flow rate, dm_f/dt and m_f are the fuel flow rate and mass respectively, n is the engine speed and imep is the indicated mean effective pressure.

The max amount of injectable water $(m_{w,max}(\theta))$ has been computed for different ambient conditions by varying just one initial parameter at a time:

- Relative humidity sensibility: $\phi_1 = 1\% - 50\% - 80\% - 100\%$;

- Ambient temperature sensibility: $T_1 = 0^{\circ}C - 20^{\circ}C - 30^{\circ}C$ with $\phi_1 = 80\%$.

The choice to do not consider ambient pressure p_1 viariation is due to the fact that either ϕ_1 or T_1 in combination with an initial relative humidity are much more affecting than the former parameter. Additionally, ambient pressure variations are not as relevant as the humidity and temperature ones.

Further assumptions for this analysis are:

- $\dot{Q} = 0$ and $\dot{L} = 0$;
- no water injection has been performed, so the water content at point 1 remains unchanged until point 2 ($m_{v,1} = m_{v,2} = m_v$) and from equation [15], $\omega_1 = \omega_2 = \omega$.

Given all this information it is possible to completely define the state 2 from which the water mass that can still be added to the air is obtained:

$$m_{w,max} = m_{sat,2} - m_{v} \tag{[17]}$$

Where $m_{sat,2}$ represents the max amount of water that can be contained in air at saturation (point 2) while m_v is the initial water content in the air, due to its initial ϕ_1 .

4.3.2. Results for IWI

From the analytical analysis performed it has been possible to plot $m_{w,max}$ as a function of the relative humidity measured at the state 2, $\phi_2(T_2(\theta), p_2(\theta))$, for each crank angle of the induction stroke. Additionally, in Table 14 and Table 15 results for a specific θ have been highlighted to easily compare effects due to different initial conditions, ϕ_1 and T_1 variations respectively. θ has been chosen after the intake valve opening (IVO) in the point of maximum depression experienced in the intake manifold during the induction stroke. The following conditions were measured:

[a]	$\theta = 4$	73° <i>CA</i>
$p_2(\theta)$	1.16	[bar]
$T_2(\theta)$	301	[K]

Table 13: Reference Crank Angle IWI.



Figure 43: Max Injectable Water Mass with φ_1 *variation for IWI.*

p ₁ =1 bar	φ1=1 %	φ1=50%	φ1=80%	φ1=100%
T ₁ =293 K				
ω [kg _v /kg _a]	0.000143	0.007	0.012	0.015
m _v [mg]	0.06	3	5	6
m _{sat,2} [mg]	9	9	9	9
φ ₂ [%]	1	36	57	71
m _{w,max} [mg]	9	6	4	3

Table 14: Max Injectable Water Mass with φ_1 *variation for IWI in [a].*





Figure 44: Max Injectable Water Mass with T₁ variation for IWI.

p ₁ =1 bar	T ₁ =0°C	T1=20°C	T1=30°C
φ1=80%			
ω [kg _v /kg _a]	0.003	0.012	0.022
m _v [mg]	2	5	9
m _{sat,2} [mg]	9	9	9
φ2 [%]	15	57	100
m _{w,max} [mg]	7	4	0

Table 15: Max Injectable Water Mass with T₁ variation for IWI.

4.3.3. Considerations for IWI

For what concerns the ϕ_1 sensibility, comparing the case of dry air ($\phi_1 = 1\%$) with the one at $\phi_1 = 80\%$ a reduction of $\Delta m_{w,max} \approx -56\%$ is shown as ϕ_1 increases. The reason is that the higher the relative humidity value, the higher will be the initial water vapour content in the air, so from equation [17] a lower $m_{w,max}$ is obtained.

In the case of T₁ sensibility, comparing cases at T₁=0°C and T₁=30°C, the reduction experienced from the former to the latter is $\Delta m_{w,max,inj} \approx -100\%$. Here the main parameter determining this reduction is the initial saturation pressure that is much higher for the case of T₁=30°C, meaning that m_v will be higher as well for the same ϕ_1 value. This huge reduction suggests that in those countries where both temperature and humidity are high, water is not able to vaporise in the intake manifold thus wasting the charge cooling effect before the beginning of the compression stroke.

Additional considerations can be made by varying both T_2 and p_2 , so changing the reference crank angle (see Table 13). By choosing θ for which both T_2 and p_2 gradually increase (see Figure 45), at point 2 a ϕ_2 reduction is perceived. This can be explained by the fact that the water vapour saturation pressure increases much faster as a consequence of a T_2 increase than its partial pressure does with a total pressure variation (p₂). For this reason m_{w,max} increases.



Figure 45: Max Injectable Water Mass Variation with p2 and T2 Increase.

The highest value of $m_{w,max}$ fixes a limit on the max WFR that can be used in any specific condition. For instance, in this case $m_{w,max} \approx 6 mg$ and since $m_f = 31 mg$ (from Table 12), the water-to-fuel ratio to be applied to avoid water condensation must be WFR<20%.

4.3.4. Results for DWI

For DWI it is assumed to inject during the compression stroke so a reference θ just after the IVC is considered:

[b]	$\theta = 6$	04° <i>CA</i>
$p_2(\theta)$	1.58	[bar]
$T_2(\theta)$	320	[K]

Table 16: Reference Crank Angle DWI.

For the IWI case both p_2 and T_2 trends show a slight oscillation during the induction stroke (see Figure 41). These oscillations are a consequence of pressure waves triggered by the intake valve opening. This means that the highest value of $m_{w,max}$ (see Figure 45) not necessarily is obtained at the end of the induction phase. Instead, as soon as the IVC both pressure and temperature gradually increase until the combustion occurs. Therefore in this case $m_{w,max}$ increases as the compression stroke proceeds and its highest value is found just before the combustion start, where the p_2 and T_2 are the biggest.



Figure 46: Max Injectable Water Mass with φ_1 *variation for DWI.*

p ₁ =1 bar	φ1=1%	φ1=50%	φ1=80%	φ1=100%
T1=293 K				
$\omega [kg_v/kg_a]$	0.000143	0.007	0.012	0.015
m _v [mg]	0.06	3	5	6
m _{sat,2} [mg]	18	18	18	18
φ2 [%]	0	17	28	35

|--|

Table 17: Max Injectable Water Mass with φ_1 *variation for DWI in [b].*

Results for T₁ variation at fixed $\phi_1 = 80\%$ are illustrated in Figure 47 and Table 18:



Figure 47: Max Injectable Water Mass with T₁ variation for DWI.

p1=1 bar	T ₁ =0°C	T1=20°C	T1=30°C
φ1=80%			
ω [kg _v /kg _a]	0.003	0.012	0.022
m _v [mg]	1	5	9
m _{sat,2} [mg]	18	18	18
φ ₂ [%]	7	28	51
m _{w,max} [mg]	17	13	9

*Table 18: Max Injectable Water Mass with T*₁ variation for DWI.

4.3.5. Considerations for DWI

The first thing that can be noticed is that in both Figure 46 and Figure 47 there is a blue line representing the injected mass of fuel. Therefore for each $m_{w,max}$ value over that line the water-to-fuel ratio will be WTF>100%. However, to avoid great amounts of water consumption WTF should be kept lower than 100%, so this line could be intended as a threshold over which no more restrictions on the maximum amount of water to be injected are present. In Figure 48 this limit is individuated by θ =620°CA. Point 2 [b] (see Table 16) has been chosen to show that for DWI the WFR is limited just at the beginning of the compression stroke. Then, as soon as pressures and especially temperatures increase, the water vapour saturation pressure at state 2 increases up to nullify the initial humidity effect on the mixture. As a consequence, water can be injected with WFR=0÷100% without any risk of air saturation. For both analysis (ϕ_1 and T_1 variation) the behaviour is the same already described for IWI. However in this last case $m_{w,max}$

values are higher than the IWI ones, meaning that with DWI greater WFR are allowed considering the same conditions at the state 1. An example of this can be seen by comparing $m_{w,max}$ values for $\phi = 80\%$ from Table 14 and Table 17. The result is $WFR_{DWI} \approx 3 \cdot WFR_{IWI}$.



Figure 48: Max Injectable Water Mass Variation with p_2 , T_2 and θ Increase.

4.4. Temperature Drop Computation

4.4.1. Major Assumptions

The main aspect of water injection is the ability of water to reduce the fresh mixture temperature when it vaporises. In the previous section a particular case with no injection has been studied to understand the influence of ϕ_1 on the WFR. Now the aim is to understand to what extent the temperature drop obtained as a consequence of water vaporisation is affected by the amount of liquid injected. This analytical approach has the meaning to give a priori estimation of the temperature reduction that could be obtained in the ideal case in which all the water injected instantaneously vaporises ($\phi_2 = 100\%$). To do that some *assumptions* have to be made:

- Water is injected;
- $\phi_2 = 100\%;$
- \dot{Q} and \dot{L} are replaced by an energy factor *EF* (see section 4.4.2).

For this study both the same approach and data applied in section 4.3 are used, so the state 1 is fixed and conditions at the state 2 vary with θ (see Figure 41 and Figure 42 page 37).

Once the final temperature has been estimated, from that value both $m_{w,max}$ and WFR_{max} can be obtained in turn. All such parameters can be finally exploited to predict the effect of water injection over an engine cycle known in advance, in order to choose the correct injection timing to maximize the temperature reduction.

4.4.2. Energy Factor Concept

Since the evaluation has been done on an open system between two points (Figure 40), to take into account of both the heat transfer and especially the compression work (in the case that

point 2 is chosen during compression), an energy factor is introduced in the energy equation ([16] page 36). In this way, for any crank angle considered, temperatures with and without water injection can be directly correlated (see equation [19]).

EF is computed applying the same energy balance between the state 1 and each state 2 (one for each crank angle of the engine cycle) but *without water injection*. Additionally, in this case T_2 is no longer unknown but it comes from experimental trends. In the end the only unknown is exactly:

$$EF = \dot{Q} - \dot{L} = \dot{m}_a (h_2 - h_1)$$
[18]

EF represents a mean value of the total heat transfer and compression work contribution experienced from point 1 and any point 2 either in the intake manifold or in combustion chamber:

$$EF = f(T_{2,noWI})_{\theta_i}$$
^[19]

Where $T_{2,noWI}$ is the experimental temperature measured at θ_i without water injection.

4.4.3. *Results*

Main steps to get the relation for the temperature reduction are highlighted in the following. First of all, by extracting T_2 from the energy balance (equation [16] page 36) a relation to compute this parameter is obtained:

$$T_{2} = \frac{EF + \dot{m}_{a}h_{1} + \dot{m}_{w}h_{w}(T_{w}) - \dot{m}_{a}\omega_{2}HOV_{0}}{\dot{m}_{a}(c_{p,a} + c_{p,v}\omega_{2})}$$
[20]

By substituting the mass balance (equation [15] page 36) in the last equation and taking into account that $\phi_2 = 100\%$, a non-linear relation for T₂ is got:

$$T_2 = f(\omega_2(T_2))$$
^[21]

Therefore, an iterative process is required to find out the value of ω_2 and then T_2 . Finally the maximum temperature drop respect to the case without water injection can be estimated:

$$\Delta T = T_2 - T_{2,noWI} \tag{22}$$

Where T_2 is the temperature value reached when all the water mass injected ideally vaporises. Once the right value of ω_2 has been found through the iterative process, the amount of water needed to saturate the air mixture ($\phi_2 = 100\%$) can be also obtained starting from the water vapour mass balance (equation [15] page 36):

$$m_{w,max} = \dot{m}_a(\omega_2 - \omega_1) \cdot \frac{m}{n}$$
[23]

Where n is the engine speed at the considered working point (see Table 12 page 37) and m=2 for four-stroke engines. Finally, from the knowledge of the fuel mass flow rate the maximum water-fuel ratio needed to ideally obtain the estimated ΔT can be computed:

$$WFR = \frac{m_{w,max}}{m_f}$$
[24]

4.4.4. Analytical Examples and Final Considerations

To better visualize such results, some examples are now shown: one for IWI and another for DWI applications. Some additional parameters must be added to the ones already listed in Table 12 page 37:

Tw	Pinj	h _w (T _w)	c _{p,a}	c _{p,v}	HOV ₀
[K]	[bar]	[kJ/kg]	[kJ/kgK]	[kJ/kgK]	[kJ/kg]
353	7	335	1	1.9	2500

Table 19: Additional Parameters for Temperature Drop Estimation.

For the IWI case the following boundary conditions have been chosen:

State 1			State 2		
T ₁	293	[K]	T _{2,noWI}	301	[K]
p 1	1	[bar]	p ₂	1.16	[bar]
φ1	70	[%]	EF	76	[W]

Table 20: Boundary Conditions Temperature Drop Estimation for IWI.

The results obtained are shown in Table 21:

ΔT _{max}	M w,max	WFR _{max}
[°C]	[mg]	[%]
-7	1	5

Table 21: Max Temperature Drop, Water Mass Allowed and WFR Results for IWI.

When performing IWI, the initial relative humidity of the air highly limits the ideal WFR that can be applied to reduce the mixture temperature. At the conditions chosen for point 2 the max

amount of water that can vaporise is very small, so the consequent temperature reduction is limited.

For the DWI case the experimental temperature considered is higher relative to the previous case, meaning that the EF will be affected. Boundary conditions for this example are shown in Table 22:

State 1			State 2		
T 1	293	[K]	T2,noWI	340	[K]
p 1	1	[bar]	p ₂	2	[bar]
φ1	70	[%]	EF	444	[W]

Table 22: Boundary Conditions Temperature Drop Estimation for DWI.

While the results obtained are listed in Table 23:

ΔT _{max}	m _{w,max}	WFR _{max}
[°C]	[mg]	[%]
-28	6	18

Table 23: Max Temperature Drop, Water Mass Allowed and WFR Results for DWI.

With DWI higher WFR are allowed as already stated in section 4.3, since the temperature increase inside the combustion chamber leads to very high values of vapour saturation pressure, so ϕ_2 values drop. As a consequence a 4 times higher temperature drop is experienced compared to IWI.

Despite this simplified analysis and even though EF does not take into account the real amount of $\dot{Q} - \dot{L}$ experienced from state 1 to state 2 when water injection is actually applied, these results give a better estimation of the phenomenon relative to the case where water injection is not considered at all.

Comparing the IWI results with and without water injection performed at the same p and T conditions, despite the lower ϕ_1 of the example with water injection, its $m_{w,max}$ is 4 times lower than the one predicted in the other case ($m_{w,max}$ results are shown in Table 14 page 39 and Table 21). It means that an even lower WFR would be allowed in real working conditions. Therefore, if the aim is to avoid air saturation, IWI shows high limitations. However, numerical outcomes of the amount of vaporised water over the total amount injected, computed for IWI in same state 2 conditions (see Table 19 and Table 20) considered for the two cases just described, have given $\frac{m_{w,vap}}{m_w} \approx 3\%$ (see Table 24 and Figure 49). This means that, in the real case, to achieve a

temperature reduction of ΔT =-7 °C by vaporising just m_{w,max}=1 mg, a WFR>100% should be employed, so basically saturation conditions would be hardly reached even with IWI.

The conclusion is that, speaking about IWI applications, the main limit of water injection strategy is not due to the amount of air initial humidity, but lies in the impossibility to vaporise acceptable water quantities before the beginning of the compression stroke.

Tint	Pint	Tw	Pinj	m _w
[K]	[bar]	[K]	[bar]	[mg]
301	1.16	353	7	15

Table 24: Input Data Numerical Analysis IWI.



Figure 49: Evaporated Water Mass Trend for Engine Point 2500x15 (IWI).

With the use of basic thermodynamic equations involving moist air it has been possible to understand the relevant influence that this phenomenon has on water injection applications. Therefore, to obtain consistent results when water injection is performed, relative humidity of the air must be considered, especially for IWI applications. For this reason, such equations have been implemented in QuickSim to improve its reliability on water injection analyses.

5. Wall Impingement

As stated in section 2.2.2, another relevant drawback of water is its high inclination to stick on engine surfaces. This problem is much more relevant for water than gasoline since both breakup and atomisation tendencies are much lower for the former, meaning that huge masses of this liquid deposit on such walls. Additionally, also the water volatility is much lower than the gasoline one, so liquid films of water are less likely to vaporise.

Up to now in QuickSim the droplet-wall interaction is computed just at droplet level. This means that no liquid film can be plotted as a continuum, but it is just represented by distinct groups of droplets. In this chapter the analysis of the *Liquid Film Model* offered by STAR-CD has been performed, in order to better visualize water injection effects and easily predict wall film dynamic characteristics thanks to graphical feedback. Since QuickSim uses the commercial CFD code STAR-CD in the background, the last goal of the present dissertation is to find the best settings of STAR-CD to implement the wall impingement model in the software. Of course, the main target is to maintain the computational time as low as possible maintaining a good result reliability.

5.1. Major Assumptions and Equations

In the development of the liquid film model the following assumptions have been stated:

- The film is thin enough for the boundary layer approximation to apply
- The film stays attached to the boundary unless an internal/separate model is used to predict film separation
- The velocity profile across the film is parabolic
- The flow is laminar and incompressible
- The work done by shear forces is negligible
- The analysis is transient

The main relations exploited by the code to describe the liquid film formation are shown in the following:

Mass Conservation Equation:

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l u_l) = \frac{\dot{m}_{imp}}{h}$$
^[25]

where ρ_l is the liquid film density, *h* the film thickness, u_l the film velocity while \dot{m}_{imp} is the mass source/sink per unit area due to droplet impingement or film separation and is assumed to apply uniformly along the liquid film depth.

Momentum Conservation Equation:

$$\frac{\partial}{\partial t}(\rho_l u_l) + \nabla \cdot (\rho_l u_l u_l) = -\nabla p_l + \rho_l g + \nabla \cdot \tau_l + S_{imp}\delta(\xi - h)$$
^[26]

where S_{imp} is the momentum source corresponding to the mass source, p_l the pressure, g the gravity acceleration, τ_l the stress tensor within the liquid film, and δ denotes the Dirac delta function. The condition at the interface is:

$$\mu_l \left(\frac{\partial u}{\partial \xi}\right)_{lint} = \mu_g \left(\frac{\partial u}{\partial \xi}\right)_{g_{int}} = \tau_{int}$$
^[27]

Where μ_l and μ_l denote the viscosity of the liquid film and gas phase, respectively *Enthalpy Conservation Equation:*

$$\frac{\partial}{\partial t}(\rho_l h_l) + \nabla \cdot (\rho_l u_l h_l) = \nabla \cdot (k_l \nabla T_l) + \frac{\dot{Q}_{imp}}{h}$$
^[28]

where h_l is the enthalpy, T_l the temperature and k_l the thermal conductivity of the liquid film. Term \dot{Q}_{imp} is the enthalpy source corresponding to \dot{m}_{imp} and is assumed to spread uniformly along the liquid film depth. The condition at the interface is given by (30). The basic Eulerian model to solve liquid film equations is based on the work of Bai and Gosman (31).

5.2. Simulation Introduction

A first analysis of the wall impingement has been performed thanks to a STAR-CD tutorial in which a diesel fuel spray was injected into the closed box shown in Figure 50. Some inputs have been then changed to understand consequences of activating different liquid film submodels. Since the interest of the analysis is on water behaviour, it has been substituted to the diesel spray in all the following simulations. Main inputs for this analysis are listed in Table 25:

d	tinj	mf	Tf	Ta	Pa
0.3	0.7	5.6	293	293	15
[mm]	[ms]	[mg]	[K]	[K]	[bar]

Table 25: Liquid Film Analysis Main Inputs.

Where d is the nozzle hole diameter, t_{inj} the injection duration, m_f and T_f are the total fuel injected and its temperature respectively, T_a and p_a are the temperature and pressure conditions of the air inside the box.



Figure 50: Liquid Film Analysis Model.

In the following sections the main liquid film sub-models have been treated to understand their influence on the film formation once they are employed. Additionally, a comparison between water and gasoline behaviours is shown.

5.3. Droplet-to-Film Transition

5.3.1. Model Description

The Droplet-to-Film Transition Model allows to treat droplets in two different ways:

- As soon as the injection starts, surrounding surfaces will be covered by just a very small amount of droplets away from each other, so droplets are treated individually;
- After a while the droplet concentration will be increased, so a liquid film will start to appear. In this case droplets are absorbed in/treated as a liquid film.

The transition from the first to the second model occurs when either a user-preset surface coverage ratio γ_c or an equivalent film thickness δ_e have been reached.

$$\gamma_c = \frac{1}{A_c} \cdot \left(\frac{\pi}{4} \sum D_{s,i}^2 N\right)$$
^[29]

$$\delta_e = \frac{1}{A_c} \cdot \left(\frac{\pi}{6} \sum D_i^3 N\right)$$
^[30]

Where D_i is the droplet diameter (D_d) , N is the number density of the considered parcel and A_c is the area of the cell face upon which the droplet parcel resides. D_s is the diameter of a spreading cylinder representing the droplet (see Figure 51).

When a liquid film spreads into a new cell face that only has individual droplet parcels on it, these parcels will be instantly absorbed into the film element.



Figure 51: Droplet-to-Film Transition Diameter Representation.

In order to implement this sub-model in QuickSim a better understanding of the way in which a variation of either γ_c or δ_e affects the liquid film formation has to be obtained. In the next two sections the sensibility on both such parameters will be shown.

5.3.2. Sensibility on surface coverage ratio γ_c

In this analysis three different cases have been considered: in the first the model is kept deactivated; in the second a value of $\gamma_c = 0.1$ is set; in the last case the STAR-CD default value of $\gamma_c = 0.8$ is used. For each case the liquid film thickness has been plotted together with liquid droplets of different sizes proportional to their diameters. Plots are taken at t=1.28 ms and t=2 ms, so after the injection event has already finished.



Figure 52: Droplet-to-Film Transition: γ_c Sensibility (t=1.28 ms).



Figure 53: Droplet-to-Film Transition: γ_c Sensibility (t=2 ms).

5.3.3. Sensibility on equivalent film thickness δ_e

Here four cases have been analysed: model deactivated; $\delta_e = 10^{-6} m$; $\delta_e = 10^{-5} m$ that is the STAR-CD default value; $\delta_e = 10^{-4} m$. Plots are now taken at just t=1.28 ms.



Figure 54: Droplet-to-Film Transition: δ_e Sensibility (t=1.28 ms).

5.3.4. Considerations

Regarding the γ_c sensibility it can be seen that with the model deactivated every droplet is absorbed in/treated as a liquid film. This can be understood by considering that the analysed surface is more "wet" in this case than in the others (see Figure 52 and Figure 53). Fixing a value of $\gamma_c = 0.8$ leads to a more uniform film formation, since only regions where droplets cover more than 80% of the total cell surface are treated as liquid film. However almost no difference can be perceived by varying γ_c from 0.1 to 0.8. One of the main goal of QuickSim is to perform simulations with the lowest waste of time as possible. If the model is not activated a $\Delta t \approx -10\%$ (computational time reduction) has been experienced.

Same considerations can be done also for δ_c variations. However only in the case of $\delta_c = 10^{-5}$ (default value) the computational time increase is just $\approx 4\%$ more than the case with no model applied.

In the end the model activation leads to a more realistic analysis of that phenomenon, so the trade-off between reliability of the result and computational time needed should be carefully analysed.

5.4. Effect of Contact Angle on Film Movement

5.4.1. Model Description

This model takes into account the liquid surface tension σ in order to simulate the film movement on inclined surfaces. This approach has been developed by Foucart (32). As first step, thanks to the solutions coming from conservation equations, it is possible to compute the drop radius R:

$$R = \left[\frac{3V_g}{2\pi \cdot f(\theta_c)}\right]^{\frac{1}{3}}$$
[31]

Where V_g is the drop volume, $f(\theta_c) = 1 - \cos\theta_c - 1/2(\sin\theta_c)^2 \cos\theta_c$, and θ_c is the drop contact angle.



Figure 55: Droplet Contact Angle Representation.

After that, from the analysis of the forces acting on a droplet lying on an inclined surface (see Figure 56), by imposing equilibrium conditions a critical drop radius R_c is obtained. From that two conditions can occur:

• if $R < cR_c$, the film adheres to the wall

• otherwise, the film continues to move



Figure 56: Forces acting on a droplet lying on an inclined surface.

In STAR-CD either θ_c or *c* can be modified during the Pre-Processing phase, so to implement this model in QuickSim the effect caused by these two parameters have to be studied, and then calibrated. In this case the injector has been rotated of 120° relative to the vertical direction (before was 180° see Figure 50), so it has been possible to analyse the effect of the film movement on a vertical surface.

5.4.2. Sensibility on the tuning parameter c

For this analysis the STAR-CD default value for the contact angle has been adopted $\theta_c = 35^\circ$, and then four different cases have been studied: model deactivated, c=0.1, c=1, c=10. The results shown represent the film thickness measured at two different instants of time, t=1.28 ms and t=2 ms.



Figure 57: Effect of Contact Angle on Film Movement: c Sensibility.

5.4.3. Sensibility on the drop contact angle θ_c

Here, same time steps considered before have been analysed by maintaining the STAR-CD default value of c=1 and varying the contact angle as follows: in the first case the model has been kept deactivated; then $\theta_c = 1^\circ$; $\theta_c = 35^\circ$; $\theta_c = 90^\circ$.



Figure 58: Effect of Contact Angle on Film Movement: θ_c Sensibility.

5.4.4. Considerations

What stands out from the previous images is that with the model deactivated the liquid film seems to have a bit less resistance against the motion relative to the case of model activated. For this reason the liquid spreads uniformly in each direction (see Figure 57 and Figure 58).

As soon as c increases (model activated) also the liquid motion resistance increases. This causes the film to spread on the side of the wall and remain more stuck when c is bigger. Comparing the case of c = 10 with the one in which the model is off, in the former situation the film motion is less homogeneous once the bottom surface has been reached by the liquid (Figure 57). Variations of c from c = 0.1 to c = 1 do not affect liquid film behaviour.

Regarding θ_c it can be seen that there is no influence at all on the film movement for different contact angle values.

Finally, negligible computational time penalty has been perceived with the implementation of this model.

5.5. Water vs Gasoline

Now the tutorial previously described will be exploited to graphically show the effect of the main differences between Water (W) and Gasoline (G) (see Table 2 and Figure 7).

Instead of C12H26 DODECANE, as liquid component the following scalars have been used:

- H2O for water analysis;
- C7H16 HEPTANE for gasoline one

Since water and gasoline have different properties, in order to inject the same amount of liquid in both cases, injection parameters have to be adapted:

- For water $t_{inj,w} = 0.69 ms$, $\dot{m}_w = 0.0081 kg/s$ have been set as injection duration and mass flow rate respectively;
- For gasoline $t_{inj,g} = 0.84 \text{ ms}$, $\dot{m}_g = 0.0067 \text{ kg/s}$.

In the following post-processing plots taken at different time steps will be shown to highlight the main differences in the liquid film behaviour for both gasoline and water. As first results film thickness and mass are represented:



Figure 59: Film Thickness Comparison.



Figure 60: Film Mass Comparison.

It is also important, in order to evaluate the atomization behaviour of these two compounds, to plot both droplet diameter and mass. To do that, in STAR-CD is possible to represent the droplet size as a function of different parameters. In this case two droplet plots are shown in which droplets size is proportional to either the droplet diameter (Figure 61) or the mass (Figure 62):



Figure 61: Droplet Diameter Comparison.



Figure 62: Droplet Mass Comparison.

Finally a representation of the amount of liquid vaporised, to show the effect of the different saturation pressure between the two components, together with the temperature reduction perceived as a consequence of such evaporation phenomenon, are illustrated:



Figure 63: Vaporised Mass Concentration (left) and Wall Temperature Distribution (right) Comparison.

From the film thickness and film mass analysis can be easily understood how much water impingement is more relevant than the gasoline one. Gasoline spreads faster than water on the impinging surface and its film mass is quite lower. The reason of this behaviour has already been explained in section 2.2 and can be further confirmed by the droplet analysis.

Regarding the droplet diameter comparison (Figure 61), at the beginning of the injection both water and gasoline droplet diameters (d_d) are more or less similar. However, after few time, due to both better atomization and break-up properties, gasoline droplets show much smaller diameter than the water one.

Considering Figure 62, since droplet mass $m_d \propto d_d^3$, the same behaviour is perceived.

A further reason why gasoline droplets almost disappear toward the injection end can be seen in Figure 63 where the greater contribution of gasoline saturation pressure causes these droplets to vaporise very easily compared to water ones. This evaporation phenomenon is confirmed by the temperature drop experienced in the box. Focusing just on the temperature plot should be clear that water is not vaporising at all. In fact, if it would have evaporated, due to its HOV value highly bigger than the gasoline one, a huge temperature reduction should have been perceived, but actually such temperature remains practically constant.

5.6. Additional Considerations

Impingement implementation in QuickSim could be a further improvement in order to obtain a more detailed analysis of water behaviour and also to give to the user a very fast understanding of the wall wetting phenomenon that lead to a high amount of water wasting. Additionally, wall
impingement analysis can be exploited to prevent severe problems of oil dilution whenever water injection is directly performed inside the combustion chamber. Finally, a further prevention can be done on the creation of a cold-water layer that would form on the combustion chamber walls. Since such surfaces are cooled, the water vaporisation capability drastically decreases leading in turn to more relevant phenomena of oil dilution as well as flame quenching against the wall.

6. Conclusion and Outlook

This work has treated the concept of water injection as an important tool to improve the efficiency of SI-engines in order to limit the production of Greenhouse gases and noxious emissions. Main properties and characteristics of water have been deeply analysed in order to gain a clear knowledge of its behaviour, so that to be able to find the correct injection strategy to completely exploit such advantages. A comparison of gasoline and water properties has shown the great difficulty of the latter to vaporise with temperature and pressure conditions generally experienced in the intake manifold, where vaporised mass values did not overcome $m_{w,vap}/m_{w,inj} \approx 1,5\%$. Among all the variables evaluated in the IWI numerical analyses the water injection temperature was found to be the most powerful tool to increase evaporation tendency of such compound, leading to values of vaporised mass of about $m_{w,vap}/m_{w,inj} \approx 20\%$. This huge increase is strictly related to the flashboiling phenomenon and to the thermodynamic characteristics of the fluid at T > 370 K, that cause the instantaneous evaporation of the jet once it leaves the nozzle. No relevant results can be obtained from a load variation point of view, $m_{w,vap}/m_{w,inj} < 1\%$.

The analytical study of moist air has shown its high influence on the total amount of water that can be injected. For $\phi_1 = 50 \div 80\%$, the maximum amount of water that can be still contained in the air before reaching the saturation condition, is highly limited. A further limitation is introduced by high ambient temperatures.

Another important drawback of water is its tendency to stick on surfaces more than gasoline. For all these reasons a unique injection strategy to maximize water evaporation does not exists. Considering the results obtained in previous chapters, the following solutions could be applied: If water is injected at ambient temperature, IWI application should be preferred. In fact, it has been understood that even if a small amount of water would vaporize in the induction phase, inside the combustion chamber, conditions that allow for a complete evaporation will occur soon. Furthermore, due to this poor vaporisation tendency in the intake manifold, it can be got rid of the limit fixed by humidity on the max injectable water mass because it will be hardly reached (see section 4.4.4). Reasons to prefer IWI than DWI mainly concern the higher costs and design efforts needed to implement the second solution relative to the first. Thicker liquid films could be expected in IWI due to the lower injection pressure. However this problem is much more severe if it occurs inside the combustion chamber, meaning that a more accurate targeting procedure is essential.

Even though no simulations have been performed in combustion chamber, due to both the thermodynamic characteristics of water and the moist air analysis developed, some considerations can be done. When water is injected at very high temperatures, in order to exploit the flash-boiling phenomenon as well as its better properties in this condition, DWI could be more suitable. In fact, while in this case humidity fixes limit for IWI, no restrictions have to be considered for DWI after few crank angles from the IVC. Additionally, DWI layout lets exploit the heat generated by the combustion process to easily warm up the water injector tip, meaning that a proper heat exchanger just for water, mandatory for IWI, could be avoided. In the end, thanks to the instantaneous water vaporisation, also the wall impingement effect could be highly reduced, relaxing the targeting effort.

Since the water injection strategy shows great potentials to overcome main SI-engine constraints and fulfil emission standards, but a complete understanding of all its effects is still not possible, in the short future further analysis to clarify every aspect of this phenomenon will be carried out. Nevertheless, as stated in section 1.1, improving engine efficiency is not the only possibility today investigated. In fact, a solution that do not require as much implementation efforts as water injection strategy and for which a good knowhow is already available in literature, is the adoption of the so called *alternative fuels*.

Different types of fuels such as compressed natural gas (CNG) or liquefied petroleum gas (LPG) have already been implemented in several applications due to their better characteristics relative to gasoline. CNG, mainly constituted by methane, has been introduced in the automotive field due to lots of reasons: larger availability relative to oil fuels, very low carbon content (H/C=4), high RON (up to 130), possibility to use $\lambda = 1$ also in full load conditions, no wall wetting in transient conditions. With these characteristics it could be considered the best solution instead of gasoline in SI-engine applications since all problems relative to CO₂ emissions, knock tendency, TWC efficiency at full load and finally the depletion of petroleum sources, can be completely solved. However, since CNG is injected just in gaseous state, as a consequence of a worse volumetric efficiency, this solution is not able to achieve the same performance as gasoline. Furthermore, due to the lack of infrastructures (CNG gas stations), safety problems caused by the high-pressure tank and other additional limits on HC emissions, this fuel is still far from completely replacing gasoline. LPG still shows characteristics similar to methane with the double advantage that can be stored and injected as liquid and has almost the same performance characteristics of gasoline. However also in this case the absence of a good system of infrastructures makes impossible to substitute it to gasoline.

Nowadays a greater interest is instead given to the so called *carbon-neutral fuels*. The big advantage of such fuels is that they do not result in a net increase in greenhouse gases (GHG). In fact, the CO₂ coming from their combustion process is the same needed to produce them. Two different families can be found: biofuels and synthetic fuels. The first one is directly obtained from biomasses, meaning that relative to oil fuels and natural gases is a renewable energy. In Europe these fuels, such as ethanol (RON up to 130), are becoming more widely employed in gasoline blends due to their ability to easily improve knock tendency of the latter reducing at the same time fuel consumption and CO₂ emissions (33). To limit their fast introduction in the automotive field there are, unfortunately, a series of social, economic, environmental and technical issues concerning both biofuel production and use, which have been discussed in the popular media and scientific journals (34). The last and more recent alternative to conventional gasoline regards synthetic fuels. Basically, the main principle is to convert carbon dioxide and hydrogen in longer hydrocarbon chains (C_xH_y) to re-create the chemical structure of the fuel. The huge advantage is that the CO₂ involved in the conversion process is directly recycled from power plant exhaust gases or derived from carbonic acid in the seawater. Therefore, the gasoline produced not only will show the same characteristics of the conventional one, but in addition it will produce neutral-CO₂. In this way no modifications have to be done to the engine structure and exactly the same system can be maintained.

Considering all these different solutions is very hard to make previsions about the future trend of the automotive field, the only certainty is that surely it will be a great period of continuous evolution and development.

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