

CFD Modelling of the Mixture Preparation in a Modern Gasoline Direct Injection Engine and Correlations with Experimental PN Emissions



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This dissertation is submitted for the degree of
Doctor of Philosophy

I would like to dedicate this thesis to my beloved wife Stefania.

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains fewer than 40,000 words including appendices and has fewer than 150 figures. Parts of the work have been published in journal papers and presented at conferences. These are specified in the text and referenced as appropriate. This PhD started in September 2017. I was enrolled as a full-time student. Then, in September 2021, I was enrolled as a part-time student. I submitted my thesis in preparation for the Viva in June 2023.

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Abstract

A detailed 3D CFD analysis of a modern gasoline direct injection (GDI) engine is carried out to reveal the connections between pre-combustion mixture indicators and PN emissions. Firstly, a novel calibration methodology is introduced to accurately predict the widely used characteristics of the high-pressure fuel spray. The methodology utilised the Siemens STAR-CD 3D CFD software environment and employed a combination of statistical and optimization methods supported by experimental data. The calibration process identified dominant factors influencing spray properties and established their optimal levels. The two most used models for fuel atomisation were investigated. The Kelvin–Helmholtz/Rayleigh–Taylor (KH–RT) and Reitz–Diwakar (RD) break-up models were calibrated in conjunction with the Rosin–Rammler (RR) mono-modal droplet size distribution. RD outperformed KH–RT in terms of prediction when comparing numerical spray tip penetration and droplet size characteristics to the experimental counterparts. Then, the modelling protocol incorporated droplet-wall interaction models and a multi-component surrogate fuel blend model. The comprehensive digital model was validated using published data and applied to a modern small-capacity GDI engine. The study explored various engine operating conditions and highlights the contribution of fuel mal-distribution and liquid film retention at spark timing to Particle Number (PN) emissions. Finally, a novel surrogate model was developed to predict the engine-out PN. An extensive CFD analysis was conducted considering part-load operating conditions and variations of engine control variables. The PN surrogate model was developed using an Elastic Net (EN) regression technique, establishing relationships between experimental PN emission levels and modelled, pre-combustion, air-fuel mixture quality indicators. The approach enabled the reliable prediction of engine sooting tendencies without relying on complex measurements of combustion characteristics. These research efforts aim to enhance engine efficiency, reduce emissions, and contribute to the development of a reliable and cost-effective digital toolset for engine development and diagnostics.

Publications

- [1] Davide Domenico Sciortino, Fabrizio Bonatesta, Edward Hopkins, Daniel Bell, and Mark Cary. A systematic approach to calibrate spray and break-up models for the simulation of high-pressure fuel injections. *International Journal of Engine Research*, 24(2):437–455, 2023.
- [2] Davide Domenico Sciortino, Mark Cary, Sunny Verma, Federico Biagiotti, Edward Hopkins, Changzhao Jiang, Dennis Witt, and Fabrizio Bonatesta. Development of a pn surrogate model based on mixture quality in a gdi engine. Report 0148-7191, SAE Technical Paper, 2021.
- [3] Federico Biagiotti, Fabrizio Bonatesta, Sadjad Tajdaran, Davide Domenico Sciortino, Sunny Verma, Edward Hopkins, Denise Morrey, Changho Yang, Adrian Spencer, and Changzhao Jiang. Modelling liquid film in modern GDI engines and the impact on particulate matter emissions – Part 1. *International Journal of Engine Research*, 23(10):1634–1657, 2022.
- Edward Hopkins, Davide Domenico Sciortino and Fabrizio Bonatesta. Modelling liquid film in modern GDI engines and the impact on particulate matter emissions – Part 2 (*Not submitted yet*).

Conference Presentations

- Davide Domenico Sciortino, Development of PN surrogate model based on mixture quality in a modern GDI engine, SAE ICE 2021, Naples 12th-16th Sep 2021.
- Davide Domenico Sciortino, Statistical and optimisation techniques for the numerical characterisation of Gasoline Direct Injection spray systems. Siemens PLM Software Simcenter Conference, Prague 3rd-5th Dec 2018.

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Nomenclature

Roman Symbols

B_0	Growing diameter calibration factor - KHRT model
B_1	Break-up time calibration factor - KHRT model
C_3	Growing diameter calibration factor - KHRT model
C_{b1}	Bag break-up calibration factor - RD model
C_{b2}	Bag break-up calibration factor - RD model
C_{s1}	Stripping break-up calibration factor - RD model
C_{s2}	Stripping break-up calibration factor - RD model
C_t	Break-up time calibration factor - KHRT model
M^+	Sum of the mass of cells with equivalence ratio above a certain threshold
q	Spread of the droplet distribution - RR model
q_w	Wall heat flux
T_L	Leidenfrost temperature
T_N	Nukuyama temperature
T_{wall}	Wall temperature
X	Reference diameter - RR model

Greek Symbols

α	EN hyperparameter
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β	Regression coefficient
λ	Ridge hyperparameter
φ	Equivalence ratio

Acronyms / Abbreviations

AFR	Air-Fuel Ratio
ASOI	After Start of Injection
ATDC	After Top Death Centre
BDC	Bottom Death Centre
BIC	Bayesian information criteria
BTDC	Before Top Death Centre
CAD	Crank Angle Degree
CD	Central Differencing
CF	Conformity Factor
CFD	Computational Fluid Dynamics
COV	Coefficient of Variance
DMC	Discrete Multi-Component
DNS	Direct Numerical Simulation
DoE	Design of Experience
EEA	European Environmental Agency
EMT	Engine Modelling Team
EN	Elastic Net
EOI	End of Injection
EUDC	Extra Urban Driving Cycle
EU	European Union

EVC	Exhaust Valve Closing
FRP	Fuel Rail Pressure
GA	Genetic algorithm
GDI	Gasoline Direct Injection
GPF	Gasoline Particle Filter
GRBF	Generalised Radial Basis Function
HPC	High-Performance Computing
HRR	Heat Release Rate
ICE	Internal Combustion Engine
ISFC	Indicated Specific Fuel Consumption
IVC	Intake Valve Closing
IVO	Intake Valve Opening
KH-RT	Kelvin-Helmholtz/Rayleigh-Taylor
LAS	Lase Absorption Scattering
LES	Large Eddy Simulation
LF	Liquid Film
LFL	Liquid Film Life
LHV	Lower Heat Value
MARS	Monotone Advection and Reconstruction Scheme
MBT	Maximum Brake Torque
MFB	Mass Fraction Burned
MFR	Mass Flow Rate
MSE	Mean Squared Error
NEDC	New European Driving Cycle

NSGA-II	Non-dominated Sorting Genetic Algorithm II
OBU	Oxford Brookes University
OLS	Ordinary Least Squares
PAH	Polycyclic Aromatic Hydrocarbons
PCJ	Piston Cooling Jet
PDF	Probability Distribution Function
PFI	Port Fuel Injection
PISO	Pressure-Implicit with the Splitting of Operators
PM	Particulate Matter
PN	Particle Number
PRESS	Prediction Error Sum of Squares
PRF	Primary Reference Fuel
RANS	Reynolds Averaged Navier-Stokes
RDE	Real Driving Emissions
RD	Reitz-Diwakar
RNG	Re-Normalisation Group
ROI	Rigion of Interest
RON	Research Octane Number
RR	Rosin-Rammler
SMD	Sauter Mean Diameter
SOI	Start of Injection
SP	Spark Plug
ST	Spark Time
TDC	Top Death Centre

TRF	Toluene Reference Fuel
UDC	Urban Driving Cycle
UI	Uniformity Index
VVT	Variable Valve Timing
WHO	World Health Organisation
WLTC	Worldwide Harmonized Light Duty Vehicles Test

Chapter 1

Introduction

Since the beginning of the XX century, the Internal Combustion Engine (ICE) has grown its penetration in the transport sector becoming the leading propulsion technology. During the decades, the entire development was focused mainly on torque and power output, depending on the specific application. Only recently, with the increased public awareness of cities' air quality and climate change issues, the focus has moved to emissions reduction to mitigate ICE's impact on the environment. Efficiency and clean technology are nowadays key words to attract new customers and investments. In the period 2000-2015, European Union (EU) governments' policies for newly registered petrol passenger light-duty vehicles have drastically reduced the allowed limit of both toxic and greenhouse emissions. The latter, together with fuel consumption figures, has become an essential factor in helping customers to make an informed buying decision. The new society's paradigm of the 'ideal car' merges three interconnected aspects: low fuel consumption (economic aspect); ultra-low emissions (ethical aspect); possibility to avoid the temporary prohibition of traffic (practical aspect).

To meet automotive market expectations and new emission legislation, the ICE research community has focused mainly on thermo-fluid dynamics analysis and optimization techniques, improving how the energy content of the fuel is converted into useful work. Other considerable developments in terms of materials, fuel composition, engine layout, emission filtering systems and electronic control strategies guarantee to achieve a thermal efficiency of almost 40% for petrol engines [7] and comply with current emission legislation [8]. On the other hand, these remarkable achievements increased the complexity of ICE over the years. For example, the transition from Port Fuel Injection (PFI) to Gasoline Direct Injection (GDI) system, required the implementation of complex electronically controlled injectors able to operate at higher pressures and temperatures. This technology yielded a fuel consumption improvement of up to 15% [9, 10]. The result highlights the importance of the fuel injection phasing, the interaction between fuel and oxidiser, and the homogeneity of the charge at

the spark event. First introduced in 1996, the GDI configuration is nowadays the dominant technology for fuel injection [11]. Developing and marketing such complex technology requires millions of pounds of investment and years of workforce. Digitalization and increased robustness of predictive models have proven to reduce the burden promoting the change from expensive real prototyping to digital model development. The implementation of models of complex mechanical systems can effectively: reduce costs and time-to-market [12]; reduce R&D impact on the environment [13]; allow a more comprehensive analysis of the phenomena [14].

The most commonly used computer-aided tools to predict fluid-related phenomena is Computational Fluid Dynamics (CFD) software. Since the '90, CFD simulations have been used in the automotive industry evolving from simple explanatory tools of hidden experimental phenomena to a fundamental step of the development process. The popularity has grown in parallel with desktop processors' capability, diffusion of remote access to High-Performance Computing (HPC) services and automation of the CFD workflow (i.e., pre-processing, meshing and post-processing). Nowadays, CFD codes can solve easily complex body aerodynamics, multi-flow interactions, combustion processes and generally multi-physics problems. Future car development will continue to use these capabilities together with big data-oriented methods, i.e., the car as an interconnected system sharing a constant flow of information to address engineer questions quickly and make new vehicles safer, cleaner and affordable.

The present study aims to use CFD analysis to define a robust correlation between CFD-based in-cylinder mixture characteristics and experimental cylinder-out Particle Number (PN) emissions. Accurate 3D modelling of fuel spray, air-fuel mixture preparation and fuel-to-wall interaction are developed to reveal how mixture quality, before the combustion event, influences toxic PN emissions. The implementation of the calibrated fuel spray model and in-cylinder wall characteristics in the model of the engine full-cycle are used to identify feasible fuel injection strategies to reduce engine-out pollutants. In this study, the CFD analysis is exploited as a substitute for the engine test bed after calibrating the models over many engine operating conditions. This PhD project is attached to the APC6 DynAMO Collaborative Research and Development project (Innovate UK Grant N. 113130).

Section 1.1 presents a snapshot of the actual situation and forecast of petrol ICE for light-duty vehicles with a focus on emissions, government policies and market trends. Section 1.2 presents an initial analysis of model development and how they have become fundamental for the future of ICE. Section 1.3 summarizes the aim and objectives of the research work along with a brief overview of significant steps followed to obtain results for both spray models

and in-cylinder solutions. The last section, 1.4, presents an overview of the thesis structure and a brief description of each chapter.

1.1 The importance of ICE development

A total of 40 million ICEs are produced each year worldwide for passenger car applications [15]. At the time of writing this thesis, around 270 million passenger cars are on Europe's roads with an average age of 11 years [16]. Moreover, the number of vehicles in use increases by 2% each year. Despite all the progress made in the last decades in terms of cleaner technologies and stringent emission regulations, still these numbers have a direct impact on the environment and consequently on people's health. In 2018, UK road transport accounts for 34% of all NO_x emissions, 12% of total PN (or Particulate Matter - PM) emissions and 20% of total greenhouse emissions [17]. It is worth noticing that the vast majority of PN emitted by a car is not generated inside the combustion chamber but is due to tyres, brake system and road wear [18]. The validity of the calculated emission figures was proven during the lockdown period due to the COVID-19 world pandemic. Comparing March 2019 and 2020, NO_x in the UK fell by 40% and PN by 12% with an estimated 1,700 avoided deaths due to air quality [19]. As a result, controlling ICEs emissions and imposing more stringent emission standards remains essential.

Table 1.1 summarises the evolution of EU emission standards in terms of NO_x and PM. CO and HC toxic emissions are not mentioned for brevity. The first two standards (EU1¹ and EU2²) did not have a specific limit for NO_x and PN emissions but had a combined limit for HC and NO_x . The regulations prescribed that cars had to be tested on a dynamometer in warm engine conditions, performing an Urban Driving Cycle (UDC) and an Extra Urban Driving Cycle (EUDC).

Both tests were characterised by a relatively low speed, loads and exhaust temperatures and hence they were not representative of a real-world scenario. EU3³ introduced the New European Driving Cycle (NEDC) to reproduce, theoretically, more realistic driving conditions. Still, the procedure was criticised for delivering emission figures impossible to replicate with the car on the road [20]. In fact, car manufacturers adopted a "cycle beating" methodology consisting of special laboratory-oriented vehicles able to minimize emissions and fuel consumption. The Worldwide Harmonized Light Duty Vehicles Test Cycle (WLTC) debuted with EU6⁴ as a replacement for the NEDC. WLTC is based on a deep analysis of a

¹UDC+EUDC. $HC+NO_x$ total limit 0.97 g/Km. Gasoline and diesel engines equal limit.

²As above but NO_x limit 0.5 g/Km. Unleaded petrol. Gasoline and diesel engines different limits.

³NEDC. Warm-up eliminated. HC and NO_x limits decoupled.

⁴WLTP, PM limit of $6e+11$ #/Km.

Table 1.1 European emission standards.

Standard	Vehicle registered	NO_x [g/km]	PM [g/km]
EU1	Jan 1993	-	-
EU2	Jan 1997	-	-
EU3	Jan 2001	0.15	-
EU4	Jan 2006	0.08	-
EU5	Jan 2011	0.06	0.005
EU6	Jan 2015	0.06	0.0045
EU6d-TEMP	Jan 2019	0.06	0.0045
EU6d	Jan 2021	0.06	0.0045
EU7	Jan 2025	0.06	0.0045

large real driving database and produces 117% more acceleration phases in comparison with the previous methodology [21]. Going from EU3 to EU6, the NO_x limit was lowered by 60% and particulate emissions changed from no limit to 4.5 mg/km and 6e+11 #/km. In the same period, the greenhouse CO_2 emission target was decreased by 50%. No changes were made in terms of emission limits from EU6 to EU6d⁵ but the introduction of the road-based Real Driving Emissions (RDE) test, complementary to the laboratory-based WLTP, has revealed the most reliable perspective for vehicle emissions and consumption figures. The discrepancy between laboratory and generally higher on-road numbers is scaled through a Conformity Factor (CF). For example, a CF = 2.1 allows a deviation in terms of emissions emitted of 110%. It is reasonable to think of a CF = 1 in the near future. EU7⁶ will introduce, in 2025, the strictest standard ever. The aim is to promote the evolution of fully sustainable, smart and affordable mobility. To meet the coming limits, car manufacturers are rethinking the R&D process, investigating how to better deploy existing technology and eventually minimise emissions without compromising efficiency. Moreover, the prospect to measure PN below the 23 nm threshold may obsolete a traditional Gasoline Particle Filter (GPF), not able to operate efficiently with such small particles.

Figure 1.1 shows the average CO_2 emissions from newly registered cars in the EU zone collected by the European Environmental Agency (EEA) [22]. From 2000 to 2018 a promising 32% reduction demonstrated the ICE efficiency improvement made in almost 2 decades but incoming targets set by the EU commission seem difficult to implement with the actual technology. The plateau reached in 2015 and the slight increase in emissions in 2018-19 was due to a combined effect of an increased number of SUVs sold and a reduction of new diesel cars registered as a result of Volkswagen's "dieselgate" [23]. Even if in 2018

⁵WLTP+RDE (CF = 1.43).

⁶It is in discussion. Measurement of PM down to 10 nm (also from brakes).

the average engine efficiency of new cars was higher than in 2017, the abnormal mass and drag coefficient of an SUV led to fuel consumption to soar [24]. As evident from the figure, the 2020 target was missed. The issue highlights the need for a combined strategy among all the actors, i.e., the automotive industry, market and policies, to pursue green mobility. Hypothetically by 2050, following the CO_2 target trend, cars should emit zero CO_2 . This is aligned with the EU's policy action to achieve climate neutrality by the same time frame [25]. According to the European Green Deal, the automotive sector must guide the switch to zero-emission cars [25].

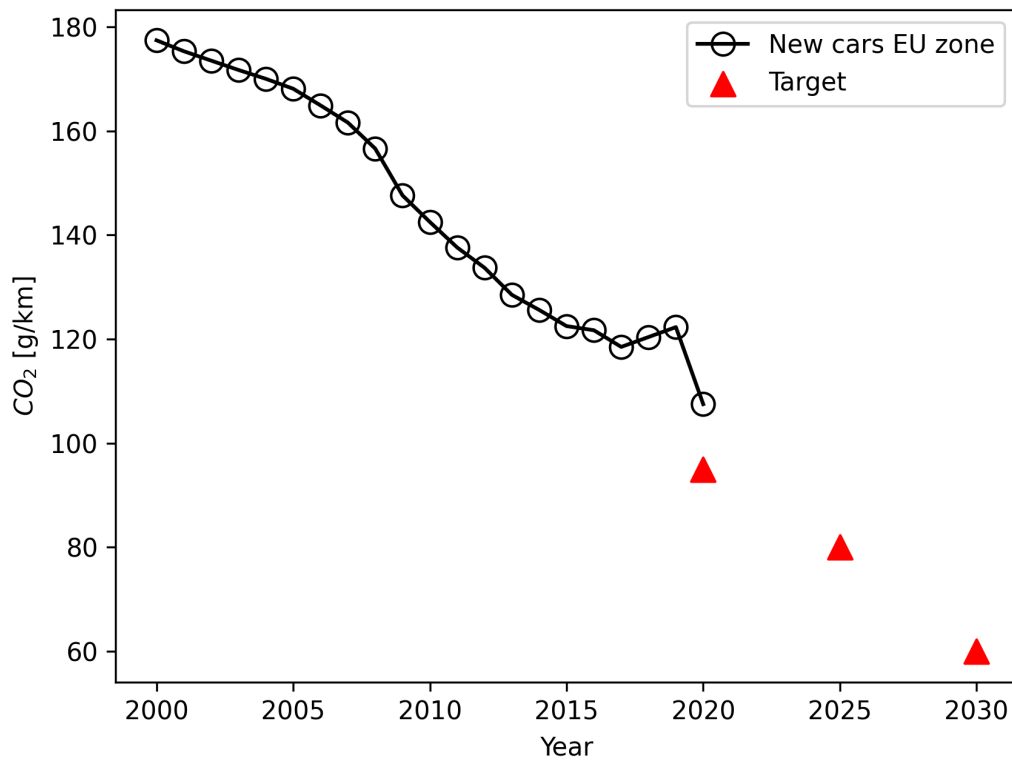


Fig. 1.1 Average CO_2 emissions of new cars registered in EU. Data from [26].

A set of real-world toxic emission figures from passenger gasoline cars operating in a normal urban situation were presented at the International Transport Forum [27]. Figure 1.2 and Figure 1.3 show the related emissions performance in terms of NO_x and PN, respectively. The results may change drastically with different road scenarios, drivers and several other factors. Nevertheless, a clear trend of emissions reduction and conformity to the latest EU standards is presented. It is evident how even EU4 cars can practically almost comply with the actual EU6 regulation. This highlights how car manufacturers tend to develop emissions

reduction strategies well in advance of the new standard being issued. In particular, NO_x has been reduced by one order of magnitude looking at the EU3-EU6 timeframe, while PN by 20%. No changes are noticeable between EU5 and EU6 cars. It is worth noticing that PN figures may get radically worse with a lower particle dimension threshold because, generally, the vast majority of engine-out particles are emitted below the regulated lower limit of 23 nm [28].

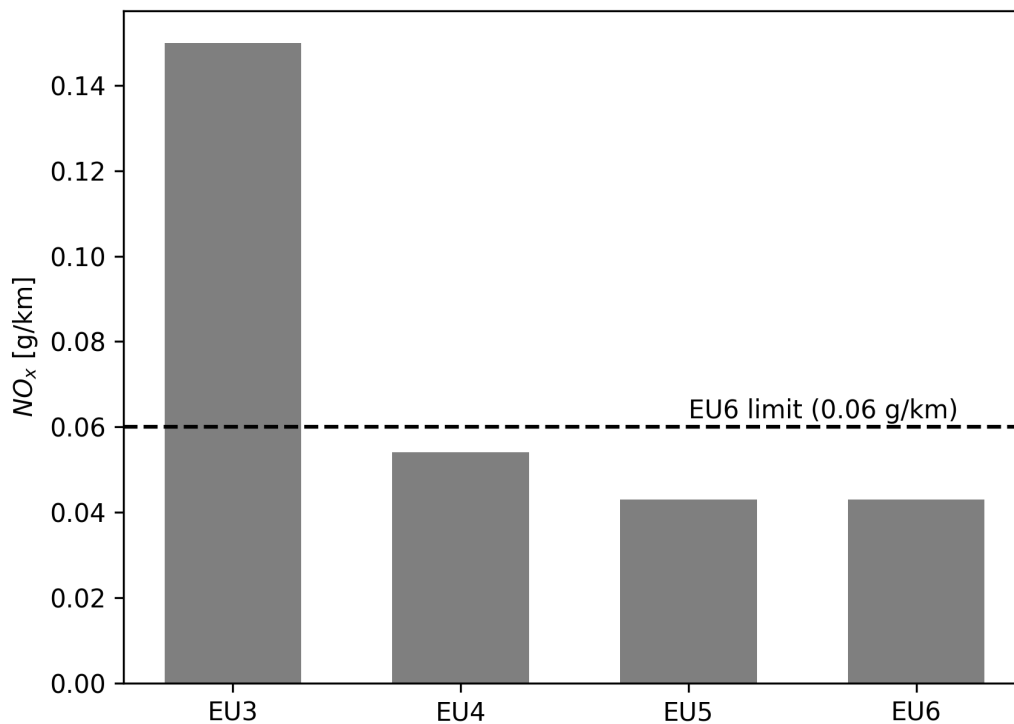


Fig. 1.2 Real-world NO_x emissions from gasoline cars registered with a specific EU standard. Data from [27].

Toxic emissions hugely affect the air quality of urban areas [22]. The effect on human health can vary from cancer to severe heart and respiratory diseases [22]. The amount of toxic emissions concentration, mainly due to the transport sector, is recorded by EEA through monitoring stations dislocated in urban districts across Europe. Figure 1.4 indicates the emission densities recorded as average by year for $PM_{2.5}$ and NO_2 , and as a daily average for PM_{10} . A different averaging time is used because different pollutants affect human health over diverse exposure times. $PM_{2.5}$ data before 2006 were not considered reliable because of the limited number of monitoring stations. Generally, emission limits were respected

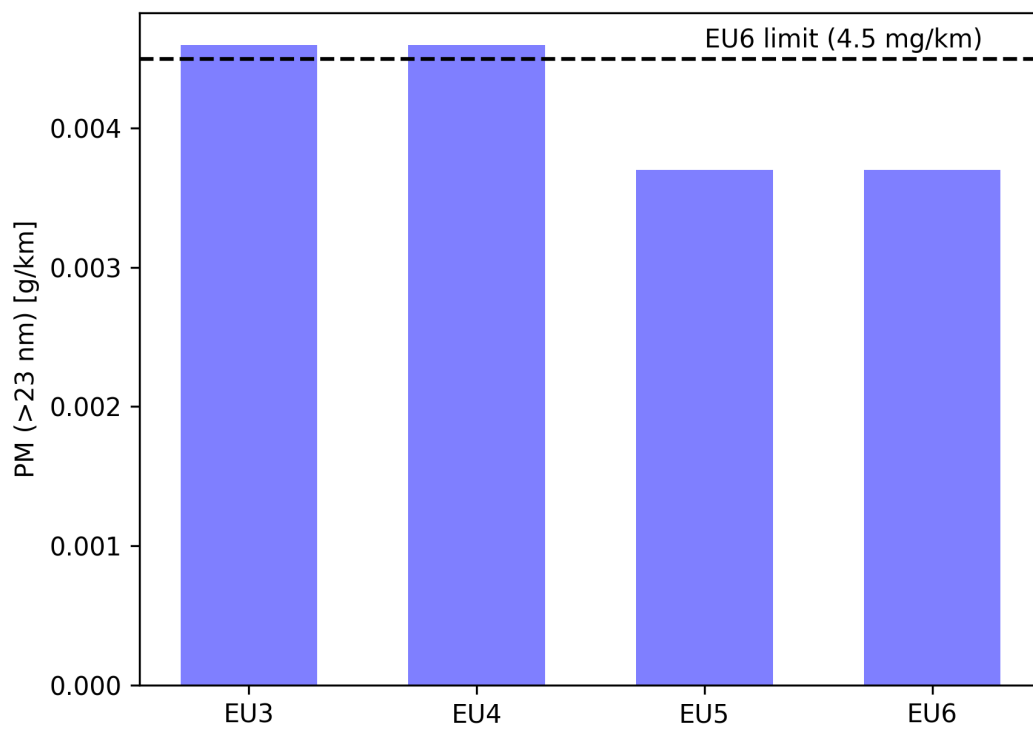


Fig. 1.3 Real-world PM emissions from gasoline cars registered with a specific EU standard. Data from [27].

with only PM_{10} oscillating in four cases across the threshold. Unfortunately, considering the worst-case scenarios over the averaged time for all the toxic emissions recorded, around 10% of the urban population has been exposed to densities around 10% above the EU limits [22]. The numbers are much higher if considering the more severe WHO air quality limits [29]. Forecasts of an increasing number of vehicles and people living in urban districts impose a clear road map on how to keep reducing the impact of toxic emissions on human health as well as a public awareness campaign about which transport solutions are environmentally sustainable. In fact, what people buy and/or use to travel involves a combination of political, economic and marketing aspects.

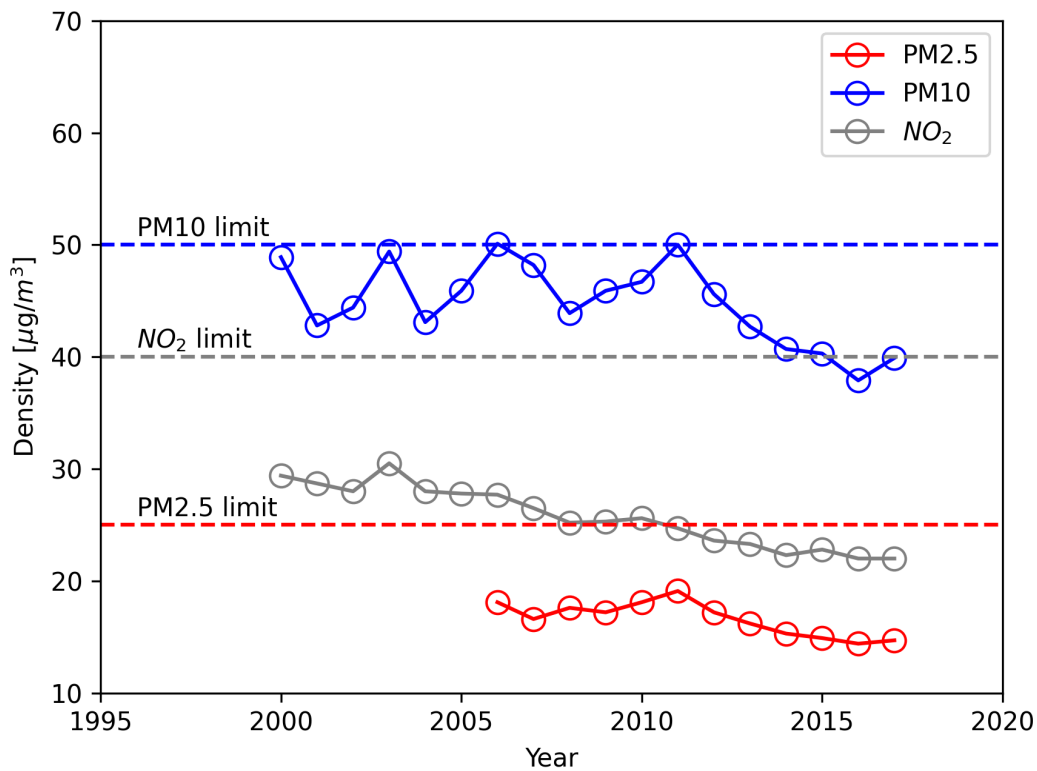


Fig. 1.4 EU average toxic emission concentrations observed at urban background stations. Data from [22].

Figure 1.5 presents the diversification by fuel specification of new passenger cars registered in the EU in the last eight years. During the period 2015-19, gasoline engines have increased their market share by 33% while diesel configuration has decreased by 41% as a consequence of 2015 Volkswagen’s “dieselgate” and the common belief that diesel cars cannot comply with future ultra-low emissions regulations [30]. Interestingly, alternative-

powered cars have grown by around 30% per year during the same time window. This particular segment includes hybrid solutions and pure electric vehicles. The latter are constantly increasing range and overall performance, undermining the establishment of the ICE and forcing car manufacturers to rethink their line-up and investments [31]. In 2020 a sea change started with alternative-powered cars reaching similar values of diesel cars and becoming the front-runner in 2021-22. Moreover, the new EU ban from 2035 on traditional gasoline and diesel engines [32] will accelerate these trends. The ban exceptions regard small-volume manufacturers and vehicles designed for use by civil protection, fire services, public order and urgent medical care. ICEs will be allowed only when using hydrogen as fuel or carbon-neutral synthetic.

Considering every possible scenario, the ICE's detrimental impact on the environment must be minimised in the following years, targeting unprecedented levels of efficiency and emission reduction. The coupling of modelling and optimization methodologies can effectively streamline the ICE design and development process, revealing complex aspects that are usually really high time/money consuming to analyse with traditional experimental techniques. The following paragraph introduces how CFD capabilities and optimisation algorithms have become fundamental tools to design the next generation of ICEs.

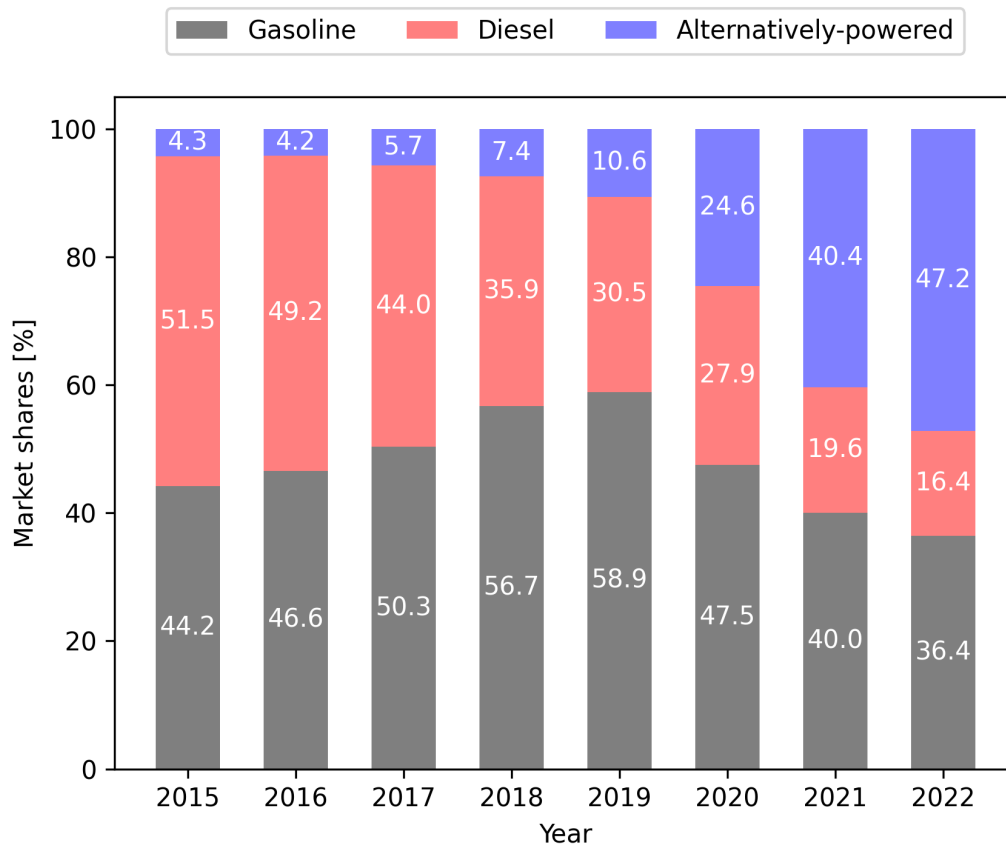


Fig. 1.5 Market share of EU new registered passenger cars by fuel type. Data from [33].

1.2 Modelling and optimization of ICE

The automotive sector, together with research institutes, must improve ICE design and control strategies to mitigate the unprecedented fuel demand from the constantly increasing numbers of vehicles on the road and to minimize to almost zero toxic and greenhouse pollutants. ICEs are complex systems involving multi-phase flows, combustion, heat transfer and gas exchange processes. Modelling these physical and chemical events through mathematical equations can reveal hidden correlations with engine control variables as well as determine a clear path to further improvements. Modelling aims to predict the reality with the minimum amount of information sampled and uncertainties in comparison with the experiments. It is possible to distinguish three groups of mathematical models used for ICEs applications:

- *Empirical models (black box)*: in such models, the equations and calibration factors are tuned with data obtained through experimental campaigns with no use of fundamental

theory governing the phenomena observed. An example is the widely used Wiebe function to describe the crank angle resolved mass fraction burned of an engine combustion process [34]. The obvious limitations of these models are interpretability and simplifications necessary with an inevitable loss of accuracy.

- *Semi-empirical or phenomenological models (grey box)*: these models describe the empirical relations of phenomena observed based on some theory but without deriving any structure from first principles. They are often used in combination with regression analysis to design statistical models useful to describe a large population of data. Popular examples are the PM model proposed by Heywood [35] and the Reitz-Diwakar (RD) liquid breakup model [36].
- *Physically based models (white box)*: these models are designed starting from the first principles of physics. The complex structure obtained makes them very difficult to implement within control strategies and generally for ICE real-world applications. An example is the description of the in-cylinder gas exchange phase using conservation and thermodynamic fundamental equations [35].

One key feature of the engine modelling tools is the possibility to analyse a large portion of the parametric spaces. The selection of the optimal designs or ad hoc solutions can be achieved rapidly in combination with optimization techniques. The number of evaluations necessary to achieve the optimal solution depends on the number of variables involved as well as the complexity of the problem. The knowledge and experience of the designer can help to reduce the parametric space with clear advantages in terms of time and costs.

Mathematical models, generally phenomenological models, are implemented on commercial high-fidelity CFD codes increasing the capabilities to predict complex phenomena. CFD software solve the Navier-Stokes equations governing the fluid flow. Partial differential equations are evaluated in a domain discretized by volume that creates a mesh. The discretization involves also a time value meaning a time-step size is defined as an input parameter. CFD capabilities are not limited to flow problems but can incorporate multi-body and multi-phase scenarios [37]. The coupling with the liquid dispersed phase, necessary to describe for example the fuel spray process, is generally done using a two-way interaction process i.e., heat and mass transfer between the carrier (gas) and dispersed phase (liquid). A more refined and computationally demanding methodology uses a four-way coupling where interactions between liquid particles are considered [38]. The number of particles is discretized by diameter groups and tracked within the flow with the coupled Eulerian-Lagrangian formulation [39]. Moreover, fuel atomization from nozzles is described with

separate phenomenological models for both the primary [40] and the secondary break-up process [1], as will be discussed in detail in Chapters 2 and 3.

The most difficult aspect to model within the fluid dynamic framework is the turbulent flow. Phenomena such as combustion, fuel spray and gas exchange through valves are hugely influenced by the turbulent flow field [41]. A well-accepted theory considers the Reynolds stresses as precursors of the large-scale turbulence that in turn initialize small-scale turbulence [42]. The latter, when sufficiently small, converts its kinetic energy into heat. State-of-the-art turbulent flow prediction can be achieved nowadays using the direct numerical simulation (DNS) method [43]. DNS solves numerically all the Navier-Stokes equations for every time/length scale without using any simplification model. The computational cost is proportional to Re^3 of the fluid analysed [44] making DNS among the highest power-demanding methodologies and therefore unsuitable for industry R&D processes.

Large eddy simulation (LES) was introduced to obtain a good prediction performance of turbulent flows while maintaining lower computational cost in comparison with DNS [45]. LES computes the large-scale turbulence while predicting the smaller scales using a sub-grid model. The additional development needed for such sub-models and the still high computational power demand make the entire methodology not the first choice for engine optimization [46].

To drastically reduce the computational cost and simplify the smallest turbulence scales, the Reynolds averaged Navier-Stokes (RANS) method has been adopted among the ICE community [47]. The compromise between accuracy and computational power is considered acceptable and hence RANS is generally used for the ICE optimization process [48]. The method defines time-averaged values of the predicted flow while the fluctuating terms are considered by means of a viscosity model (usually the so-called $k-\epsilon$ model [49]). The significant disadvantage of time-averaged values is the inability to capture highly unsteady behaviours, common when dealing with in-cylinder phenomena.

Figure 1.6 shows the difference between DNS, LES and RANS methodology for the same turbulent flow. It is evident the deterioration of the small perturbations predicted shifting from DNS to LES as a consequence of small-scale turbulence simplification, and their total disappearance with RANS due to the time-averaged approach.

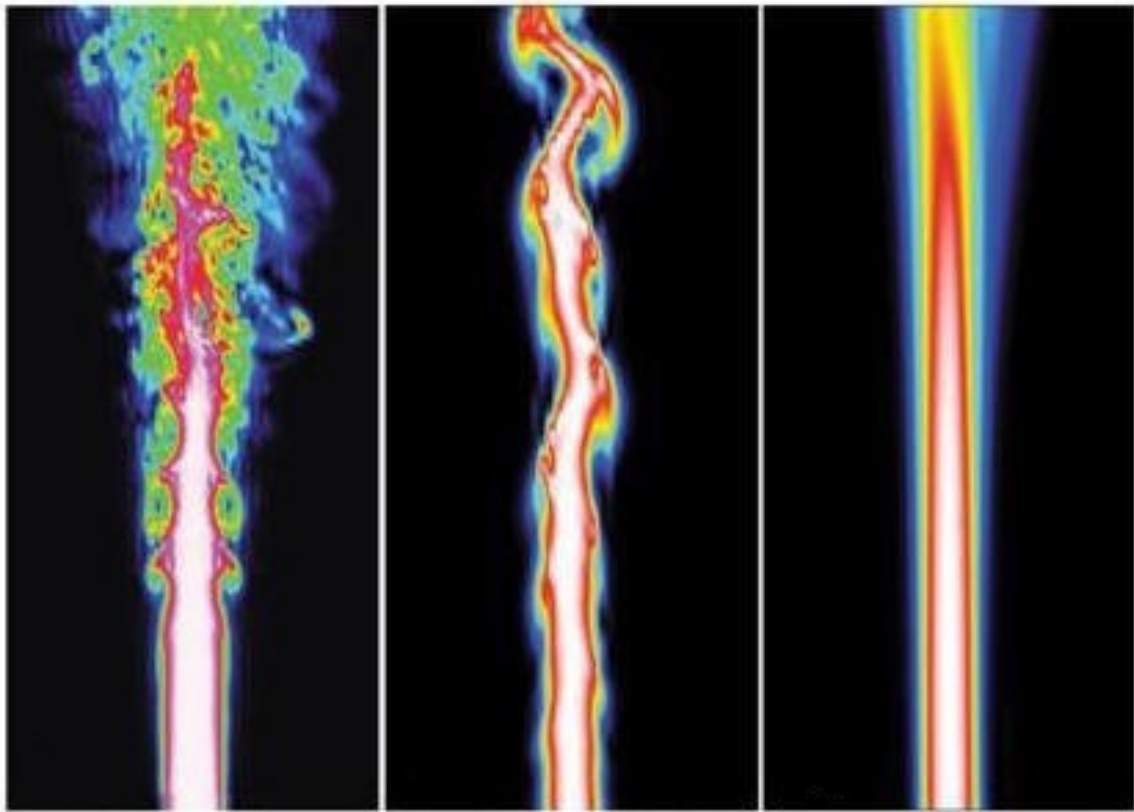


Fig. 1.6 Comparison of a turbulent flow predicted with a) DNS, b) LES and c) RANS approach. Image from [50].

It has been proved how parametric investigation in combination with CFD simulations and ad hoc engine testing considerably improved the understanding of in-cylinder phenomena and considerably speed up the optimization process [51]. The latter often relies on objective-oriented techniques that maximise (or minimise) a cost function based on data analysis and implementing design changes to address the identified area of improvement. Specifically, air-fuel mixture preparation [28], fuel spray impingement [3], knocking tendency [52] and pollutants production [53] are among the most investigated topics. The common workflow for these studies may be summarized in four steps:

1. Definition of the equations and models implementation on a CFD code.
2. Models calibration and validation with experimental quantities.
3. Objectives definition and optimization.
4. Drawing of novel strategies/techniques and final validation with experimental tests.

Still, state-of-the-art engine modelling is affected by a certain quantity of error in comparison with values obtained experimentally, especially when trying to predict unstable/transient phenomena [54]. As a result, searching for new ways to increase prediction performance as well as introducing new optimization workflows are essential to meet future standards faster.

The common engine optimization methodology relies on evolutionary or gradient-free methods as a distinction from non-evolutionary or gradient-based methods. To find the optimal solutions (local or global) of a differentiable function a vast quantity of spatial information (for example, the local gradient) from the response surface is needed. Real-world ICE problems are usually complex, non-linear and not differentiable making the definition of such surfaces not doable from an engineering point of view. A typical scenario of an engine optimization problem consists of the definition of multi-objective parameters (for example, fuel consumption and NO_x emissions) to be minimised (or maximised depending on how the objectives are defined) by tuning certain engine-related, ‘control’ variables (for example, injection pressure and injection phasing). Genetic algorithm (GA) in combination with computational power has been used to tackle complex optimization problems mimicking the Darwinian idea of “survival of the fittest” [48]. The variable combinations are randomly generated to initialize the algorithm. These methods improve the algorithm capability preventing the optimiser from collapsing into the local optimum, exploring deeper the solutions space and increasing the chance to catch the global optimum [55]. When dealing with multi-objective problems, the optimization of one objective function leads to the deterioration of the others. As a result, a trade-off between objectives is necessary to find the best engine variables combination that guarantees reasonable values for all the objectives. The concept of Pareto fronts is generally used to define sets of solutions that outperform or dominate others in the solution space [56]. Still, the experience and judging capabilities of the user are fundamental to speeding up the analysis of the parametric space and identifying the best possible design. Recently, optimization processes have been used to tune models and sub-models for spray calibration [57]. This can be further developed by revealing the physical relationship between calibration factors and the spray characteristics as will be shown in the next chapters. Finally, once the design space is optimized to produce accurate spray models, the resulting mixture processes can be exploited to find consistent relations with other in-cylinder parameters such as post-combustion emissions. An overview of how advanced statistical tools and optimisation were used for the CFD spray calibration and the development of a novel PN surrogate model are introduced in the next section.

1.3 Aims and Objectives

The project aims to find a robust correlation between air-fuel mixture characteristics obtained through CFD analysis and PN emissions obtained experimentally. The correlation was found by means of a PN surrogate model where the model features are mixture-related. In the context of PN description with pre-combustion characteristics, to the best of the author's knowledge and after an extensive review of the existing literature at the time of writing this thesis, it is evident that the surrogate model presented in this work is the first of its kind. Therefore, the proposed PN surrogate model stands as a pioneering contribution in the field, addressing interpretability and overfitting issues that have not been previously explored or addressed in the literature.

The objectives can be summarized according to the following seven points:

1. Review of the current state of the art of CFD simulations on fuel spray, air-fuel mixing, spray wall interaction and liquid film (LF) formation.
2. Application of statistical methods to identify the best/most suitable models and sub-models within the Siemens SimCenter STAR-CD commercial software environment to predict the fuel injection process in modern GDI engines.
3. Use of advanced statistical and optimisation approaches for spray model calibration, supported by an extensive experimental dataset.
4. Application of the calibrated spray model and sub-models within a virtual combustion chamber that reproduces a full cylinder of a new Ford GDI engine.
5. Conducting the CFD analysis over a wide range of engine operating conditions, covering a large proportion of the engine operating envelope.
6. Application of advanced regression methods to prioritise pre-combustion mixture quantities over a large dataset obtained through CFD simulations. Prioritising pre-combustion parameters is essential to reduce the computational effort and speed up the regression analysis.
7. Analysis of injection strategies and how they influence the film formation and mixture performance.

A novel calibration methodology was developed to predict quickly and accurately, within a commercial 3D CFD software, the fundamental characteristics of high-pressure fuel spray in a quiescent, constant-volume, vessel. The purpose was to replicate, in a digital environment,

the experimental setup used to collect fuel spray data. After the design and test of the virtual vessel, the novel methodology consisted of the implementation of a combined statistic and optimization approach to select and calibrate the best breakup numerical models among the most used in literature. A large set of experimental data, provided by Ford Vehicle Evaluation & Verification Powertrain, supported the model calibration phase. The calibrated fuel spray model was then implemented in a virtual combustion chamber environment, reproducing the real setup of a new Ford GDI engine. The engine simulations revealed the dependency between injection characteristics and mixture properties, and served as a virtual test bench to develop a novel PN surrogate model able to predict harmful emissions over a wide range of operating conditions.

The spray model assessment and optimization constituted an essential framework to outline low emissions fuel injection strategies. The work has led to a conference presentation (Siemens SimCenter Conference, Prague December 2018) and, after further developments, to a journal paper [1]. The development of the PN surrogate model was carried out by analysing numerical results with advanced regression techniques and experimental PN data provided by DynAMO project partner Loughborough University. The response equations were obtained and evaluated through various statistical operators reaching statistically significant solutions. The development of the PN surrogate model was the subject of a second journal publication [2]. The final stage of the research project was devoted to investigating optimal spray and mixing strategies to reduce PN, without compromising the typically high thermodynamic efficiency of the Ford Eco-Boost GDI engine series. Injection strategies relied on split injections to improve the air-fuel mixture indicators and minimise the fuel LF formation. The contribution to knowledge can be summarized according to the following three points:

1. New statistical and optimization approaches for spray modelling calibration, and definition of new standards for GDI fuel spray modelling.
2. Development of a novel PN surrogate model able to correlate experimental engine-out PN with modelled in-cylinder pre-combustion mixture indicators.
3. Contribution toward the use of CFD modelling as a virtual test bench, i.e., the numerical analysis used as a valid substitute to experimental engine testing to deliver an innovative R&D approach that reduces costs and time to market.

1.4 Thesis Outline

The thesis is structured as follows:

Chapter 2 (Literature review) examines the modelling techniques and optimization approaches used in relevant literature to improve ICE performance and emissions. Gaps within similar methodologies are highlighted and then used as starting point to define the novel comprehensive methodology proposed in this research work. Reviews of injector studies for gasoline applications have revealed the peculiar characteristics of the multi-hole configuration and how they influence engine performance. Experimental and numerical investigations on general approaches for air-fuel mixture evaluation are reviewed in connection with cylinder-out emissions analysis. Then, state-of-the-art injection strategies for low emissions are analysed. Moreover, a detailed analysis of PN formation and main characteristics is introduced to unveil the complex phenomena that lead to particle emissions. The latter is intrinsically connected to the thermo-physical and chemical properties of fuels. An analysis of fuels and their influence on mixture properties and emissions is hence presented. Finally, the state-of-the-art of fuel break-up modelling and calibration is shown by comparing the widely used trial-and-error approach and the most advanced optimisation techniques.

Chapter 3 (Models Implementation) outlines all the models and sub-models implemented in this research work. Specifically, the spray breakup, the fuel surrogate, the spray-to-wall interactions and the mixture performance parameters. From a simplified vessel to the complex engine geometry, the model implementation is described together with the meshing process. The operating points investigated are presented together with the methodology used for the boundary conditions and the initial model validation process, and how the model was able to replicate the real counterpart in terms of cylinder pressure and air-trapped mass. At the end of the chapter, a summary scheme of the entire model calibration and implementation is presented.

Chapter 4 (Models Calibration and Optimisation) describes the novel approach used to obtain the best model combination for the fuel spray break-up and the approach to calibrate the models over a wide range of injection pressures. In particular, how statistical and optimization techniques are combined to develop a faster and more accurate approach that can replace the time-consuming trial-and-error method. A fundamental part is the definition of the objective functions and ranking procedure to select the optimal set of calibration factors. Factorial design and nested optimization are described highlighting the importance of specific constraints. Lastly, regression techniques and feature engineering approaches are discussed with the aim of developing a robust PN surrogate model that combines experimental data (PN) with numerical mixture properties.

Chapter 5 (Spray Model Validation Results) shows the effect of calibration factors on spray/injection model responses and which spray model combination provides the most consistent and accurate results in comparison with the experimental counterpart. Then, the

definition of the physically acceptable set of optimal calibration factors is discussed in detail. The validation section describes the set of tests used to evaluate the performance of the model when varying the boundary conditions within the range available experimentally. Then an accurate morphology comparison between numerical and experimental quantity is presented. Finally, the prediction capabilities of the model in terms of fuel-to-wall interactions are analysed using the most relevant experimental data available in the literature.

Chapter 6 (In-Cylinder Mixture Analysis Results) presents a detailed analysis of the outcomes of air-fuel mixing characterization and LF deposit with a simplified isooctane fuel and a more complex surrogate blend. The analysis is focused on how engine parameters such as wall temperature influence the equivalence ratio distribution as well as the formation of the LF. The wide range of engine operating conditions investigated, with ad-hoc engine variable sweep, helps to define a statistically relevant data set of pre-combustion mixture indicators that are then used as a search matrix for the PN surrogate model. The piston cooling effect due to the spray-to-wall interaction is introduced to prove the necessity of fine-tuning boundary conditions of the 3D domain when certain injection strategies are considered. Then the concept of piston limiting temperature is introduced within an engine operation map, identifying the necessary temperature to either minimise the liquid deposit or to produce its complete evaporation. Finally, the end of the chapter describes the design of fuel split injection strategies for PN reduction. The technique offers the maximization of mixture homogeneity and minimization of liquid deposits that have been proved to strongly affect the engine-out PN. The guidelines provided can be used as starting point to develop on-board emission reduction strategies.

Chapter 7 (PN Surrogate Model) presents the novel PN surrogate model designed to correlate mixture-related quantities with experimental PN emissions. The Elastic Net (EN) regression technique used to construct the model is described together with the statistical performance. The latter consists of a set of parameters used to compare model complexity and prediction performance. Since this is the first version of a cascaded PN surrogate model developed on a single engine platform, the limitations of the model are discussed with a particular focus on the design of the dataset and the capabilities of the model in providing realistic trend-wise predictions.

Chapter 8 (Conclusions) summarizes all the relevant achievements of the present work. Four sections are presented starting with the main conclusions related to the fuel spray model calibration and selection of the best model combination to predict the atomisation from modern GDI injectors. The conclusions from the mixture analysis are presented providing important guidance for engine developers that want to implement advanced modelling techniques able to capture liquid deposit behaviour and better understand the complex

processes related to PN. The latter is described with the conclusions drawn from developing the surrogate model. The final section presents a description of future works to enable an increasing sophistication and generalisation of the proposed models.

Chapter 2

Literature Review

An analysis of the most relevant literature regarding GDI engine characteristics and phenomena that lead to PN formation is presented in this chapter. GDI technology offers tangible advantages in comparison with traditional PFI engines with better fuel economy and control of the charge quality. However, fine-tuning and control of fuel injection are necessary to avoid excessive fuel deposition on the cylinder and piston walls that might increase harmful emissions. It is also shown how a comprehensive understanding of the mixture preparation phase, dictated by the high pressure with which the fuel is injected inside the combustion chamber, is fundamental to predict the emission behaviour. Digital models, in particular CFD, have been proven to be a necessary tool to reduce the cost of prototype testing and provide a comprehensive insight into the mixture and fuel-to-wall interaction phenomena. The representation of the fuel within the engine CFD model also plays an important role in determining the evaporation characteristics and mixture distribution. Regarding the model implementation, the not trivial calibration of the models and sub-models during the years has been shifted from the trial-and-error approach to a more rigorous methodology using advanced statistics and optimisation methods. Finally, a summary of the literature review is presented highlighting the main findings and best practices.

2.1 GDI Technology

The concept of gasoline direct injection recalls one of the fundamental working principles of diesel engines where the intake stroke is characterized by the introduction of pure air through the valves, and fuel is injected directly inside the combustion chamber. GDI engines evolved from PFI technology using ad-hoc electronically controlled injectors capable of one order of magnitude higher fuel pressure and around one order of magnitude smaller mean fuel droplet diameters [58]. The increased fuel atomization is necessary to compensate for the limited

time available for the air-fuel mixture preparation before the spark time (ST). Figure 2.1 shows a comparison between GDI and PFI architectures. The latter relies on a homogeneous air-fuel ratio (AFR) distribution to maximise efficiency, injecting the right amount of fuel within the airflow sucked through the intake valves. The homogenous air-fuel mixture to be ignited is created outside the combustion chamber. The GDI solution, using the advantage of the injector closer to the spark plug, can operate in both homogeneous or stratified charge modes. For homogeneous operation, the injection is carried out during the intake stroke with the fuel evaporation rate enhanced by both the flow field within the combustion chamber and the finer fuel atomisation. The stratified operation consists of one or multiple injections during the compression stroke with the creation of a rich region (AFR < 14) near the spark plug while maintaining a lean distribution (AFR > 20) in the rest of the chamber.

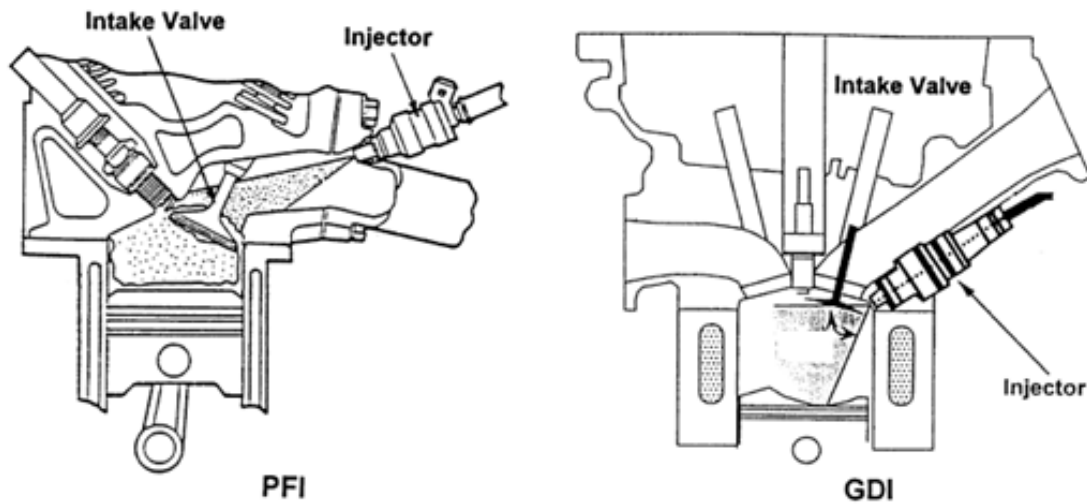


Fig. 2.1 Comparison between PFI and GDI architecture [58].

The advanced fuelling control obtained with GDI technology can improve the fuel economy by 15% in comparison with traditional PFI engines [9, 10]. The substantial advantage is due to three main factors:

- *Cooling effect*: the in-cylinder evaporation of the fuel absorbs heat from the surrounding air improving the volumetric efficiency and reducing the knock tendency [59]. Moreover, increased knock resistance allows the use of higher compression ratios and ST advance leading to a further enhancement in both efficiency and power output.
- *Unthrottled control*: when operating at partial load conditions, the engine can be regulated by the amount of fuel injected instead of the throttle valve. This reduces the pumping losses with clear advantages on overall efficiency [60].

- *Lean operation:* with the stratified charge mode, the overall lean AFR reduces fuel consumption with a beneficial effect also on CO and NO_x emissions [61]. Lean mode is limited to a narrow range of low-load operating conditions due to flame propagation instabilities that may arise with ultra-lean combustion [62].

Figure 2.2 describes the increase of volumetric efficiency of the GDI over the PFI engine as a function of the injection timing [63]. The maximum gain is obtained for an SOI between 300 and 240 CAD where the turbulence intensity and distance of the piston from the injector nozzles facilitate the fuel evaporation and hence a better cooling effect. For early injection, the volumetric efficiency gain decays rapidly due to fuel-to-piston impingements and consequently inhomogeneous AFR distribution. Similarly, for late injections, the reduction of turbulence intensity when the piston is approaching the top death centre (TDC) and the reduced time available for the mixing have a detrimental effect on fuel evaporation [60]. Since the injector is electronically controlled, the injection strategy can be promptly adapted to the actual operating condition with substantial advantages during transient operations. The GDI technology is often combined with turbo units, Variable Valve Timing (VVT) and down-sizing philosophy showing, in comparison to traditional PFI engines, much higher power density [64–66].

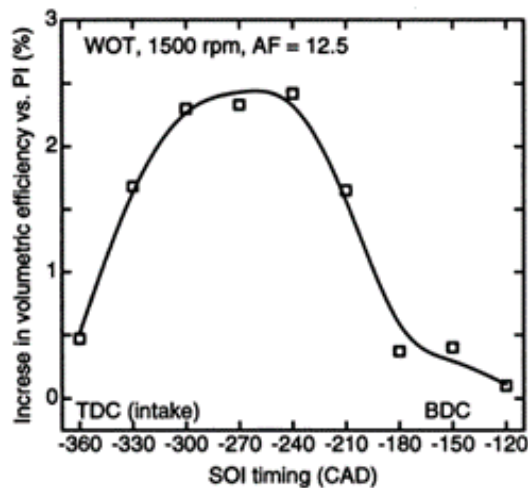


Fig. 2.2 Volumetric efficiency variation of a GDI engine operating at different SOI in comparison with a PFI engine [63].

Injectors for GDI applications are designed to operate internally with a high level of fuel pressure and externally with cyclic variations of both ambient temperature and pressure due to the engine cycle. Figure 2.3 shows the cross-section of a typical injector for GDI applications. The fuel is pressurized by a mechanical pump and enters the tube maintaining

both the valve stem and the steel ball at the close position with the help of the pre-loaded spring. When an electric current passes through the coils, the resulting magnetic field moves both the valve stem and the ball upwards (to the left in the image), allowing the passage of the pressurised fuel through the nozzles and creating an atomised spray. Details of the spray process and calibration of the most used phenomenological break-up models can be found in section 2.6. A dumping spring mitigates the bounce of the stem, a typical issue that is detrimental to the fuelling control and increases both fuel consumption and emissions [67].

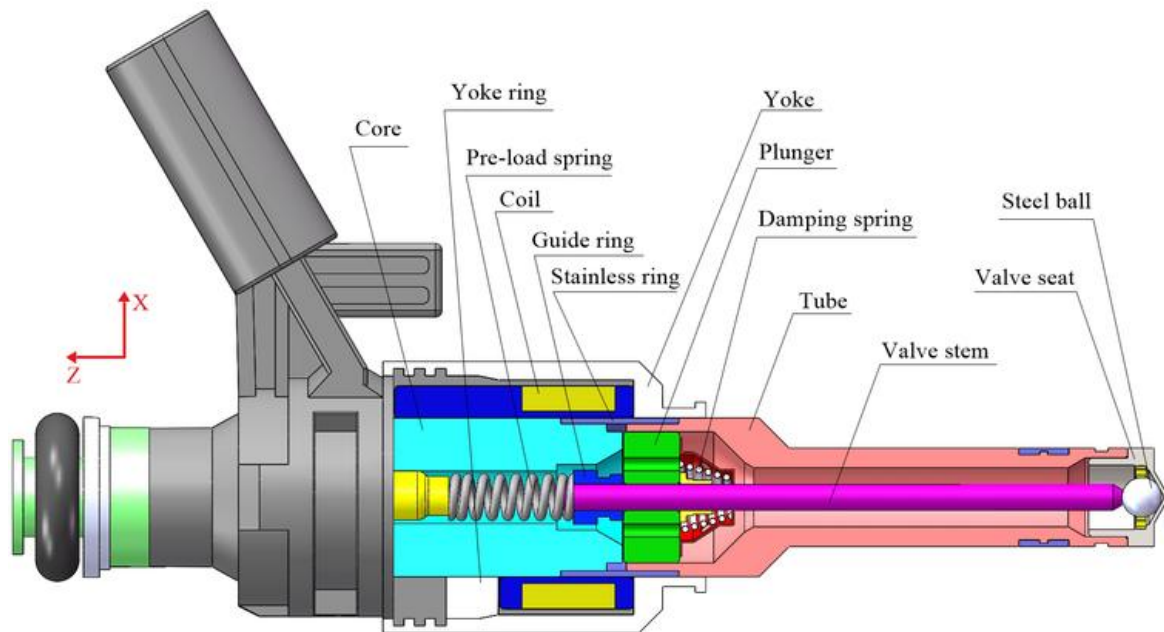


Fig. 2.3 Cross section of a typical solenoid fuel injector for GDI applications [68].

The optimal configuration for the injector, the spark plug and the valves should be changed, ideally, for each operating condition in order to maximize the engine performance [58]. The actual positions and geometries are a trade-off between different areas of the engine operating envelope. Both performance and emissions are affected by the injector location. Figure 2.4 shows the two most used layouts for GDI injectors and the resulting performance characteristics in comparison with the PFI solution. The side injector, also called wall-guided GDI, provides higher emission levels and fuel consumption when compared with the top-mounted or spray-guided GDI. The location of the injector near the cylinder walls, closer to the piston, facilitates fuel impingements, air-fuel mixture inhomogeneity, and pool fire phenomena that are well-known sources of harmful pollutants [69]. The spray-guided configuration seems to offer the best overall performance with a slight increase of NO_x levels in comparison with traditional PFI probably due to mixture inhomogeneity issues [70].

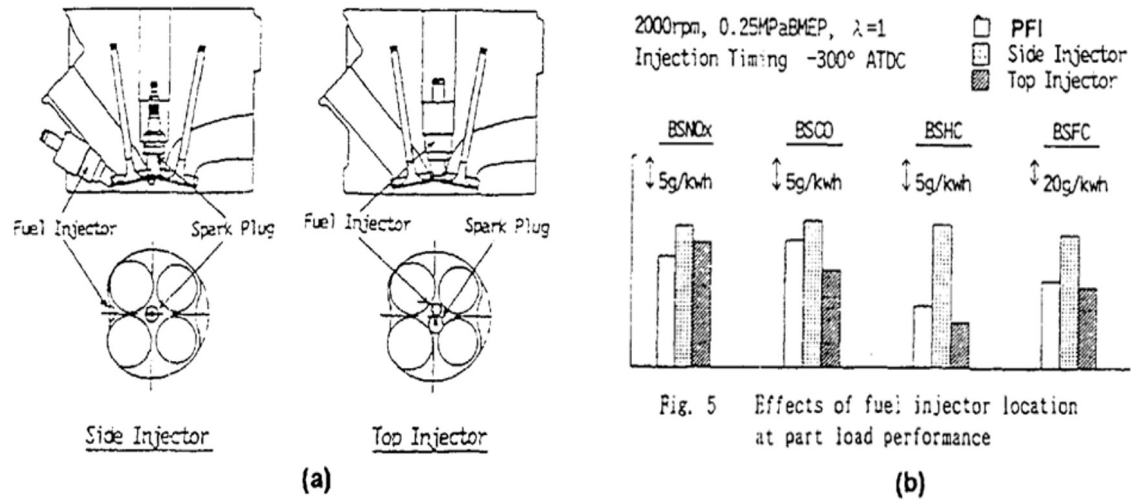


Fig. 2.4 GDI combustion system comparisons; (a) comparison between the side (wall-guided) and top (spray-guided) configuration; (b) effect of injector position on engine emissions and performance [71].

A noticeably shorter time is available for air-fuel mixture preparation when comparing GDI with PFI engines. The mixing could remain incomplete and the presence of sub-stoichiometric mixture pockets promotes soot formation and uHC during the combustion process. It has been found that fuel-rich zones lead to abnormal combustion processes [72] and the over-cooling effect of these zones inhibits fuel vaporisation with detrimental effects on particle emissions [73]. Moreover, the combination of thermal stress and injector tip wetting leads to coking issues that deeply affect the overall performance of the injector [74]. Resulting problems include the variation of fuel mass delivered in comparison with the requested quantity and an abnormal mixing process that in turn creates flame propagation issues and increases the emission levels (uHC , soot and NO_x).

2.2 Air-Fuel Mixture Preparation and Correlation with PN

In GDI engines, the lack of mixture quality (homogeneity) is the main driver of PN formation [75, 76]. Even when operating at theoretically homogeneous, stoichiometric operating conditions, some levels of charge stratification persist. Depending on the location and surrounding conditions, the stratification can trigger particle inception that leads to soot emissions. The poor mixture quality can derive from:

- Mal-distribution of AFR at ST and during combustion.
- The LF deposited on the piston crown or walls.

- Residual droplets remaining after ST.

The short time available between the end of injection (EOI) and ST results in incomplete fuel distribution and the formation of sub-stoichiometric regions. These regions have an over-cooling effect that reduced both fuel evaporation and mixture formation speed. The fuel film formation is mainly governed by injection characteristics such as fuel injection pressure and spray angle/pattern. High injection pressure may lead to deep spray penetration resulting in spray-to-wall impingement phenomena. As the fuel film is formed, three scenarios are possible:

- The fuel film does not participate in the combustion process.
- The fuel film participates in the combustion process and is exposed to high temperatures. As a result, a notable quantity of particle emissions is expected.
- The fuel film participates in the later stages of combustion and is exposed to lower gas temperatures. This may result in a relevant presence of unburned hydrocarbon (*uHC*).

The residual droplets are generally related to cold start engine operating conditions or specific strategies such as late injection and stratified combustion mode [77, 78]. If a reduction of fuel atomisation occurs, it leads to larger-than-normal droplets that take longer to vaporize. Fuel liquid droplets that move towards the periphery of the combustion chamber also experience a lower vaporisation rate, as they remain precluded from the main chamber motion. As most of the available oxygen is consumed by the main flame front, the periphery droplets struggle to find oxygen to mix with. In turn, this causes abnormal combustion and relevant particle emissions. Moreover, the phenomenon of direct carbonization of remaining liquid droplets is also possible [79]. Several studies have been conducted to find out how mixture-related engine parameters correlate with particle emissions [80, 69, 81]. Even if the results are sometimes unclear or discordant for specific engine operating conditions, all the parameters investigated may be listed in descending order by influence on PN emissions, as follows:

1. Fuel type
2. Fuel Rail Pressure (FRP)
3. Coolant and oil temperatures
4. AFR
5. Injection timing

6. ST

Lucchini et al. [60] investigated the correlation existing between CFD-based mixture parameters and experimental PN data from a GDI engine. A mixture uniformity index (UI) was defined as an indicator of the mixture quality. For a full load operating condition, the two injectors tested gave similar levels of UI at ST, but the injector featuring a wider spray pattern and reduced wall impingement produced up to two orders of magnitude lower PN. Figure 2.5 indicates how the wider spray pattern of injector 2 had the best AFR distribution, creating a more uniform cloud of droplets and less liquid deposit. The similarity of UI values at ST between the two injectors demonstrated the necessity of more than one parameter to accurately describe the mixture distribution and homogeneity. To correlate pre-combustion phenomena to PN emissions, the focus should be given to fuel atomisation, distribution and interactions with walls. Moreover, the authors described the correlation without providing a regression analysis of the quantities involved.

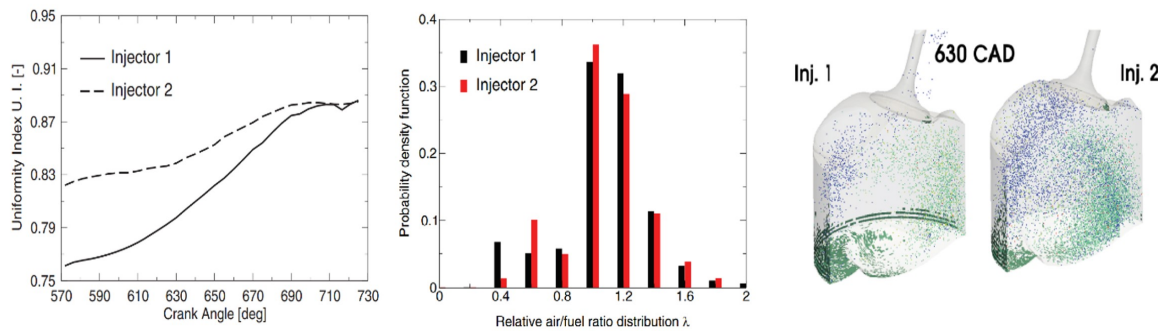


Fig. 2.5 CFD mixture parameters in terms of UI (left), AFR equivalence ratio distribution (middle) and liquid droplets and film deposit (right) [60].

Jiao and Reitz [75] analysed the influence of the equivalence ratio in theoretically homogeneous/premixed, part-load, GDI engine operating conditions. PN was found in higher concentration and dimensions near the cylinder walls during both lean and rich operating conditions, as shown in Figure 2.6. The cylinder periphery had a combination of lower temperatures and oxygen species that inhibited PN oxidation. Moreover, the mixture in these locations might be characterised by fuel-rich pockets that are a source of soot emissions.

Lou et al. [82] used a spray-guided engine to correlate ultra-high pressure injection strategies with combustion characteristics and emissions. The injection strategies were expressed in Crank Angle Degree (CAD) as Start of Injection (SOI) Before Top Death Centre (BTDC). The highest injection pressure investigated largely reduced the overall PN emissions for both early (310 CAD BTDC) and late injections (250 CAD BTDC), as indicated in Figure 2.7 (left). The trend was consistent through all the PN modes and particularly in

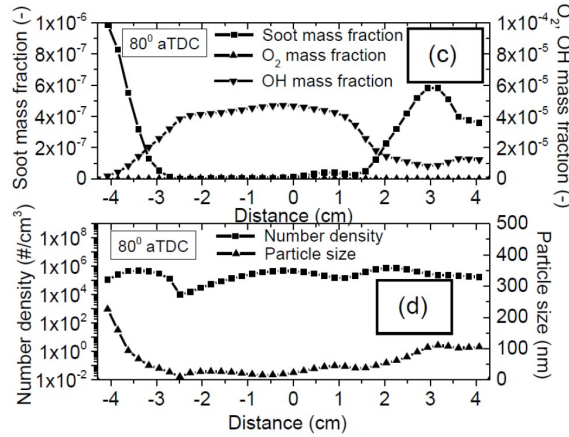


Fig. 2.6 Localised presence of soot mass and *OH* (top), PN number density and size on a reference line for a lean premixed operating condition (bottom) [75].

the sub-23 nm region, as shown in Figure 2.7 (right). Sub-23 particles formed the larger portion of the total PN and increased with late injection due to a reduction of the mixing time. However, delaying the SOI improved combustion velocity with benefits on the overall efficiency and hence on the fuel consumption.

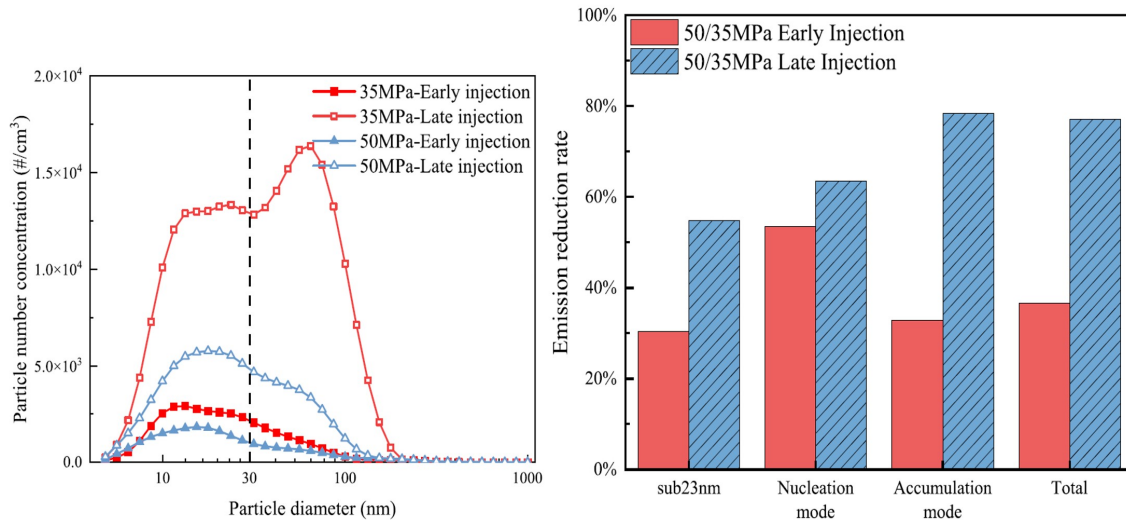


Fig. 2.7 Particle size distribution (left) and percentages of emission reduction (right) for 350 and 500 bar injection pressure at 5 bar BMEP [82].

Potenza et. al [83] studied the effect of injection strategies on PN morphology, dimension and concentration. Considering a reference operating condition with SOI of 270 CAD BTDC and 50 bar fuel rail pressure (FRP), the increase of both Start of Injection (SOI) and FRP produced up to one order of magnitude increase in soot emissions. As shown in Figure 2.8,

both pre-catalytic and exhaust port trends were similar indicating a higher soot production due to a stronger fuel impact on the piston crown when increasing FRP (Figure 2.8 left) and SOI (Figure 2.8 right). The presence of metallic particles, together with carbonaceous clusters, revealed how fuel impingement might promote piston wear. Even if the results seem discordant with other studies when considering the impact of FRP on PN [3, 82, 28], they exposed the importance of a correct calibration for both FRP and SOI to improve the mixture homogeneity, avoid/minimise fuel impingement and ultimately reduce soot emissions.

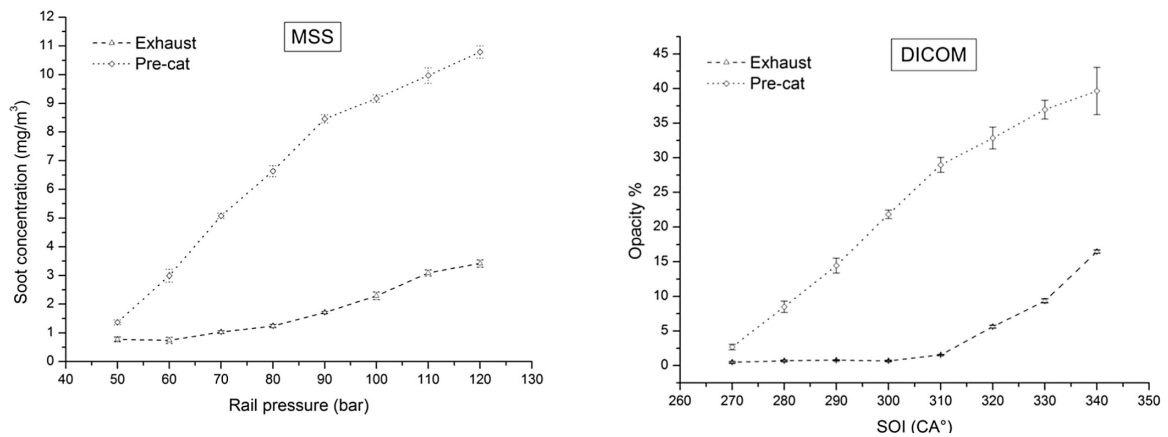


Fig. 2.8 Engine-out soot as a function of FRP (left) and SOI (right) [83].

Sciortino et al. [28] investigated the PN number density distributions in a passenger car wall-guided 1.6 litre 4-cylinder GDI engine, for a combination of low-load and part-load engine operating conditions with FRP and SOI set according to the manufacturer Electronic Control Unit (ECU). The increase in engine speed and load led to lower peaks in both nucleation and accumulation mode, as shown in Figure 2.9. Increasing engine speed promoted a proportional increase in in-cylinder turbulence intensity, speeding up the mixture formation and homogenisation. The reduction of PN associated with greater engine load suggested that the higher injection pressure used in this case exerts the greatest effect on charge homogeneity and, in turn, on the process of particle inception. Figure 2.10 confirmed this theory as CFD images of the combustion chamber revealed how the higher load had a noticeable enhancement of both UI and equivalence ratio uniformity.

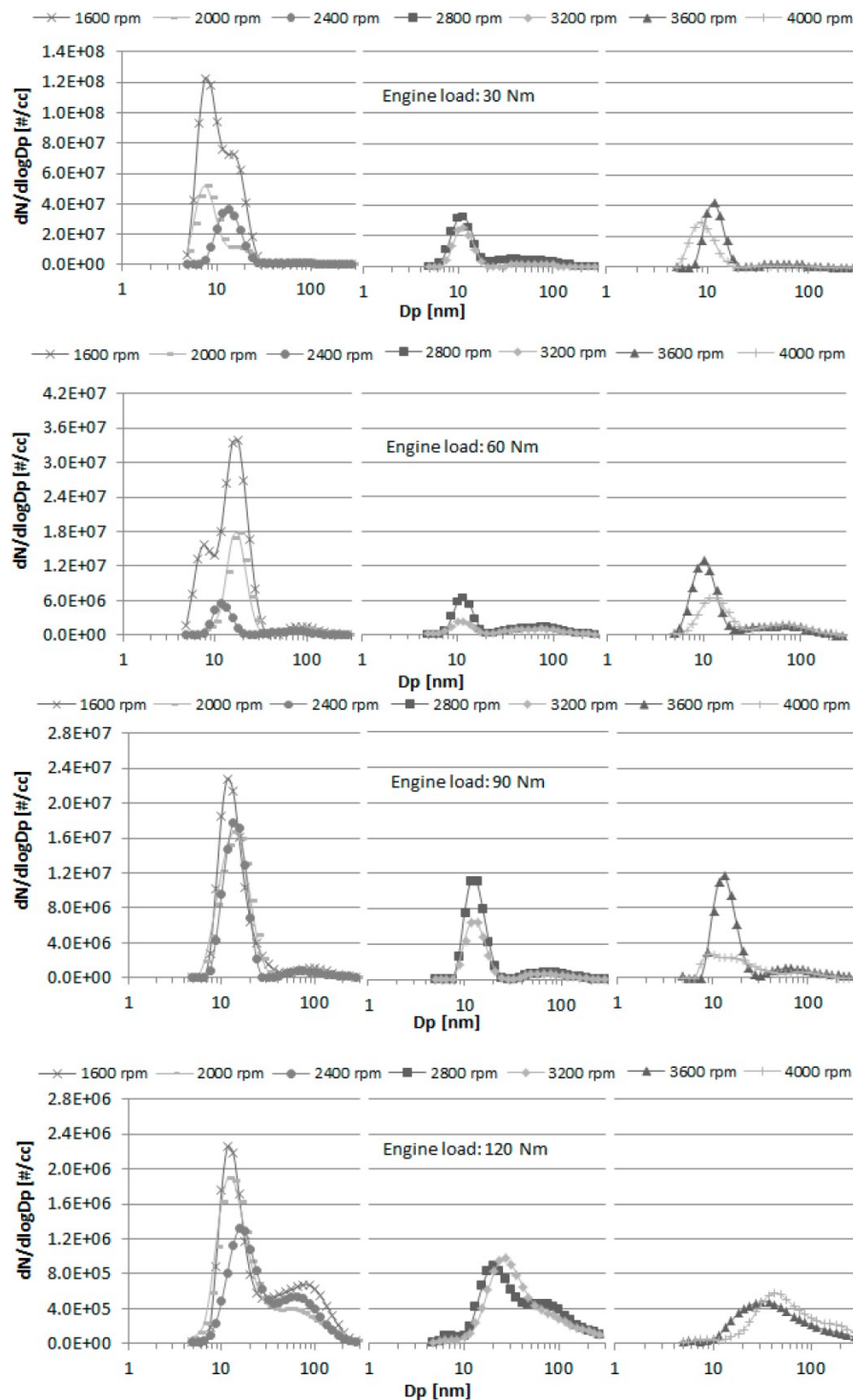


Fig. 2.9 PM number density for different engine operating conditions. For each load (30-120 Nm) the engine speed is increased from 1600 to 4000 rpm [28].

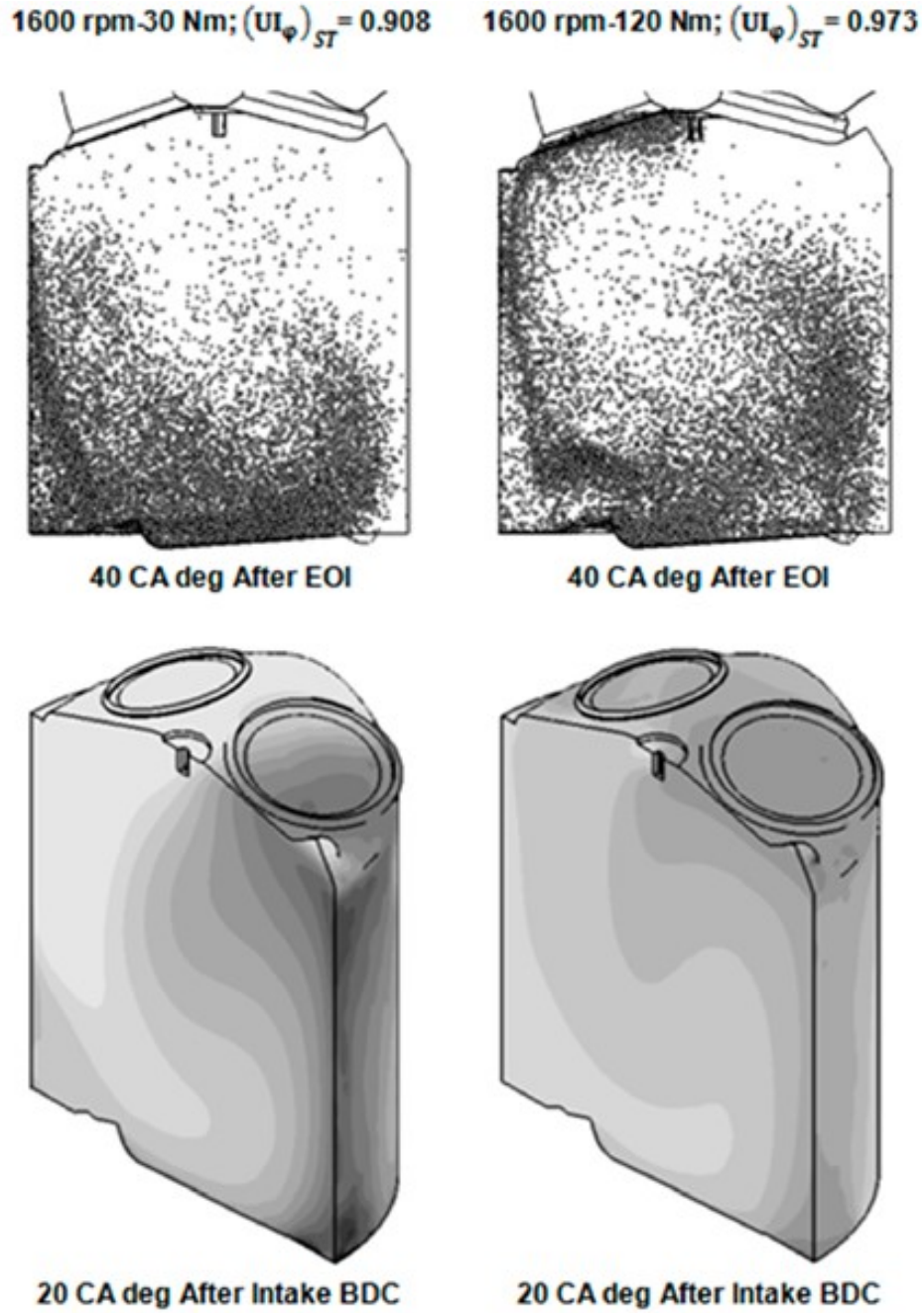


Fig. 2.10 CFD images of liquid droplet distribution (top row) and equivalence ratio (bottom row, darker colour means richer mixture). UI was defined for the two operating conditions at ST [28].

2.3 Split Injection Strategy for Emission Reduction

The use of split injection can yield efficiency optimisation and emission reduction [84–86]. Unfortunately, such strategies require intensive tuning and they heavily depend on the specific engine operating point. While splitting the injection process reduces the spray penetration and the possibility of film deposits, the decreased amount of mixing time and the development of rich regions around the spark plug might translate into intense nucleation of particles and combustion instabilities. The base idea of split injection is to have an initial shorter fuel spray during the intake stroke to form a lean mixture and then, in the second stage, towards the end of the compression stroke, the rest of the fuel is injected to create a stratified charge. Costa et. al [85] analysed a split injection strategy aiming to improve combustion performance and minimise emissions. The investigation combined experimental data from an optical GDI engine and numerical results used to optimise both injections and ignition timing. The authors found that for a constant amount of fuel, a double injection not only reduced NO_x , HC and PN emissions, but also the heat release rate (HRR) was faster with obvious advantages for overall efficiency. Fine-tuning the second injection phasing was fundamental to reducing the PN levels. In fact, if the injection occurs too late in the compression stroke, the formation of LF on the piston crown might promote localised rich diffusive combustion with consequent increments of PN emissions.

Park et al. [87] analysed the performance and emission levels of a GDI engine operating with an overall lean mixture ($\lambda=2$) adopting split injection strategies. The flammability limit was achieved with fuel injections through the compression stroke, i.e., stratified charge operation. Figure 2.11 shows how the 2-stage injection with asymmetrical delivering (3:7) created combustion instabilities (1.2% Coefficient of Variance - COV) and a higher level of exhaust gas opacity (directly correlated to PN), while NO_x and HC emissions were reduced in comparison with the symmetrical (1:1) reference case. The results were directly correlated to mixture preparation, fuel impingement and over-richer stratification before the spark event. A symmetrical 3-stage injection produced the best performance in terms of efficiency (indicated specific fuel consumption – ISFC) and PN but had an abnormal increase for both NO_x and HC probably due to a combined effect of reduced air-fuel mixing time and catalyst system performance.

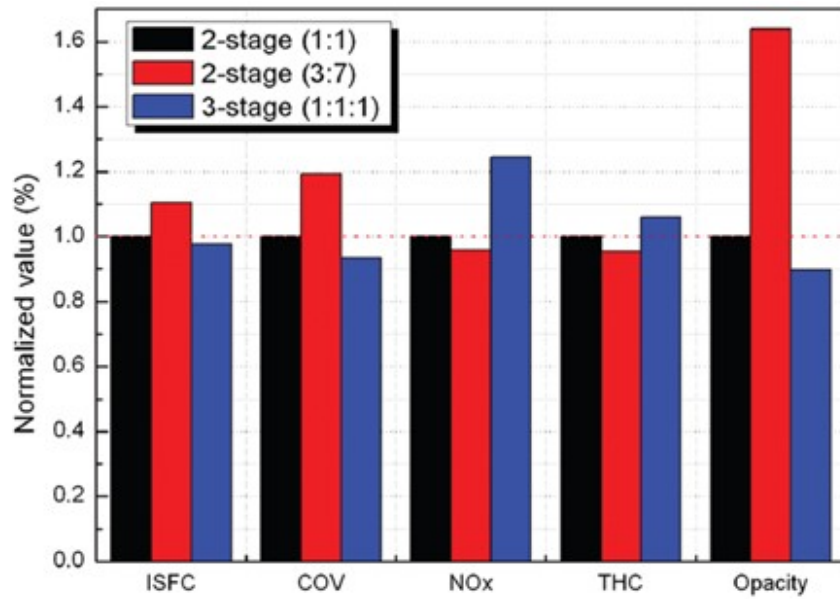


Fig. 2.11 Lean-burn performance and emissions for three split injection strategies. Data are normalised with the 2-stage (1:1) injection where a fixed amount of fuel is equally portioned between each injection [87].

Li et al. [88] investigated the effect of split injections on mixture formation utilising a Laser Absorption Scattering (LAS) technique. With an FRP of 46 bar and ambient pressure of 6 bar, a comparison in terms of fluid velocity is presented in Figure 2.12 where images are taken at 2.5 ms after SOI (ASOI). For the single injection case (Figure 2.12 left), the liquid accumulated at the leading edge of the spray produced a higher penetration in comparison with the split injection case (Figure 2.12 right). The air entrainment in the tail and vortices toward the bottom had the effect of diluting the spray region and hence promoting a lean equivalence ratio. For the split injection case, the second injection penetrated the tail region of the first. This reduced the liquid accumulation due to an enhanced evaporation rate. Moreover, the spray was more compact, and penetrated less considering the leading edge, and the regions with over lean equivalence ratio were reduced. Ultimately, the split injection proved to be the best candidate for a better mixture formation and hence had the potential to reduce both *HC* and *PN* emissions.

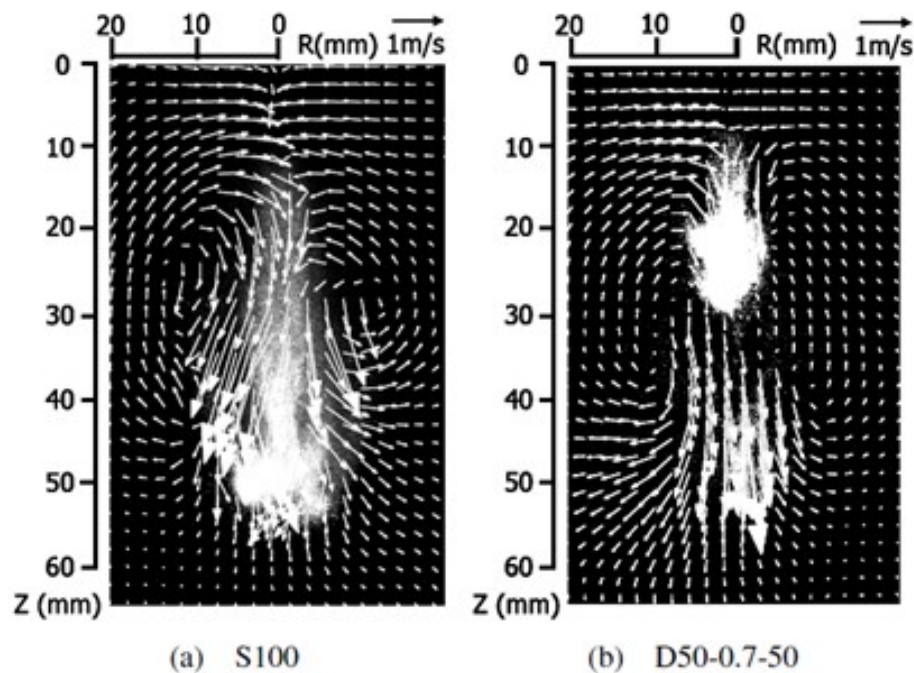


Fig. 2.12 Air entrainment velocity for the single injection (left) and split injection (right) with 50% of the total fuel quantity delivered for each injection with a dwell of 0.7 ms. Images were taken at 2.5 ms ASOI [88].

2.4 PN Formation Process and Characteristics

The combination of chemical and physical events that lead to PN formation can be summarised as follow:

1. Oxidation and/or pyrolysis of fuel under fuel-rich conditions and temperature between 1000 and 2800 K.
2. Production of precursor molecules from hydrocarbons species, leading to the formation of Polycyclic Aromatic Hydrocarbons (PAH) gas species molecules.
3. Polymerization of hydrocarbon rings.
4. Particle inception or nucleation, as a result of the interaction between polymerized structures.
5. Particles growth due to interactions between PAH species and particle surface.
6. Coagulation of particles due to collision.

7. Oxidation of particles in the presence of oxygen species (O_2 , OH , CO_2 , H_2O) in a high-temperature environment (during and post-combustion).

In-cylinder thermal conditions and chemical species determine the formation of PAH (equivalent diameter around 0.5 nm) and the inception of the first PN particle (1 nm) as shown in Figure 2.13.

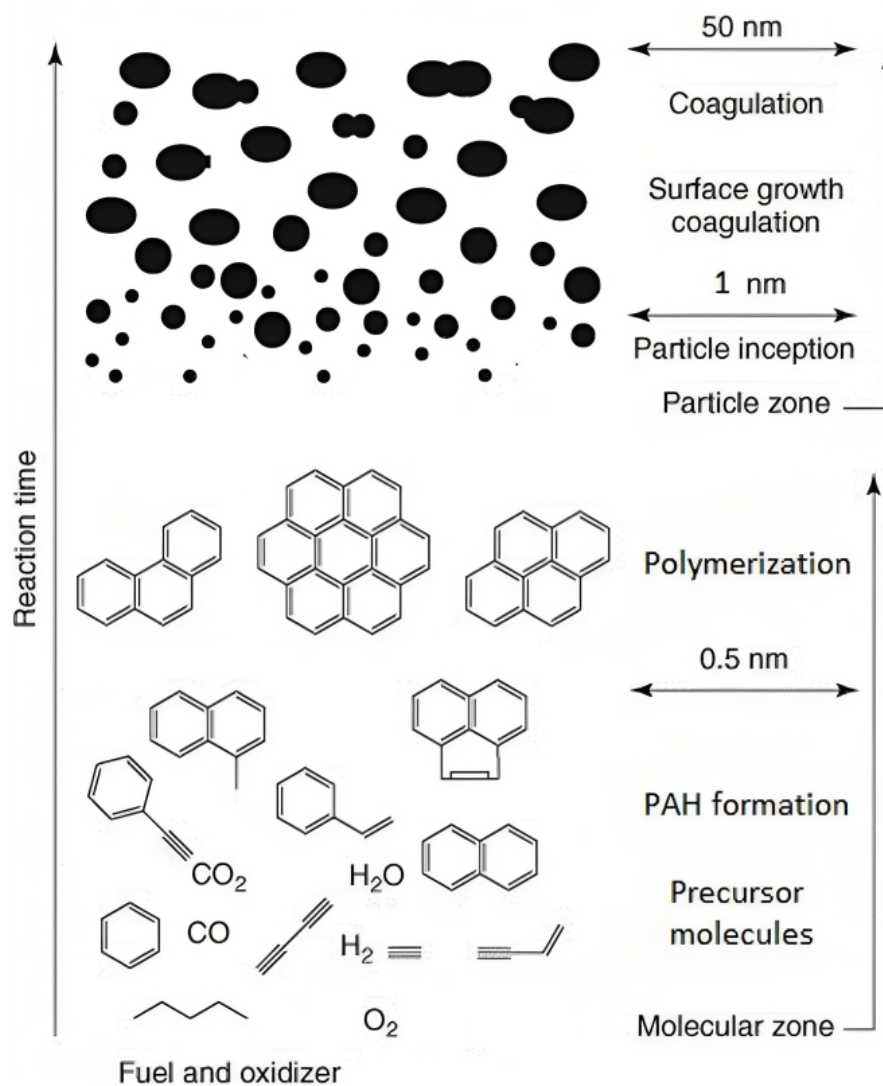


Fig. 2.13 PN formation process from a combination of fuel and oxidizer [89].

The composition of engine-derived PN is a blend of volatile and solid components. *uHCs* from fuel and oil are the main constituents of the volatile part. Solid components are mainly ash, sulphur and metal. Among them, agglomerated carbonaceous particles (solid), commonly known as soot, may absorb both organic and inorganic compounds on their

surface. During and after combustion, with high-temperature variation, several events can modify PN characteristics in rapid succession by means of nucleation, oxidation, evaporation or condensation of volatile deposits and self-nucleation. More specifically, considering a GDI engine operating at stoichiometric conditions, the vast majority of soot produced during combustion is oxidised before the end of the combustion [90, 91, 80]. Only around 1% might be oxidised by passing through the exhaust pipe [80]. This is evident by analysing the production of soot and how it follows, with some delay, the evolution of combustion as shown in Figure 2.14. The delay is due to the time needed for particle inception and growth following the high-temperature pyrolysis starting phase. Interestingly, the peak of soot is aligned with 50% of the mass fraction burned (MFB); the bell-shaped curve then decays drastically when approaching the end of combustion (90% MFB).

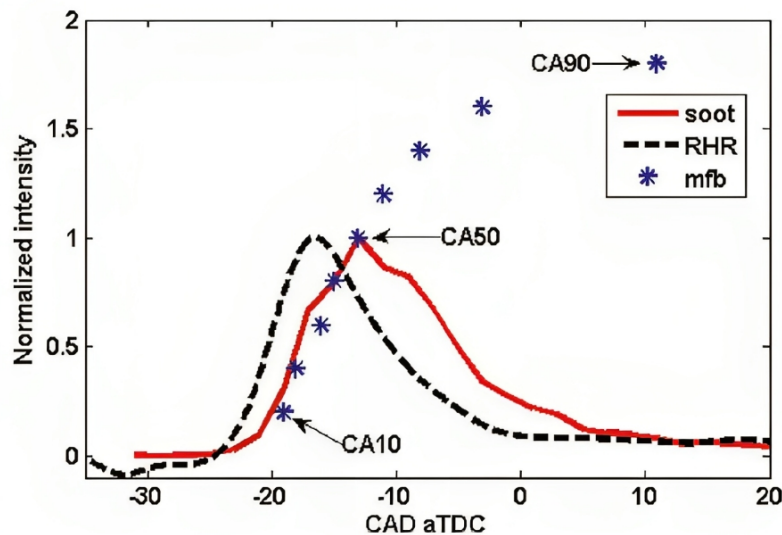


Fig. 2.14 Soot evolution during the combustion process in comparison with heat release rate and MFB [92].

The detailed dimension analysis of PN from exhaust pipe reveals how it can be divided into three main modes:

1. *Nucleation*: it comprises nanoparticles with a diameter smaller than 50 nm. The main constituents are volatile droplets.
2. *Accumulation*: generally, this mode features particles with a dimension smaller than 100 nm (ultrafine particles) consisting of agglomerated solid carbon particles and volatile deposits on the surface.
3. *Coarse*: similar to accumulation mode but with larger dimensions (>1000 nm).

Figure 2.15 presents the dimension analysis of the normalised concentration of PN from a typical gasoline engine. Considering the number concentration, the bimodal distribution shows a peak at around 10 nm (nucleation mode) and a second peak near 100 nm (accumulation mode). Generally, the vast majority of PN emitted by number is volatile within the nucleation mode [93]. The mass analysis inverts this behaviour, with most of the mass emitted in the accumulation and coarse mode. A complete account of these modes in relation to the functional form of the experimental particle number density distributions is due to Kittelson et al. [93]. The average diameter for GDI application can be approximated at 25 nm when considering the number density [29]. More precisely, Sciortino et al. [28] found that 72% of particles are emitted on average in the 5–23 nm size range, while over 80% fall in the nucleation mode range. Only 10% of particles are emitted in accumulation mode (51–100 nm). The very high frequencies in the sub-23 nm range expose the limitations of the EU6d emission regulations which do not consider particles below this threshold. This finding is aligned with a more recent study from Lou et al. [82] where sub-23 nm particles account for >50% of the total engine-out PN.

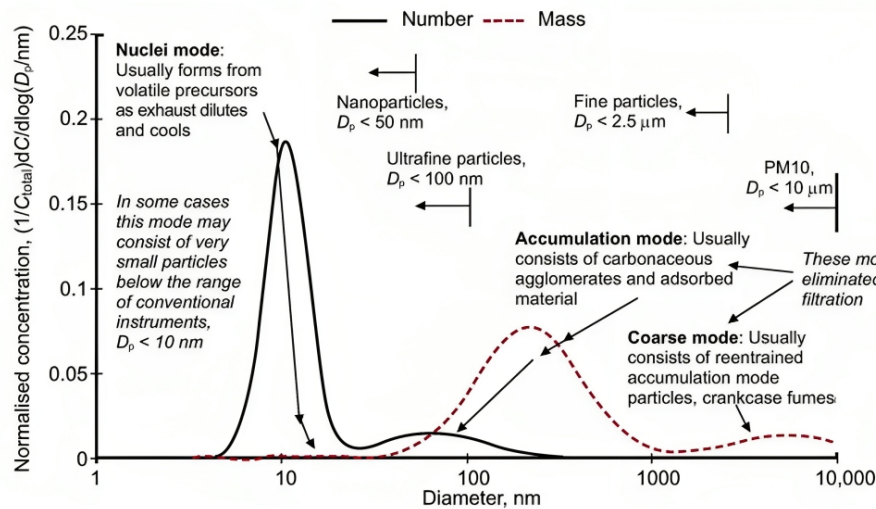


Fig. 2.15 Typical trends for PN number and mass density as a function of equivalent droplet diameters [93].

A schematic representation of the three modes is provided in Figure 2.16. It is evident the volatile nature of the nucleation mode and how this state creates layers above the mainly carbonaceous solid state.

Sampling PN is a non-trivial practice due to the volatile nature of the highest concentration mode, the nanoscale of the particles and other uncertainties related to the engine characteristics. It requires expensive equipment and well-trained operators. The sampling point of the exhaust stream, the engine characteristics and operating conditions as well as

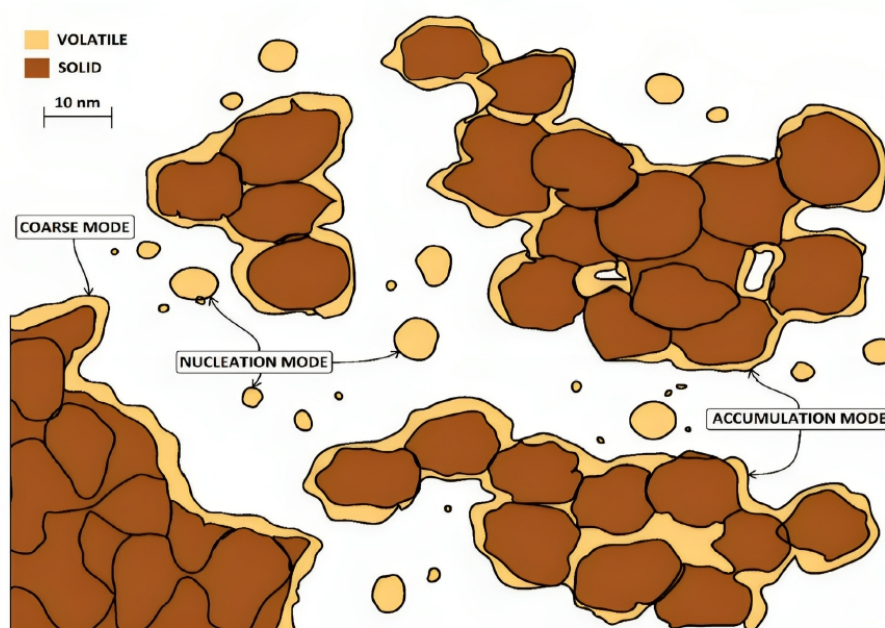


Fig. 2.16 Schematic representation of the main PN modes [86].

the dilution and temperature of the sampling line, all affect the measurement of PN numbers and characteristics [80, 94]. For example, the dilution of the exhaust gas necessary for PN sampling inevitably creates condensation and adsorption phenomena of the volatiles with the consequent creation of new non-volatile compounds [80]. Other phenomena such as diffusion, thermophoresis, agglomeration and electrophoresis directly influence the formation of solid components [80, 94]. Consequently, PN measurements and conclusions in literature are sometimes in conflict [63, 39]. As suggested in [95], a way to improve the repeatability and precision of engine-out measurements is to locate the sampling point in the proximity of the exhaust valves.

2.5 Fuel Properties and Their Influence on In-Cylinder Phenomena

The thermo-physical and chemical properties of the fuel directly influence mixture quality, combustion characteristics and emissions. Commercial gasoline is a blend of many hydrocarbons. The precise composition is directly correlated to the initial oil used, the production methodology and environmental conditions. Considering typical gasoline for ICE applications, the bulk is usually formed by a relatively homogeneous mixture of lightweight

hydrocarbons, e.g., C_4 - C_{12} . A simplified description of fuel composition can be obtained through chemical *HC* groups as follow:

- *Aromatics/Olefins*: both groups produce advantages in terms of knock resistance and combustion rapidity with clear benefits in terms of thermal efficiency. On the other hand, these chemical groups have been demonstrably associated with an increase in NO_x , CO and PN emissions when increasing their percentage in fuel blends [96, 97].
- *Naphthenes*: they are used to produce high-octane gasoline [98].
- *Oxygenates*: these are added to improve combustion characteristics and reduce emissions. For example, ethanol proportions have beneficial effects on thermal and volumetric efficiency and mitigate carbon emissions [99].
- *Paraffins*: also known as saturated alkanes, their structure and percentage content have a direct effect on thermal efficiency as well as on CO , HC and NO_x emissions [100].

Roque et al. [101] investigated the impact of fuel film properties on evaporation rate and soot production. The experiments were performed on a hot plate reproducing realistic engine conditions. Figure 2.17 shows the evaporation of light (hexane and isooctane, left column) and heavy components (dodecane, right column) for a LF deposit at different plate temperatures. Region of interest (ROI) 1 was the region nearest the injection point. It is evident how light components vaporise at a lower temperature in comparison with heavy components. This increases the percentage of heavy components in the film with a direct effect on soot production. For both types of components, the maximum evaporation is not obtained at the maximum plate temperature (200 °C) because of faster evaporation not captured by the selected time window, and because of interactions between components that modified the saturation curve of the fuel reducing the boiling temperature of heavier components. A greater quantity of soot is produced at 80 °C and 120 °C due to film thickness, fuel composition, and fuel interaction with the entrainment flows generated by the combustion. At the highest temperature, the reduced quantity of fuel film reduces the pool fire intensity and hence the soot formed.

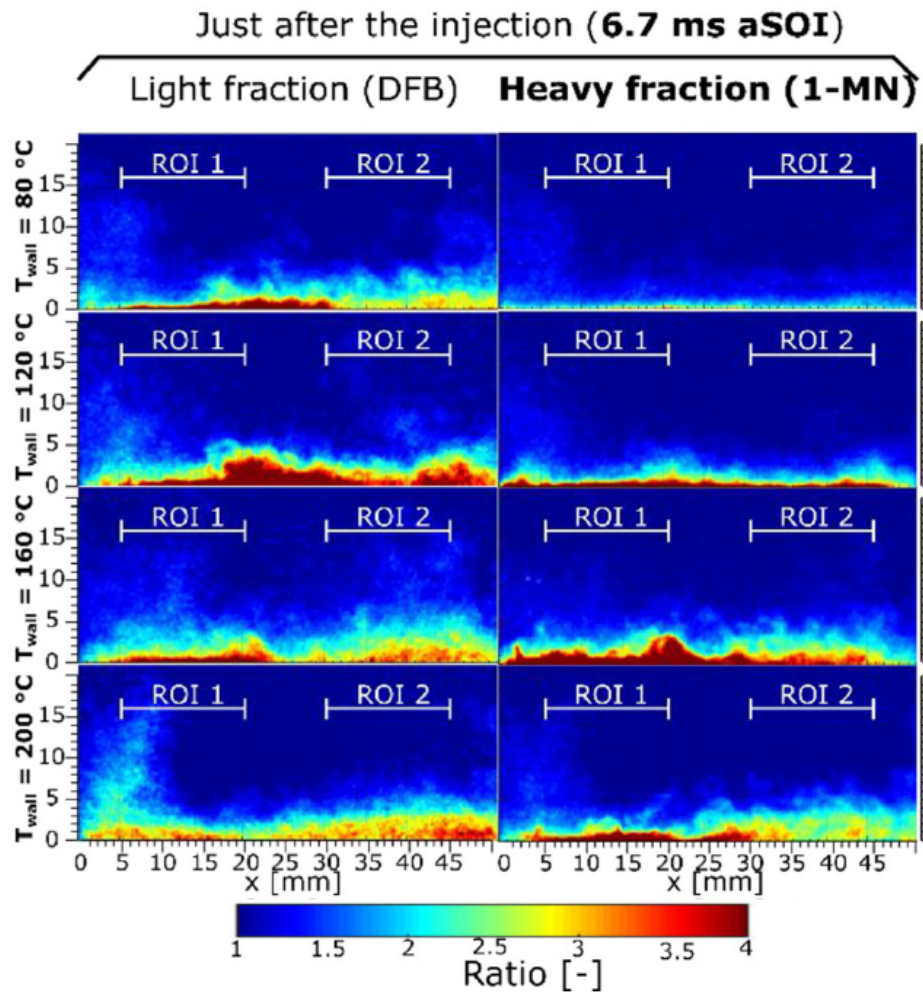


Fig. 2.17 Evaporation of light (left column) and heavy (right column) components on a plate at different temperatures. The ratio is obtained by comparing the images with evaporation and the reference images with no injection [101].

Numerous CFD investigations over-simplify the fuel characteristics using single component models, e.g., N-Heptane and Isooctane [102, 103, 75]. The simplification drastically reduces the computational time but deteriorates the possibility of accurately predicting the LF formation and its retention, the pool fire and generally all the phenomena that rely on a precise distinction between heavy and light fuel components. Basic surrogate models have been developed recently to determine a trade-off between computational power and simulation accuracy [104, 105, 28]:

- Primary Reference Fuel (PRF): a mixture of n-heptane and isooctane
- Toluene Reference Fuel (TRF): a mixture of n-heptane, isooctane and toluene

While PRF and TRF have demonstrated good prediction performance of the combustion phase, they are unable to accurately replicate the non-reacting phases of spray, air-fuel mixing and fuel-to-wall interactions [106]. More complex surrogate fuel models, that integrate a great variety of light and heavy components, are hence essential if the aim is to use the digital model to explore the engine behaviour outside the experimental dataset available [107].

Even if not accurate to model in-cylinder phenomena, isooctane can be used in the initial state of the model development to calibrate the fuel spray external characteristics, i.e., penetration and morphology [108]. Lucchini et al. [109] used optical experimental results to calibrate isooctane spray penetration and morphology in a GDI engine varying the injection pressure between 100 and 200 bar. As concluded by the authors, a more refined investigation of the Leidenfrost effect and refinements of fuel components are mandatory to better understand the spray impingement on walls. Similarly, Habchi et al. [102] used isooctane to determine the importance of piston temperature in predicting the fuel film deposit. The authors found that more than 20% of fuel injected was retained as a liquid deposit on the piston crown while complete evaporation was obtained when the piston temperature exceeded a threshold temperature. The latter was an average between the boiling and the Leidenfrost temperatures of the fuel.

Jiao et al. [80] investigated the effect of fuel composition on the mixture preparation process and soot formation indicating how the boiling curve heavily influences the spray process, the wall film deposit and the combustion characteristics. Light components, vaporising earlier during the spray, tend to distribute around the spray plumes. On the other hand, low-volatile components influence the life of the wall deposits and the related emissions. A multi-component fuel (39 species and 184 reactions) model replicated the gasoline used in the experimental campaign. The surrogate included n-heptane, iso-octane, toluene and PAH. The authors used a discrete multi-component (DMC) fuel vaporisation model where several components were selected to replicate both the thermo-physical and chemical properties of the real fuel. The flame vicinity to LF accelerated the evaporation with the consequent formation of rich regions. While the lack of oxygen mitigated the oxidation, pyrolysis can occur due to the high temperatures involved. Radicals, e.g., H atoms, accelerate pyrolysis with the subsequent formation of soot particles in hot fuel-rich regions.

Following a TRF fuel approach with 109 species and 543 reactions, Wang et al. [104] carried out a sensitivity analysis to identify the main reactions that lead to PAH formation. The toluene content unrealistically enhanced the mixture formation and soot oxidation resulting in an underestimation of soot prediction.

Sciortino et al. [28] used a method where TRF was treated as a mono-component fuel by the CFD code, optimised to reflect the Lower Heating Value (LHV), aromatic content

and the Research Octane Number (RON) of commercial gasoline. The thermophysical properties of liquid and gas phases were assumed to be temperature-dependent, and NIST tables were used to estimate these properties. The method revealed the importance of the mixture preparation in determining PN emissions but was limited in regard to the complex vaporisation phenomena of liquid deposits.

2.6 Modern Trends in Calibration and Implementation of Spray Break-up Phenomenological Models

Fundamental characteristics of fuel spray such as droplet dimension, distribution and overall morphology are mainly influenced by 1. atomiser geometry; 2. ambient condition in which the spray evolves and 3. Thermo-physical properties of the fuel [110]. A fuel stream is atomised when the kinetic energy produces instabilities or disturbances [110] that grow until the break-up occurs with the formation of small droplets. While the viscosity of the fuel and hence the surface tension are responsible for the delay of the break-up, turbulence and aerodynamic phenomena have the opposite effect promoting the formation of small droplets. Figure 2.18 describes the fuel injection for a diesel, multi-hole, injector where instabilities grow inside the nozzle due to cavitation and turbulence in the liquid stream. Similarly for gasoline, liquid ligaments and big droplets are formed at the nozzle exit [111] and the entire initial region is involved in what is called primary break-up [112]. The secondary break-up takes place further away from the injector nozzle and is due to pressure instability, producing a region with a great variety of droplet dimensions [113, 36].

The tip of the spray plume is characterised by a high concentration of fuel vapour [57]. In fact, in this region, droplet disintegration is mainly governed by evaporation. Depending on injection characteristics and wall distances, spray-to-wall impingement may create a liquid deposit with detrimental consequences for the emission levels, as described above.

The most used break-up models for GDI applications are the Reitz-Diwakar (RD) and the Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) models. A detailed description of these models is presented in Chapter 3. Some authors discuss the importance of modelling the internal flow of the nozzle [114] to accurately predict spray evolution. Others prefer a simpler and computationally lighter approach imposing a droplet size distribution at the nozzle exit [28, 1]. Internal flow simulations require a detailed mesh sensitivity analysis, the validation of internal flow phenomena and the accurate internal geometry of the injector. On the contrary, a droplet distribution imposed at nozzle exit requires a more refined calibration of break-up constant. Whichever methodology is chosen, it is important to underline the need

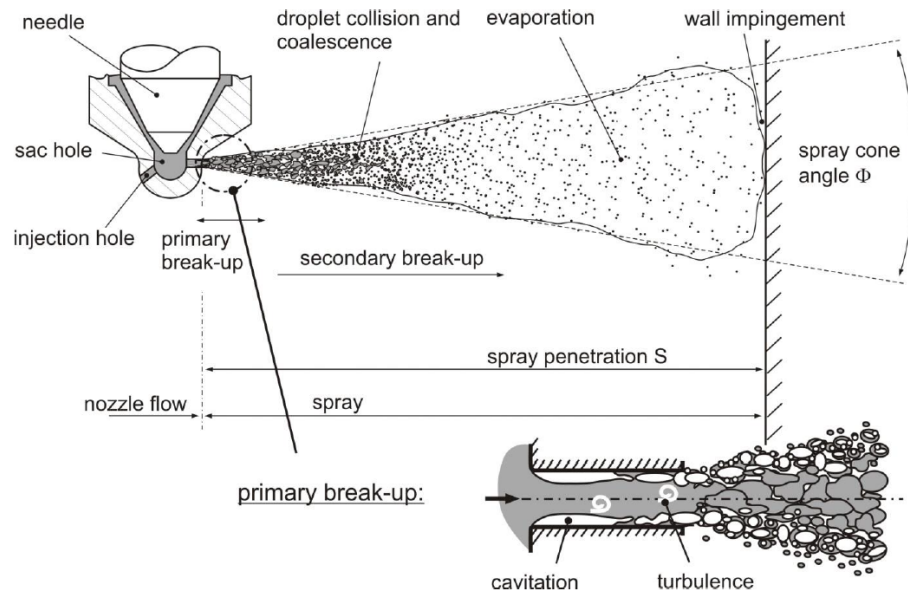


Fig. 2.18 Direct injection fuel schematic [111].

for coherent calibration and validation of the models to correctly predict the characteristics of the spray.

In a study by Wang et al. [115], the performance comparison of RD and KH-RT models was presented as prediction capabilities of a high-pressure isooctane spray from an outward-opening injector in a quiescent vessel. The models were calibrated using three levels of the most influential calibration factors, and the initial droplet size distribution was provided by the Rosin-Rammler (RR) equation with fixed calibration factors for all cases studied. The RD model outperformed the KH-RT model, as one set of calibration factors was able to capture the real injector behaviour for the two vessel back-pressures investigated. The KH-RT model had an abnormal central flow motion and stronger break-up that led to an inaccurate spray penetration and morphology.

In a similar study by Braga et al. [116], the KH-RT instability model was used to predict the high-pressure injection of ethanol from a 7-hole injector. The authors used a similar calibration methodology found in [115] selecting four levels for each calibration factor and analyzing their effect on spray characteristics. A validation analysis was performed using spray experimental data. The RT droplet diameter break-up factor and KH break-up time were found to be the parameters that most influenced spray Sauter Mean Diameter (SMD), penetration, and morphology, highlighting the importance of fuel droplet size in improving the prediction performance of the model.

Ho Teng [117] used empirical equations from experimental fuel Mass Flow Rate (MFR) profiles to mimic the spray characteristics from a GDI multi-hole injector. The droplet

size distribution for a fully spatial developed spray (i.e., EOI) was obtained from an RR cumulative function that allowed the prediction of SMD and droplet diameter corresponding to a particular volume fraction. Increasing the injection pressure resulted in a shift of the cumulative curve towards smaller diameters due to enhanced atomisation.

Costa et al. [12] applied a statistical approach to calibrate spray models for GDI engine applications. An initial droplet distribution located in proximity to the nozzles was reproduced by means of a log-normal Probability Distribution Function (PDF). The latter was influenced by fuel properties and ambient conditions. The model tuning parameters were the variance of the PDF and the break-up time. The calibration was performed through a DoE space where the tuning parameters were optimised reducing the error with the experimental spray penetration at different injection pressures. Results highlighted how the pressure strongly affect the initial droplet size distribution and in particular how an increase in injection pressure result in a narrower distribution.

Perini et al. [56] performed calibration and optimisation of a spray model able to predict diesel spray behaviour. The 3D model was a combination of a blob injection and a KH-RT to reproduce the droplet break-up. Six tuning factors were selected from the KH-RT break-up model and the sub-grid developed in the nozzle region. Five objective functions, all related to spray characteristics, were designed to perform a multi-objective optimisation able to minimise the error between numerical and experimental quantities. The optimisation methods relied on a Non-dominated Sorting Genetic Algorithm II (NSGA-II). Interestingly, the Pareto front study indicated that both liquid and vapour penetrations were accurately predicted with analogous values of calibration factors. The sensitivity analysis of the calibration constants was performed against the objective functions but not against the spray characteristics.

For example, in [118] a linear relation was presented between the time scale of the secondary break-up and the chamber equivalence ratio confirming the fundamental relation between spray modelling factors and spray characteristics, i.e., spray penetration and droplet dimensions.

2.7 Summary

1. The spray-guided configuration of injection in a GDI engine provides the best engine performance and reduces emission levels in comparison with other injection configurations. Theoretical homogenous charge or stratified charge can be produced with reduced quantities of LF. However, FRP and SOI must be tuned appropriately, depending on the specific operating conditions to avoid the creation of fuel-rich pockets within the mixture at spark timing, and mitigate film deposits

2. Air-fuel mixture properties and PN emissions are dependent quantities. When a relatively high level of mixture inhomogeneity occurs, the consequence is an increase in PN formation. How the fuel is distributed within the combustion chamber (stratification, liquid deposit and/or residual droplets) heavily influences the creation of localized sub-stoichiometric regions that are likely to trigger the particles' nucleation.
3. CFD analysis can be used to accurately predict in-cylinder phenomena and better understand the connections between pre-combustion properties and PN emissions. Detailed modelling of the fuel composition and wall conditions is mandatory. Single component or PRF/TRF can be used when reproducing the combustion phase and the spray external properties, but they are unable to accurately replicate the non-reacting phases of spray, air-fuel mixing and fuel-to-wall interactions. More complex surrogate models, that integrate a great variety of light and heavy components, must be used to replicate the complexity of air-fuel mixing and fuel-to-wall interaction.
4. UIs cannot entirely describe the mixture distribution and homogeneity. To correlate pre-combustion phenomena to PN emissions, the focus should be given to fuel atomisation, distribution and interactions with walls.
5. Since mixture properties depend on engine parameters, it is fundamental to understand the most influential parameters to control the mixture and in turn the PN levels. Based on this literature review, the fuel type, FRP and wall temperatures have the greatest impact on PN emissions.
6. Most of the soot produced during combustion is oxidised before the end of the combustion. The oxidation drastically reduces particle dimensions. Consequently, around 70% of particles are emitted in the 5–23 nm size range. The very high frequencies in the sub-23 nm range expose the limitations of the EU6d emission regulations which do not consider particles below this threshold.
7. A direct correlation exists between the fuel film thickness and PN emissions. When the fuel liquid deposit is formed, the evaporation of light components produces sub-stoichiometric regions while heavy components persist in liquid form facilitating the conditions for pool fire to occur.
8. Spray break-up phenomenological models rely on the tuning of several calibration factors to replicate the experimental counterpart. KH-RT and RD are the most used models, often in combination with a RR initial distribution that heavily reduces the computational time avoiding modelling the phenomena inside the injector's nozzles.

The calibration of these models can be done with advanced statistical and optimisation techniques, but these might yield physically implausible quantities.

This study focuses firstly on the requirement for a systematic spray calibration methodology that produces physically plausible calibration constants. The scope is to evaluate the relation between calibration constants and spray characteristics through the application of advanced statistical and optimization methodologies. Secondly, a diverse array of mixture indicators, contingent on both temporal and spatial parameters, is employed to discern the relations between mixture properties and PN emissions. In contrast to prior works that confined their analyses to visual comparisons, this project adopts a more stringent approach, relying on an advanced regression technique. The resultant PN surrogate model demonstrates a solid level of performance, successfully predicting the intricate PN experimental emissions with a minimal set of computationally derived mixture characteristics.

Chapter 3

Models Implementation

The first step to implementing the numerical model of the fuel spray within the combustion chamber is an accurate description and understanding of the equations and calibration constants involved. Experimental spray characteristics are traditionally analysed first within a quiescent volume to easily capture quantities like spray tip penetration, orientation, droplet dimensions and plume morphology. The exact replication of these characteristics through the tuning of models' constants might ensure the correct estimation of post-injection phenomena that influence the engine performance, e.g., mixture preparation, combustion phase and engine-out exhaust composition. The interaction between spray plumes and solid walls requires further ad-hoc modelling that includes the dynamics and thermodynamics of the droplets impacting on a surface, the surface characteristics and ultimately a balanced setup that covers a wide range of operating conditions. The set of equations is solved by the CFD code within a mesh domain. An analysis of the mesh for both the quiescent volume and the combustion chamber, together with the solving methods adopted, is presented in this chapter. The CFD work focused on the air exchange, fuel spray and mixture preparation stages of the engine cycle.

A description of the engine operating conditions investigated is reported together with the mixture characteristics used to draw the correlations with PN experimental emissions. A large number of operating conditions were investigated with the aim of improving the statistical robustness of the PN surrogate model proposed in this study. The model was developed through a range of part-load operating conditions and single-variable sweeps where control parameters such as the start of injection and injection pressure are varied in isolation. Eventually, a multi-component surrogate fuel blend model is presented and used to reproduce the relevant characteristics of the E5 95RON gasoline used in parallel experiments.

The general methodology is complex and formed by several models. As a result, the author suggests first reading through Figure 3.22 on page 81 and then following the detailed description provided in this chapter and Chapter 4.

3.1 Quiescent Volume Reproduction

The injector investigated in this study is a modern, high-pressure, Continental 5-hole GDI injector. The maximum rated injection pressure is 300 bar. The higher pressures facilitate the fuel spray atomisation hence the charge mixture [108]. However, the injection strategy should be tuned to avoid spray-to-wall interactions and consequently the formation of liquid deposits [60].

The tip view of the nozzle and a schematic representation are shown in Figure 3.1. In the representation, S_ϑ is the circular distance between two consecutive holes, D_i is the diameter of a hole (180 μm for this injector), R is the distance between the centre of the hole and the centre of the injector and ϑ is the angle between the centre of two consecutive holes. Since this injector has a $S_\vartheta/D_i > 3.5$ (i.e., wide-hole configuration), the interactions between spray plumes during injections are limited preventing the phenomena of flash boiling [119].

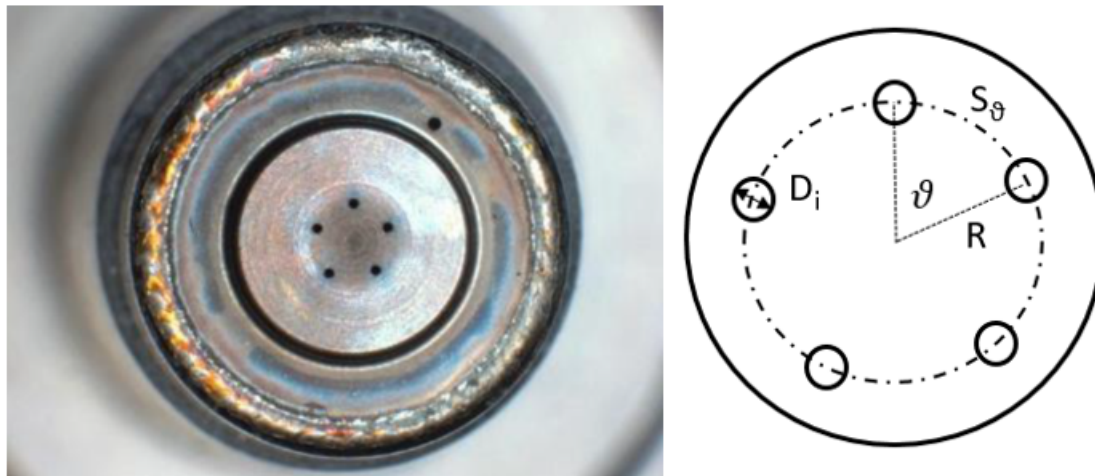


Fig. 3.1 Tip view of the Continental 5-hole injector (left) and a schematic representation (right) [1].

The experimental test campaign for this injector analysis was carried out by Ford Vehicle Evaluation & Verification Powertrain and Fuel Subsystem Laboratory, USA. A detailed account of the test setup and experimental methodology is beyond the scope of this study that instead is focused on the development of the digital counterpart. The type of data shared by the lab were aligned to what similar studies use to characterise the fuel spray

process [60, 120, 116]. Moreover, several details cannot be disclosed due to confidentiality as requested by Ford. As a result, only a brief description is conducted. The data were recorded from four different experiments and served to characterise the spray process:

1. Spray pattern visualization test
2. High-speed imaging test
3. Laser diffraction droplet size test
4. Fuel MFR test

For all the tests, an N-heptane fuel was used as recommended by SAE J2715 practice [121]. N-heptane has similar properties in comparison with isooctane but it is less volatile making it safer to be used for experimental testing. Nitrogen was used instead of air for imaging acquisition tests to improve the signal-to-noise ratio. Test 1 and 2 served to understand the injection direction and plume morphology from each hole. In particular, test 1 used a digital camera pointed to a calligraphy paper. The injector, mounted on top of the paper at 50 mm, was activated at a pressure of 35 bar with a certain pulse width and the footprint was captured by the camera. The images provided a top view of the spray pattern.

The spray penetration length was obtained from test 2 where an imaging chamber (two optical access) was used to capture the propagation of the spray plumes in comparison with reference measuring labels. The test was repeated sweeping the injection pressure from 50 to 200 bar at 50 bar intervals and one bar back-pressure. Test 3 used a laser beam through two of the five plumes on a plane at 50 mm down the nozzle and a rapid data acquisition system to measure the droplet dimensions and in particular Dv_{10} , SMD and Dv_{90} . These three reference diameters describe the percentages (10%, 32% and 90%) of droplets, within the overall distribution, with diameters equal to or below that reference value. While more reference planes would have produced a more comprehensive characterisation, the use of a single reference plane at a certain distance is a common practice [1]. If increasing the distance between the reference plane and the nozzle might introduce inaccuracy in determining the droplet dimensions, the higher pixel density in the proximity of the nozzles means that imaging post-process is possible only at a certain distance [121].

Test 4 was done in a constant volume chamber and the fuel flow was acquired through a Coriolis flowmeter. To reduce the errors, averaged results of several shots at different pulse widths were used to obtain precise MFRs for the same range of injection pressure utilised in test 2.

Siemens Simcenter STAR-CD CFD package v4.32 was used to develop the fuel spray digital model and correlate the numerical results with the experimental counterparts¹. A coupled Lagrangian/Eulerian framework was selected following similar studies [57, 122]. In this framework, discretized droplets (fuel) enter the computational domain formed by a continuous matter (nitrogen) and are solved by means of RANS equations. The $k-\epsilon$ Re-Normalisation Group (RNG) turbulence model predicted the complex interactions between the two fluids. This sub-model is generally a good trade-off between accuracy and computational power [123, 1]. The discretised fluid domain (mesh) and the related flow characteristics were treated by means of the multi-dimensional second-order Monotone Advection and Reconstruction Scheme (MARS) [1]. The numerical time-step Pressure-Implicit with the Splitting of Operators (PISO) algorithm was used to solve the momentum-pressure and the discretised equations [124].

Regarding the Lagrangian phase, parcels of droplets with identical thermo-physical properties were treated assuming no interactions among them and between plumes and the wall domain. These simplifications were possible by deactivating the collision sub-model, which did not improve the spray pattern sufficiently to justify the extra computational time required, and the LF model. In fact, to reproduce the test environment where spray penetration data were collected (test 2) the wall domain was sufficiently far away from spray plumes to avoid any contact and indirect influence. Since the injector is a wide-hole configuration which mitigates flash boiling [119], the related sub-model was deactivated. In [119], the authors found experimentally almost no spray cone interactions and hence collapsing for the ratio $S_g/D_i > 3.5$. In this project, the injector has $S_g/D_i = 5$. Thermo-physical properties of the droplets (liquid) and gaseous components within the computational domain were treated as temperature-dependent from the NIST tables [125].

During the fuel spray event, three main components interact constantly: liquid fuel, fuel vapour and ambient matter. The nature of the injection process influences the spray characteristics, and these can be grouped into external and internal parameters [117]. For example, droplet dimensions and distribution are classified as internal parameters, while spray penetration and plume morphology as external parameters. Accurate predictions of both internal and external parameters are essential to developing a spray digital model and correctly reproducing the air-fuel mixture formation [117, 60].

In order to reproduce the test chamber of test 2, a quiescent/constant cylindrical volume was designed and meshed. The geometry had a bottom-pressure boundary and a wide wall configuration to mitigate the influence of the computational boundaries on the spray process.

¹The methodology presented in section 3.1, continued in Chapter 4, section 4.1 and 4.2, and the related results presented in Chapter 5, section 5.1 – 5.4, led to a publication [1].

The five holes, reproducing the tip of the injector, were positioned at the top of the vessel, in a central position as can be seen in Figure 3.2. Four levels of mesh refinement were used to reach a good balance between spray prediction accuracy and computational time. Table 3.1 presents the main features of the vessel. A total of 800,000 cells were used. The numbers strictly depend on the level of mesh refinement. In particular, the base mesh size was 3.5 mm, while the refinement was 0.5 mm in the proximity of the nozzle. This region is the most difficult to predict because of the higher velocity of the droplets and the level of uncertainty of experimental values making difficult the calibration process [113]. Moreover, the 0.5 mm value corresponds to the level of refinement typically used in the injector region of a GDI engine CFD model [124, 1].

The routines available in STAR-CD to quickly create a fuel spray case and post-process the outcomes were not sufficient to quickly obtain the numerical values that mimic the experimental setup and hence new subroutines were designed to calculate the spray penetration length and the droplet size distribution at every time step on a plane 50 mm down the nozzle.

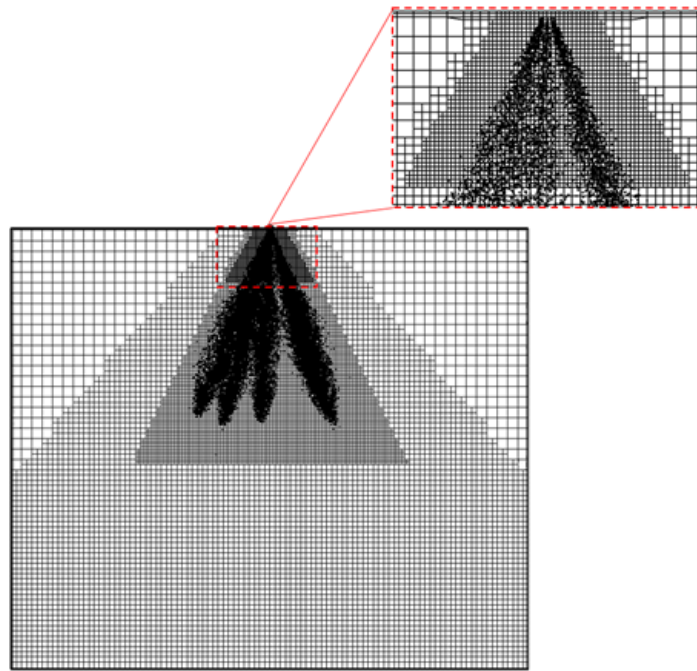


Fig. 3.2 Quiescent vessel cross-section with four levels of mesh refinements and zoom-in on the nozzle exit location [1].

A comparison between the experimental and the reconstructed MFR profiles is presented in Figure 3.3 for three injection pressures. Even though the software can handle the real profiles, the use of simplified/trapezoid MFRs simplified the setup of each simulation and reduced the computational time without losing the prediction accuracy. Each simplified

Table 3.1 Setup and characteristics of the 3D model of the quiescent vessel [1].

Parameter	Value/Setting
Vessel dimension	D = 200 mm, L = 170 mm
Mesh refinement	3.5, 2, 1, 0.5 mm
Number of cells	800,000
Bottom face	Pressure boundary
Top face plus side walls	Adiabatic
Back-pressure (absolute)	1 bar
Vessel temperature	293 K
Vessel fluid	Nitrogen
Physical run-time	2 ms

profile was optimised to match the area of the real counterpart (i.e., the total mass injected) and the opening/closing ramps. The initial velocity of each droplet injected depends on the slope of the opening ramp and hence the accuracy in reproducing this slope is fundamental to predict both internal and external spray parameters.

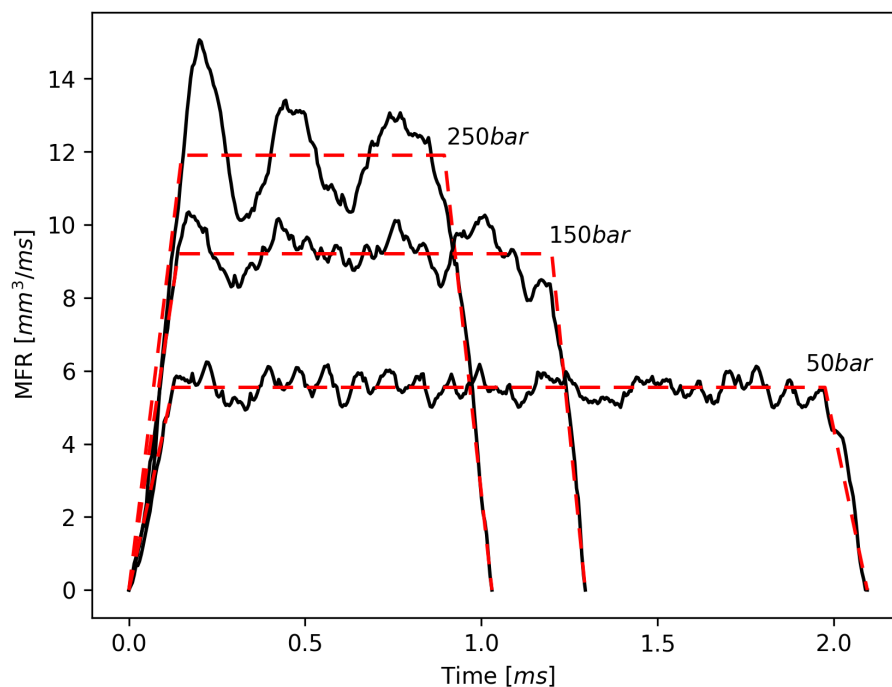


Fig. 3.3 MFR profiles for three injection pressures (50, 150 and 250 bar). Black lines represent the experimental data while red dashed lines are the reconstructed profiles used in the spray simulations [1].

While slight differences might exist between each hole in terms of MFR, the available experimental data provided by Ford were an average of the five holes and hence this was imposed as the MFR of each hole in the simulation. To account for the effect of vena contracta at the nozzle, a discharge coefficient as a function of the injection pressure, was obtained from the Bernoulli equation [126]. The coefficient is applied to each hole's geometrical diameter reducing the dimension to an effective dimension. In particular, the change was from 132 to 128 μm going from 50 to 250 bar FRP.

The proposed approach did not investigate the internal flow of the nozzle and instead utilized a predetermined droplet distribution that then was atomised following the most used break-up models. Despite the potential decrease in the overall spray model's generality, the significant reduction in computational time can serve as a valid justification for adopting this approach, as supported by similar studies [113, 115]. If the internal flow was considered, an accurate representation of the injector's internal geometry and validation of difficult-to-obtain internal flow characteristics would have been necessary. In particular for the internal flow, the calibration of cavitation and vena contract phenomena. In terms of the final results of the spray model proposed in this study, if the internal flow had been implemented and if the aforementioned requirements had been satisfied, a marginal improvement in the prediction performance was expected.

The phenomenological models used within the fuel spray framework rely on the fine-tuning of calibration constants to accurately predict the experimental counterpart. A detailed analysis of the related equations is fundamental to understanding the correlations between these constants and the numerical responses. The following analysis was done by the author and extrapolated from [1].

The RR cumulative function, Equation 3.1, was selected to characterize both the initial droplet distribution at the nozzle exits within the CFD model and the experimental spray droplet size distribution on a reference plane 50 mm down the nozzle:

$$Q = 1 - e^{-\left(\frac{D}{X}\right)^q} \quad (3.1)$$

In Equation 3.1, Q is the total volume fraction of droplets with a diameter up to D ; X and q are model calibration factors. For D equal to X , Q takes the value 0.632 and hence X represents the reference diameter for which 63.2% of the total liquid volume exists as droplets with a diameter smaller than X . The exponent q indicates the spread of size distribution, with narrower distribution for greater values. Despite this function not being able to describe multi-modal distributions, the RR model has been proven to consistently predict the droplet size distribution of GDI injectors [127]. The SMD can be obtained as a function of X and q [117], where the latter is defined as an argument of the gamma function Γ , as follows:

$$SMD = \frac{X}{\Gamma\left(1 - \frac{1}{q}\right)} \quad (3.2)$$

Combining Equation 3.1 and Equation 3.2:

$$\frac{D}{SMD} = -[\ln(1 - Q)]^{\frac{1}{q}} \Gamma\left(1 - \frac{1}{q}\right) \quad (3.3)$$

Equation 3.3 is of a general nature, being able to correlate different volume fractions for a given droplet distribution. This permits the evaluation of the distribution spread. For example, for $Q = 0.9 \rightarrow D = D_{v90}$ and knowing the ratio between the latter and SMD it is possible to obtain q . The same equation can be used to obtain D_{v10} .

The SMD is a crucial spray parameter. It is often convenient to represent SMD using a continuous probability density function (PDF), which summarises the droplet distribution [117, 110]. Knowing X and q , the PDF is obtained from Equation 3.1 as the numerical derivative of Q with respect to D :

$$\left(\frac{dQ}{dD}\right)_i = \frac{Q_{i+1} - Q_{i-1}}{D_{i+1} - D_{i-1}} \quad (3.4)$$

The equations from Equation 3.2 to Equation 3.4 were used to reconstruct the droplet distribution from experimental spray on a plane 50 mm down the injector.

Starting from the RR initial drop distribution, parcel/parent droplets are introduced in the 3D domain. To recreate the spray atomization process, parent droplet break-up occurs due to forces produced by their interactions with the continuous gas phase. The resulting instabilities generate child droplets that can be predicted, as for the RR, with phenomenological constant-sensitive models. The two most common break-up models for GDI applications have been analysed in this work: KH-RT [122] and RD break-up models [128]. The KH-RT is a hybrid model formed by the combination of two sub-models, both based on instabilities growing within the liquid-gas interface. For the KH model, the instability is generated by aerodynamic forces. The RT model, instead, predicts the break-up as a result of droplet deceleration and density difference between the two involved fluids. For each parcel injected, the two models evaluate the break-up simultaneously, with the faster dominating over the slower and hence used as a break-up mechanism at each time step. Both KH and RT models depend on two calibration constants each, that influence the child droplet dimension and the break-up time rate. Equation 3.5 and Equation 3.6 indicate the diameter of the child droplet D_{KH} and break-up time τ_{KH} for the KH model, respectively:

$$D_{KH} = 2B_0\lambda_{KH} \quad (3.5)$$

$$\tau_{KH} = \frac{3.726B_1D_{KH}}{2\lambda_{KH}\omega_{KH}} \quad (3.6)$$

In these equations, λ_{KH} is the instability wavelength, ω_{KH} is the growth rate of the fastest-growing wave and B_0 and B_1 are the calibration factors. When the parent droplet assumes a radius equal to the perturbation wavelength, the break-up will produce a new parent and a child droplet. B_1 depends on turbulence and/or cavitation phenomena within the injector and has a strong effect on fuel spray evolution [129]. The RT model has a similar structure, both in terms of equation form and calibration factors. Equation 3.7 and Equation 3.8 represent the diameter D_{RT} of the child droplet and break-up time τ_{RT} for the RT model, respectively:

$$D_{RT} = C_3\lambda_{RT} \quad (3.7)$$

$$\tau_{RT} = \frac{C_t}{\omega_{RT}} \quad (3.8)$$

In these equations, C_3 and C_t are the calibration factors.

The RD model [128, 124] predicts the break-up based on two mechanisms: ‘bag break-up’, due to pressure instability and expansion of the droplet towards lower pressure regions, with subsequent separation of the child droplet; and ‘stripping break-up’, which produces the child droplet by means of a shearing process from the parent droplet surface. The following equations outline the role of each break-up mechanism and their correlation with calibration factors. The Weber number threshold value for bag break-up is:

$$We \equiv \frac{\rho|u - u_d|^2 D_d}{2\sigma_d} \geq C_{b1} \quad (3.9)$$

where u and ρ are the gas velocity vector and density, respectively; D_d is the droplet diameter, σ_d the surface tension and u_d the velocity vector. C_{b1} is a tuning parameter; if the droplet Weber number is smaller or equal to C_{b1} , then the droplet is stable; otherwise, a break-up will take place. The characteristic break-up time rate τ_b is related to the same parameters as follows:

$$\tau_b = \frac{C_{b2}\rho_d^{1/2}D_d^{3/2}}{4\sigma_d^{1/2}} \quad (3.10)$$

In this equation, C_{b2} is another calibration factor and ρ_d is the droplet density.

The stripping break-up threshold involves the droplet Reynolds number to take account of the dynamic viscosity as follows:

$$\frac{W_e}{\sqrt{Re_d}} \geq C_{s1} \quad (3.11)$$

In this equation, C_{s1} is the tuning parameter with a similar role as C_{b1} . The stripping break-up time rate is given by:

$$\tau_b = \frac{C_{s2}}{2} \left(\frac{\rho_d}{\rho} \right)^{1/2} \frac{D_d}{|u - u_d|} \quad (3.12)$$

where C_{s2} is the fourth calibration factor of the model.

3.2 Fuel-to-Wall Interactions

Fuel-to-wall interaction and fuel deposit vaporization rate are strongly affected by [3]:

1. Wall properties and condition
2. The relative velocity between drops and wall
3. Fuel composition
4. Ambient condition

The evaporation/boiling regimes experienced by the fuel film deposit may be classified as a function of the wall temperature T_w as indicated in Figure 3.4. For T_w above the saturation temperature T_{sat} of the fuel used, three boiling regimes may be defined: nucleate boiling, transition boiling and film boiling. The transaction among the boiling regimes is accompanied by an increase in the dry fraction of the wall [130] that in turn affects the wall-to-liquid heat flux. The latter has a crucial effect on the deposited liquid lifetime and hence it may be used to describe the LF behaviour. The limiting temperatures for the three regimes, i.e., the Nukiyama temperature T_N and the Leidenfrost temperature T_L , are obtained experimentally from the lifetime curve of a liquid droplet deposited on a hot plate as described in [130].

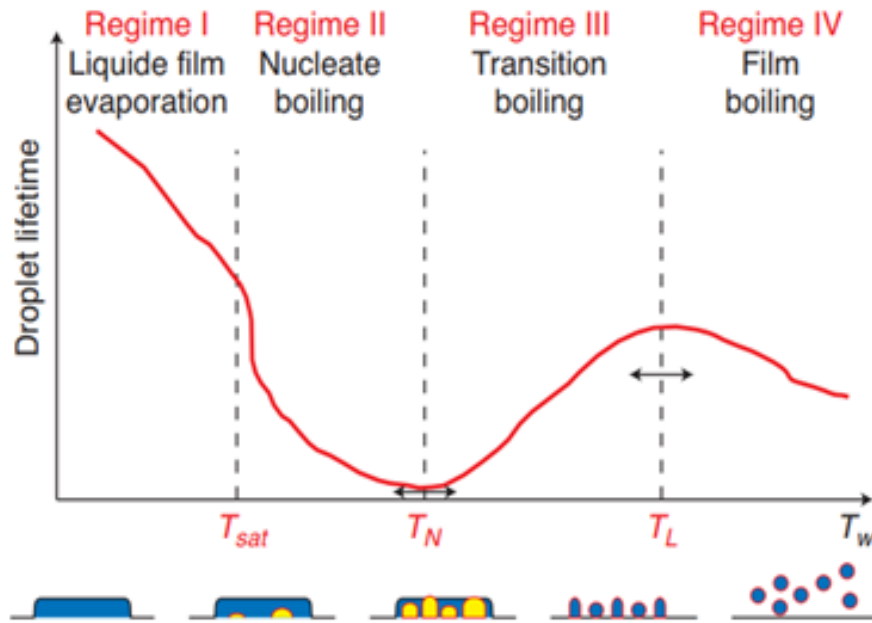


Fig. 3.4 Droplet lifetime deposited on a plate with variable temperature and various regimes [130].

To validate the LF model used in this work, experimental methodologies found in the literature [130, 5, 6] were taken as reference cases. A numerical CFD investigation was conducted using STAR-CD v4.32 reproducing a 3D quiescent vessel with a bottom hot wall. The vessel dimensions were 30x200 cm with mesh size refinement between 3 – 1.5 mm and a total cell count of 170,000. Isooctane was used as fuel to replicate the experimental counterparts. The injector geometry was identical to the one described in the previous section. Calibrated factors were used to reproduce the droplet break-up and to obtain realistic spray behaviours.

Figure 3.5 provides an example of the 3D domain and the impact of the injected fuel on the hot surface. Two sets of simulations were performed:

1. Droplet life analysis on a hotplate. Considering the subsequent ICE implementation of the spray model, instead of reproducing a single droplet, the lowest injection pressure available in this study (50 bar) and the associated calibration were selected to deliver a fuel quantity on the plate. Within the limitations of comparing the behaviour of a single droplet on a hot plate with that of a high-pressure fuel spray after impact, the deposited LF is expected to follow a similar trend as in Figure 3.4 and hence correlate with the physical behaviour experienced in [5]. The test conditions for these numerical simulations are summarised in Table 3.2.
2. LF deposition on a hot plate due to high-pressure fuel injections. The film quantity retained at 5 ms ASOI was evaluated for two injection pressures (150 and 300 bar). The injected quantity was one order of magnitude higher than the previous numerical test and hence more adequate to replicate traditional ICE conditions. The spray model calibration was performed to match the given experimental levels of SMD and D10 of the droplets size distribution at 150 bar, 11 mm and 8 mm respectively. For the 300 bar injection, experimental droplet sizes were not available, but the spray model was altered to reflect the expected enhanced atomisation. The test conditions are described in Table 3.3.

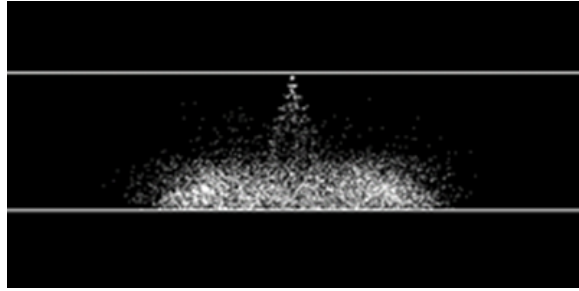


Fig. 3.5 The quiescent vessel was designed to investigate the interactions between the fuel spray and a hot wall (bottom wall).

Table 3.2 Test conditions for the analysis and comparison of the Stanglmaier experimental test where a single droplet is positioned on a hot plate [5].

Parameter	Value
FRP[bar]	50
Fuel injected [mg]	1.5
Injection duration [ms]	0.39
Wall temperature [K]	sweep 370 - 484 K
Fuel temperature [K]	300

Table 3.3 Test conditions for the Schulz analysis [6] of the LF retained on a hot plate injecting fuel at high pressure.

Parameter	Value
FRP[bar]	150, 300
Fuel injected [mg/hole]	3.4
Injection duration [ms]	2.1
Wall temperature [K]	353, 413, 453
Fuel temperature [K]	300

The droplet-to-wall interaction was predicted with the Bai-ONERA model [131, 3]. Considering the thermo-kinetic characteristics of droplets impacting on the surface, the model can predict three possible outcomes, i.e., deposition, splash and rebound. The correct behaviour is obtained as a function of a normalised temperature T^* and a kinematic quantity K . Equation 3.13 and Equation 3.14 define the two quantities where T^* includes T_w , T_N and T_L (temperatures related to the fuel composition and operating conditions) while K is defined as the product between the Weber number We and the Ohnesorge number Oh . The numbers are in turn functions of ρ_d , V_d , D_d , σ_d and μ_d that indicate respectively the droplet density,

volume, diameter, surface tension and viscosity. Figure 3.6 represents the Bai-ONERA model with the three main regions [3]. If deposition occurs, droplets lose all the momentum and form a LF on the surface. In the splash regime, droplets break-up with some of them sticking to the surface and others moving away depending on T^* . In the rebound regime, droplets bounce off from the wall without deposition due to the creation of a vapour layer. For a given fuel, a relatively high K , i.e., fast droplets and/or big diameters, increase the possibility of a splash regime.

$$T^* = \frac{T_w - T_N}{T_L - T_N} \quad (3.13)$$

$$K = We \cdot Oh^{-0.4} = \frac{\rho_d V_d^2 D_d}{\sigma_d} \left(\frac{\mu_d}{(\rho_d D_d \sigma_d)^{0.5}} \right)^{-0.4} \quad (3.14)$$

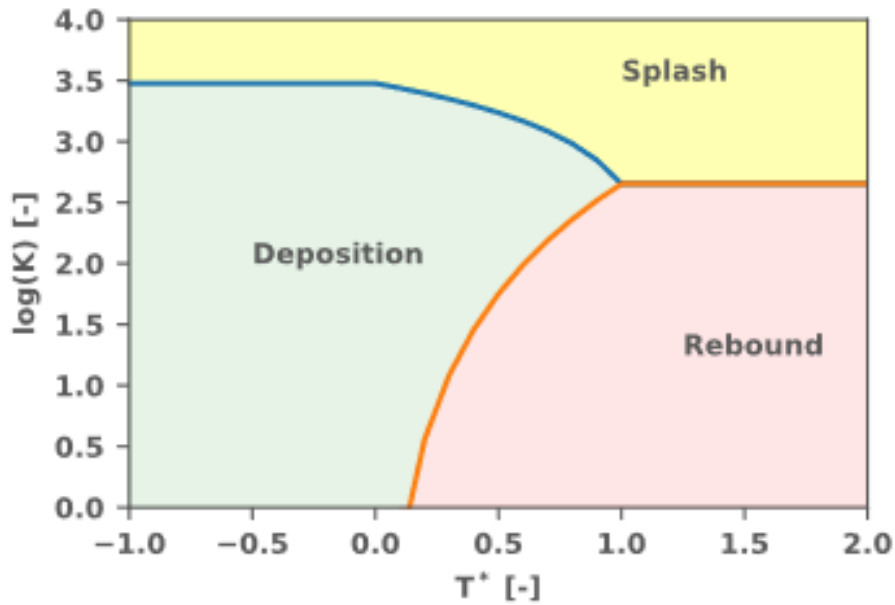


Fig. 3.6 Bai-Onera spray-to-wall impact regimes [3].

Within STAR-CD, once droplets stick to a surface, three main factors can be tuned to reproduce the LF behaviour:

$$T_N = B_s \cdot T_{sat} \quad (3.15)$$

$$T_L = T_{sat} + \Delta T \quad (3.16)$$

$$q_w = f(\rho_g, \rho_f, h_{fg}, \sigma_f, \mu_f, c_{pf}, Pr_f, C_i, T_w) \quad (3.17)$$

Equation 3.15 introduces the factor B_s which multiplies the saturation temperature to yield the T_N of the isooctane used for this investigation. Following [3], a value of 1.1 was selected for this investigation as the best compromise across all operating conditions investigated and used consistently. In fact, the value provided an accurate representation of liquid deposits within the model and results were validated through available experimental data and literature. To implement the T_L , the Habchi model was used [130]. As evident from Equation 3.16, the model uses a ΔT which is the difference between T_L at 1 bar and the boiling temperature of the fuel at normal conditions. Figure 3.7 shows the variation of the T_L as a function of the pressure. The trend follows the T_{sat} and highlights how the temperature limits depend on the ambient conditions at which the fuel is injected. The behaviour highlights a limitation of the software that does not allow the variation of the B_s value while the pressure is changing within the combustion chamber. However, the approximation made and the correct tuning of the parameter might yield consistent and accurate results [3]. A vapour-liquid equilibrium-state model was adopted to model the evaporation from spray droplets and from the deposited LF. Temperature-dependent thermophysical properties from the NIST tables were used for all gaseous and liquid components during the CFD analysis [124]. The wall heat flux was modelled by means of the Angleberger wall function [132].

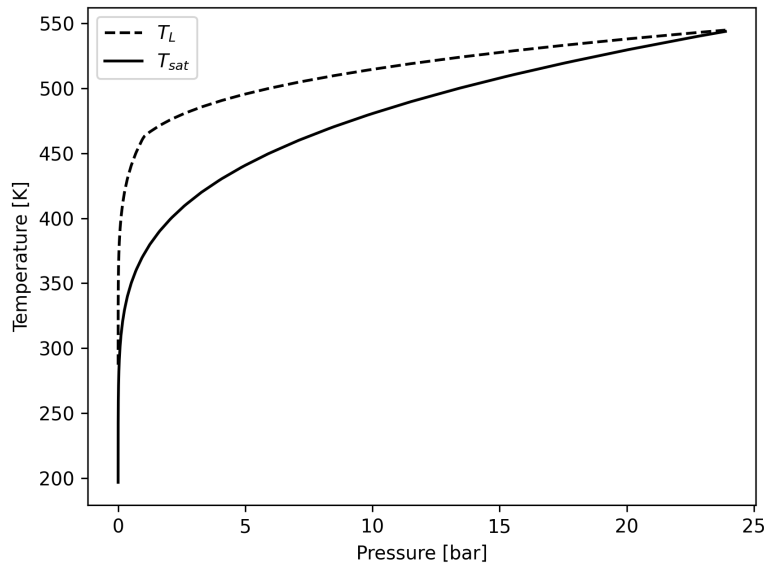


Fig. 3.7 Saturation (T_{sat}) and Leidenfrost (T_L) temperature for isooctane as a function of pressure.

Table 3.4 Boiling parameters and the corresponding values used for isooctane tests.

Boiling Parameter	Value
C_{sf}	0.0014
N	4.11
ΔT_L	90.55
C_s	353, 1.06
C_{max}	0.15
C_{min}	0.09

Equation 3.17 describes the independent variables of the heat flux model. The parameters serve to design the heat flux curve and specify the point at which the different boiling regimes occur. In the equation, ρ_g , ρ_f , h_{fg} , σ_f , μ_f , c_{pf} , Pr_f and C_i are respectively the gas density, the liquid density, latent heat of evaporation, surface tension, viscosity, heat capacity, Prandtl number and the calibration constant to modify the heat flux curve. The latter are C_{sf} and N for the nucleate regime and C_s , $C_{(max/min)}$ for the transition/film regime, as evident from Figure 3.8. The suggested values used for isooctane analysis are reported in Table 3.4. In the figure, it can be noticed how in the nucleate boiling regime the maximum heat flux is achieved. The reduction in the transition regime is due to the creation of bubbles within the film that reduce the heat transfer surface. Minimal values of heat flux exist in the film boiling regime where a vapour cushion between the liquid and the hot wall creates thermal insulation.

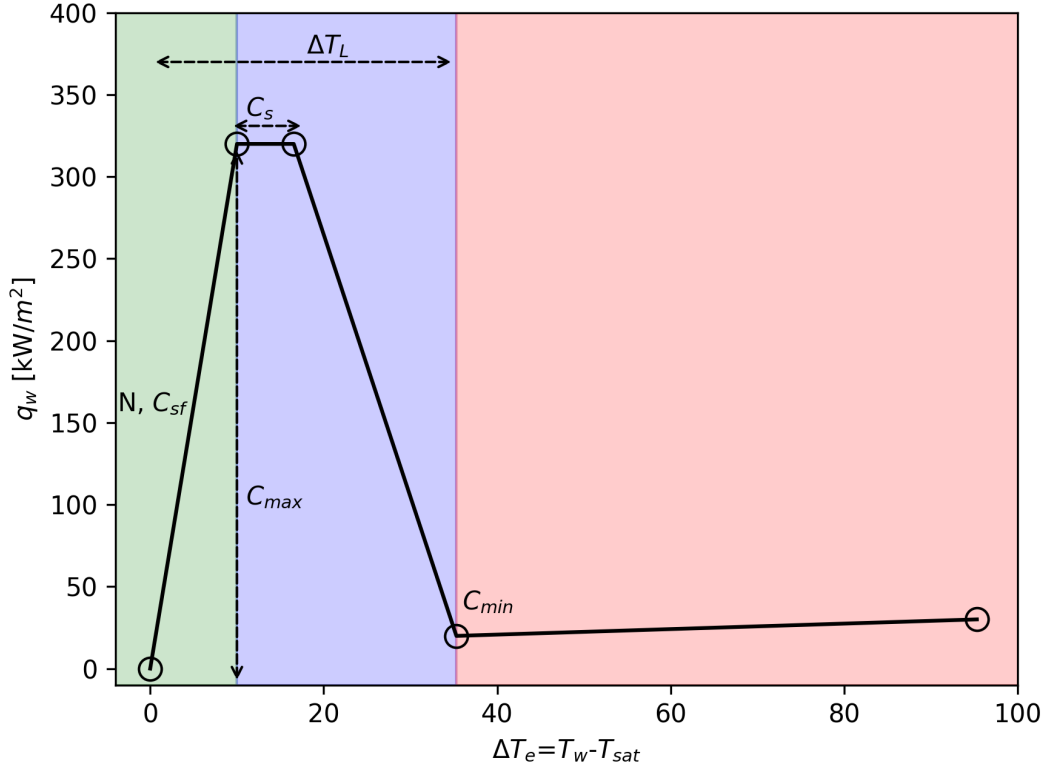


Fig. 3.8 Heat flux model and calibration factors. Highlighted the three regions corresponding to the boiling regimes: nucleate (green), transition (blue) and film (pink).

3.3 In-Cylinder Meshing and Spray Implementation

The in-cylinder CFD analysis of mixture preparation and LF deposition used the Siemens Simcenter software package that included STAR-CCM+ for surface mesh generation from CAD data, ES-ICE for volume mesh and STAR-CD v4.32 for solving. The original CAD of the Fox UG XM, 3-cylinder, GDI engine was provided by Ford Motor Company (for the general technical specs of the engine please refer to [1]). The CAD geometry was analysed and repaired to isolate the fluid domain, as shown in Figure 3.9. To speed up the analysis and reduce the computational costs, only one cylinder was modelled. The method is vastly used in literature because it is considered a reasonable trade-off between the prediction performance of the overall engine and analysis costs [1, 60, 75]. The original geometry had relatively long intake ducts to optimise the engine performance and in particular the volumetric efficiency.

On the other hand, the short exhaust ducts were integrated into the cylinder head to reduce the engine dimension and turbo-lag. The surface repair operations included:

- Liner straightening
- Valve closing
- Geometry re-orientation
- Feature lines
- Surface smoothing
- Open entities filling

The surface re-meshing was done with a base size of 1 mm and a minimum cell size of 0.1 mm. For the volume meshing in ES-ICE, this study adopted a semi-automatic trimming method with hexahedral volume cells and local refinements provided in the proximity of both the injector and spark region. Two cylinders “wrap layers” (0.25mm thick) were implemented to capture the complex behaviour of the crevice flow while a single prism layer (0.3mm thick) was selected for all the remaining surfaces. Figure 3.10 shows the resulting mesh after the aforementioned operations.

A cut through a valve symmetry plane of the initial base mesh is shown in Figure 3.11. It is possible to notice the valves at the close position for which the default valve lift is 0.1 mm. Above this threshold, the valve curtain interface permits mass, momentum, and energy transfer between the cylinder and the intake/exhaust volumes. At the close position, the valve curtain interface is considered an impermeable adiabatic wall [124].

Even if the injector location was provided through the original CAD, accurate analysis of the spray plume directions was necessary to replicate the experimental data available. As shown in Figure 3.12 (left), the plume directions were approximated with 5 cones at a certain orientation and their imprint (middle figure) was calibrated on a plane 50 mm down the injector location (right figure) as obtained in the real counterpart. The correct prediction of spray characteristics is fundamental to understand the complex phenomena involved during the mixing process and fuel-to-wall interactions [60].

Once the initial volume mesh was obtained, a grid sensitivity study was carried out to identify the maximum cell base size which delivers the best trade-off between computational time and accuracy. Simulations for the mesh sensitivity and subsequent post-processing were done by a member of the Engine Modelling Team (EMT) at Oxford Brookes University (OBU) and the final mesh setup was discussed among the team members to have a final mesh

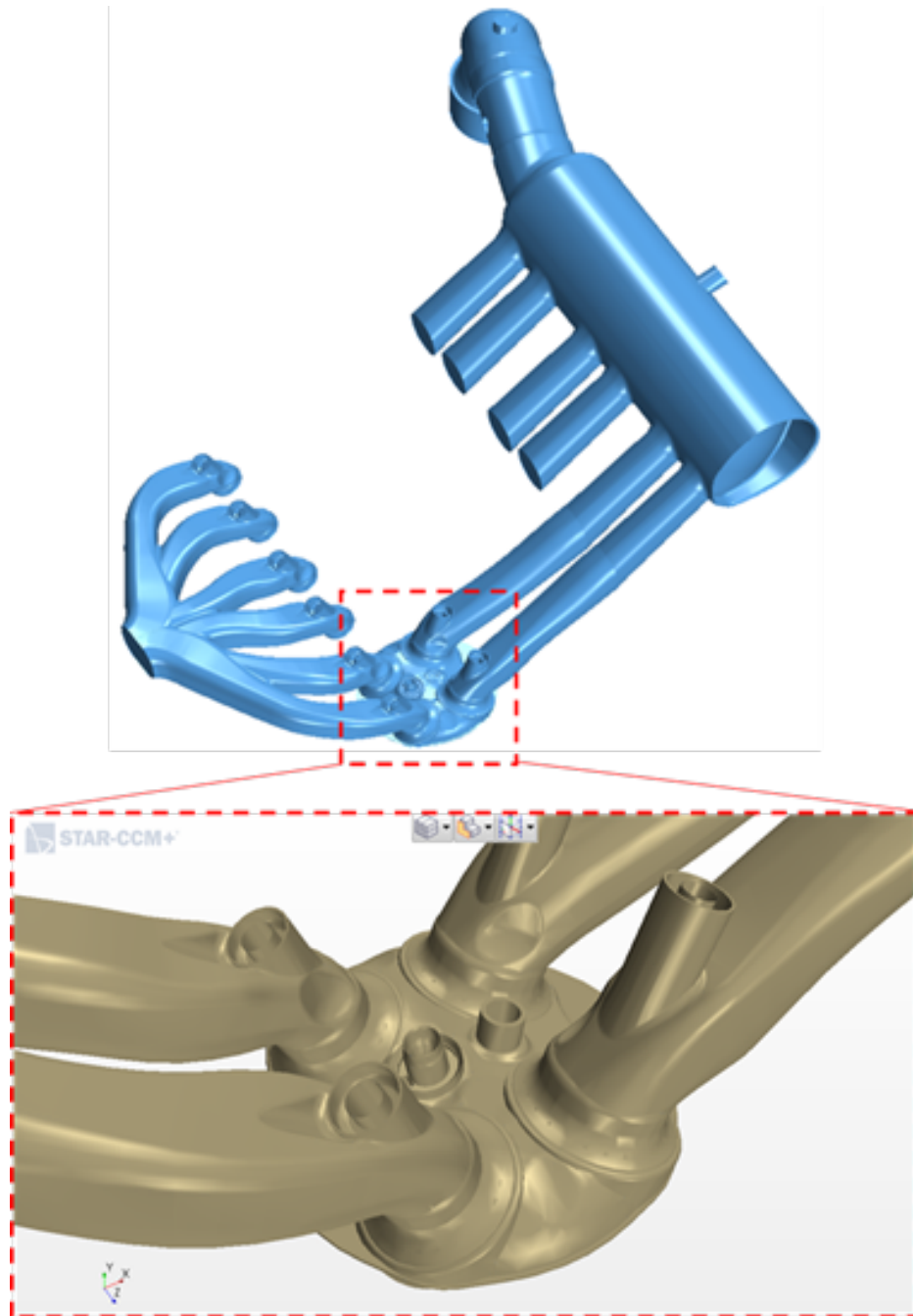


Fig. 3.9 Fluid domain extracted from the original CAD geometry. In detail, cylinder number one with intake and exhaust ducts, the spark plug and the injector.

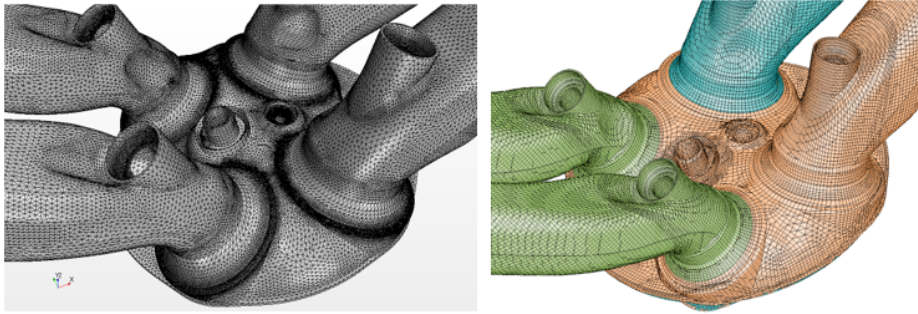


Fig. 3.10 Cylinder surface mesh (left) and trimmed volume mesh (right).

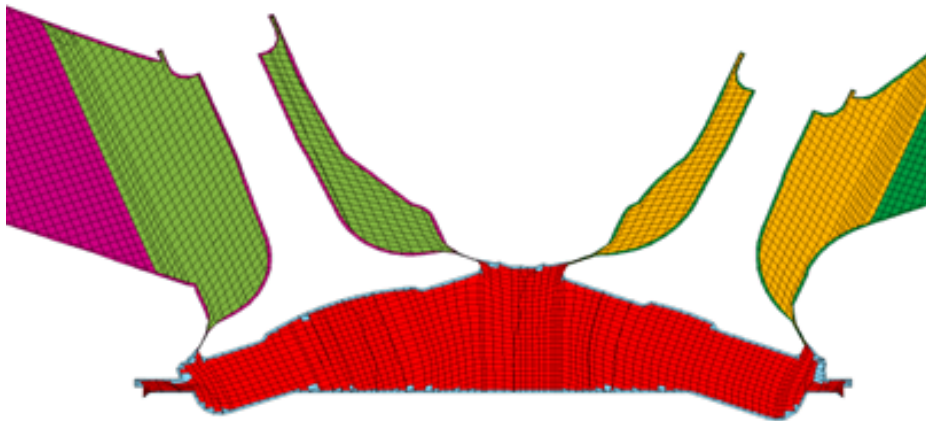


Fig. 3.11 Cut of the cylinder and detail of intake (left) and exhaust (right) ducts.

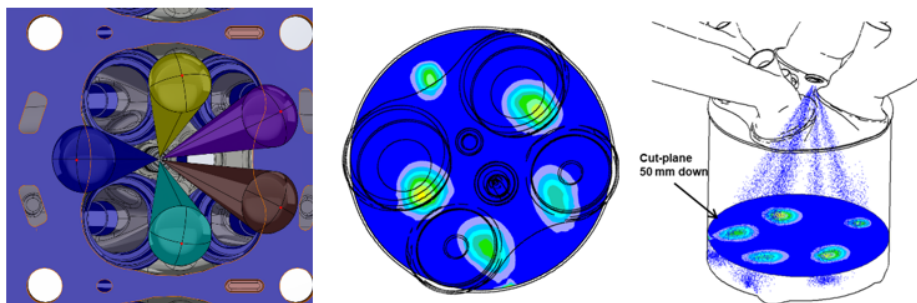


Fig. 3.12 Injector position analysis. Plume orientations (left), plume imprint from cylinder top view (middle) and side view (right).

Table 3.5 Operating condition for the mesh sensitivity analysis.

Parameter	Value
Engine speed [rpm]	5000
MAP [bar]	1
Intake temperature [K]	311
Exhaust pressure [bar]	1.2
IVO [CAD BTDC]	5
EVC [CAD ATDC]	50

that was able to produce accurate results not only in terms of mixture properties but also during combustion and emission production. Three different grids, i.e., 1.15, 1 and 0.85 mm were created and simulations were run using identical cold flow settings. The operating condition selected and the corresponding boundary values are reported in Table 3.5.

Simulation results and post-processing in terms of in-cylinder pressure, mass, turbulence, number of cells and computational time are reported in Figure 3.13. The simulations were performed from 60 CAD after TDC (ATDC) of combustion, i.e., a few degrees before exhaust valve closing (EVC), for one cycle (720 CAD) without combustion and a simplified injection process. The analysis showed that a base size of 1.00 mm could be an acceptable compromise in cold flow conditions as it produced similar values to the 0.85 mm size. The peak pressure value (Figure 3.13-a), the peak tumble location in CAD (Figure 3.13-b), the air trapped (Figure 3.13-d) and the tumble ratio were almost identical despite the consistent reduction of cell count, from 1.2 million to 800 thousand at bottom death centre (BDC), and overall solving time (from 25 hours to 14 hours). However, considering the complications expected from spray and combustion/soot formation (to have a standard mesh among the rest of the OBU research team working on post-spark and post-combustion events), and the computational power available through the project, a base size of 0.85mm was selected. To ensure an accurate prediction of the ballistic region of the spray and correct development of the flame front, a local refinement with half-cell size (0.425mm) was performed in the proximity of the injector and the spark plug as shown in Figure 3.14, yielding a total cell count of 1.42M (million meshes) with the piston at BDC position and 360k with the piston at TDC. With the mentioned settings, the overall computational time to simulate from EVC until ST was, depending on the engine speed selected, around 13 hours with an HPC cluster consisting of 92 cores.

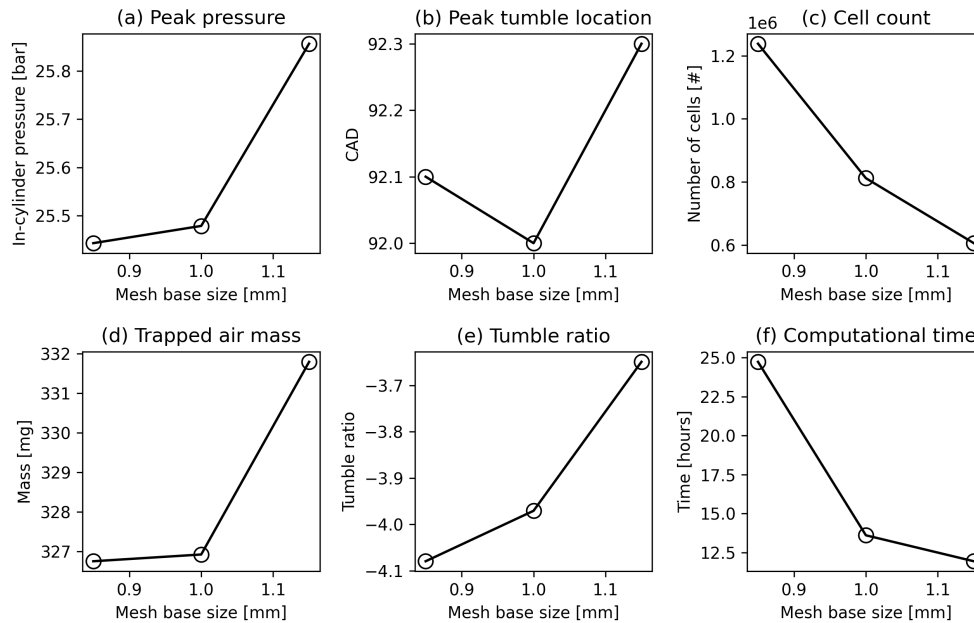


Fig. 3.13 Mesh sensitivity analysis. Three levels of base size mesh (0.85, 1 and 1.15 mm) were tested against the cylinder peak pressure (a), the peak of tumble location in CAD (b), the total number of cells at TDC and BDC (c), the air trapped mass (d), the tumble ratio (e) and the computational time (f) to run an entire engine cycle without combustion.

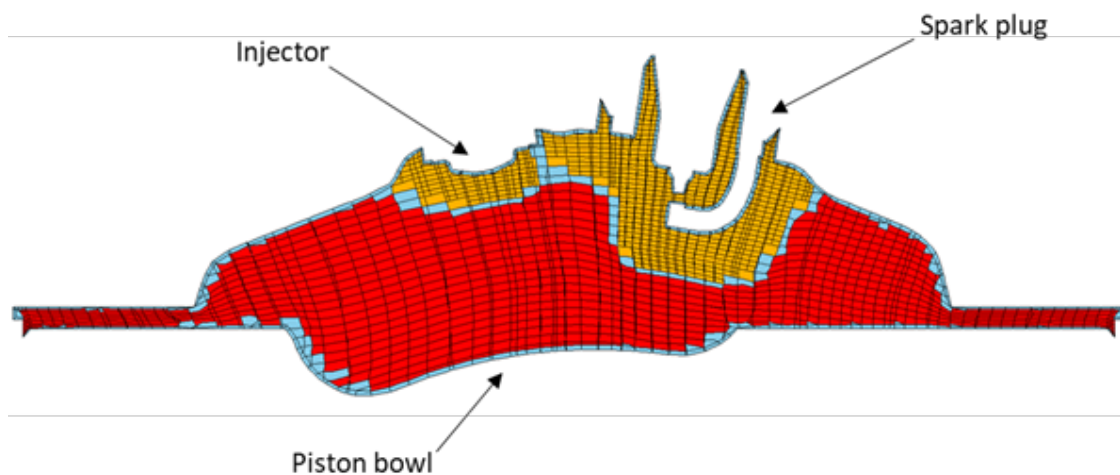


Fig. 3.14 Cylinder cut with mesh refinement in the proximity of the injector nozzle and the spark plug region.

3.4 In-Cylinder Simulation Setup and Mixture Parameters

The boundary conditions were imposed as time-dependent with both temperature and pressure profiles for intake and exhaust runners obtained through validated Ricardo Wave 0D-1D simulations. The post-processed, experimental-based, engine data were passed to a member of the EMT who executed these 0D-1D simulations and shared the results in a database available to all the team members.

Figure 3.15 shows an example of the crank angle resolved boundaries for two operating conditions, low speed and load, and mid-engine speed, high load. The three peaks, more evident in the pressure traces, replicated the fluid dynamics at the intake and exhaust port of the three-cylinder used for parallel experimental tests. In the figures as for the rest of this work, the engine cycle arrangement is such that 360 CAD correspond to the TDC combustion.

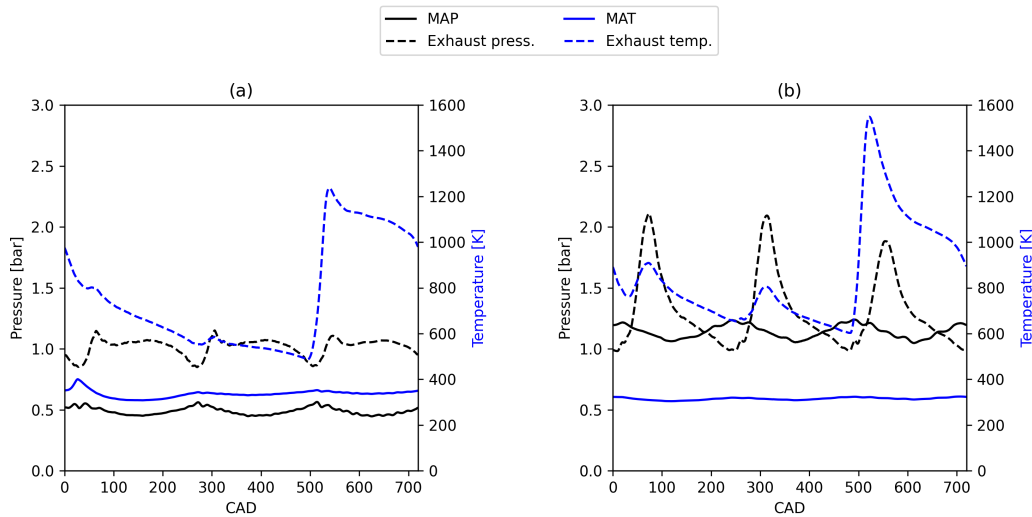


Fig. 3.15 Engine boundaries from the 0D-1D model in terms of air/exhaust pressure and temperature. Only 1500 rpm – 20 Nm (a) and 2500 rpm – 100 Nm (b) are shown for brevity.

Constant region-specific temperature boundary conditions were applied to the walls within the computational domain, with piston crown temperature based on experimental (telemetry) data obtained by installing thermocouples on the piston. These data were generated by previous R&D work of DYNAMO project partners and made available to the consortium. Telemetry data served to construct a wall temperature map as a function of engine speed and load. The engine was equipped with a Piston Cooling Jet (PCJ) system that sprays oil directly into the underside of the piston, in the proximity of the connecting rod, through a dedicated gallery. The system is automatically controlled by a solenoid that follows an operational map. Cooling the piston with lubricant oil with specific strategies is a common technique to control both engine performance and emissions [133], and to ensure structural integrity.

In order to capture the effects of spray impingement and consequent local cooling, the piston surface temperature within the simulations was reduced linearly as a function of SOI timing, with a reduction of 30 K for an early SOI timing equal to 330 CAD BTDC [3]. The values were selected by validating the result with available experimental data, literature and ensuring that the variation of temperature was consistent with the saturation curve of the surrogate fuel blend.

The initial parameter to predict and test the validity of the proposed methodology is the air-trapped mass at Intake Valve Closing (IVC). Compared to experimental data, the model was able to predict the trapped mass with an error consistently below 3% for all the operating conditions analysed. A visual comparison between the experimental and the CFD results of the in-cylinder pressure traces is shown in Figure 3.16. Three different operating conditions, at increasing speed and load, are presented. The CAD window is centred at compression stroke up to ST.

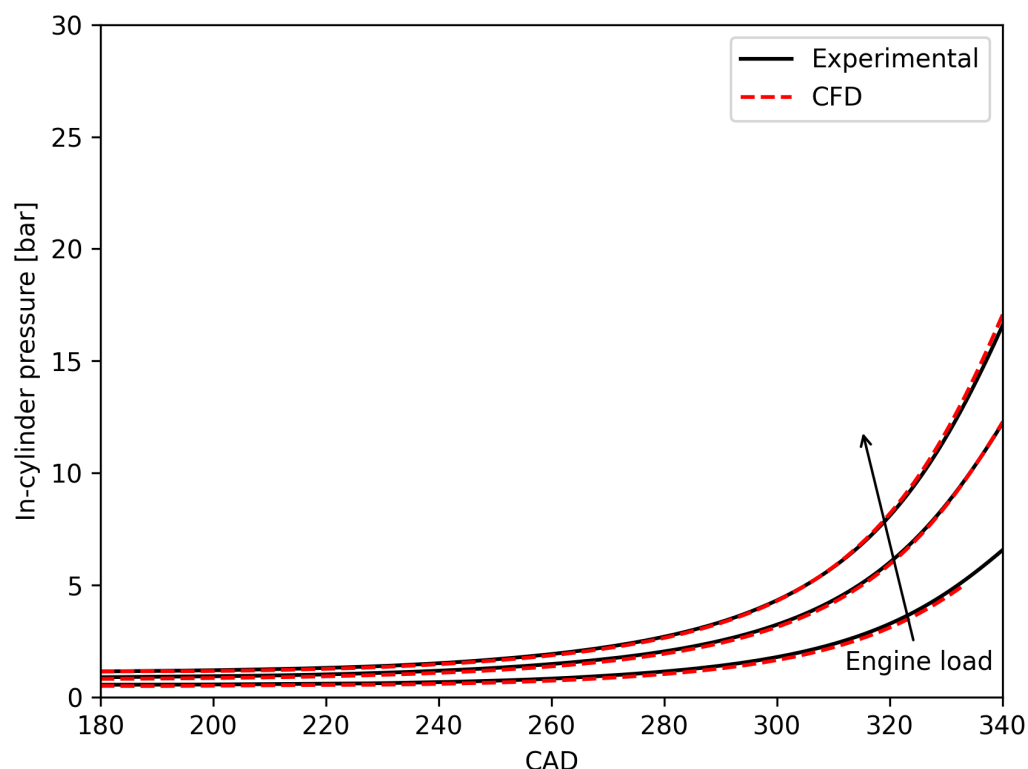


Fig. 3.16 The prediction capability of the CFD model in terms of in-cylinder pressure traces during compression stroke until ST. Only 1500 rpm – 20 Nm, 2167 rpm – 61 Nm and 2500 rpm – 100 Nm are shown for brevity [2].

For the sake of brevity, the results related to other operating conditions are not reported as they exhibited identical levels of correlation. The satisfactory agreement between the numerical and experimental data regarding the engine's overall geometry, trapped mass, and in-cylinder pressure traces established the reliability of the CFD results throughout the entire simulated period (IVO – ST). The engine CFD simulations were conducted remotely, utilizing the HCP cluster facilities at the STFC Hartree Centre. The simulations were performed with a 3-node or 96-core configuration to maximise the computational efficiency and with an average solution time of 36 hours.

For the purpose of this investigation, which aims to perform a regression analysis to correlate PN output to mixture quality characteristics, the CFD simulations were commenced 20 CAD before Intake Valve Opening (IVO) timing and terminated at ST, covering gas exchange and in-cylinder mixing processes. The selection of final stage of the exhaust stroke was selected to guarantee uniform thermodynamic conditions between the cylinder and exhaust ducts, and to fully capture the effect of the valve overlap period [60].

An example of the valve profiles used in the simulation is presented in Figure 3.17. As evident from the figure, the simulation window is centred in the period IVO – ST (350 CAD for the specific operating condition). The reconstructed profiles were based on experimental data and adapted for each operating condition knowing the IVO BTDC and EVC ATDC. Each opening/closing stage was characterised by three reference points: the first is the nominal opening/closing value; the second is the one adopted by the ES-ICE software; the third is the experimental reference.

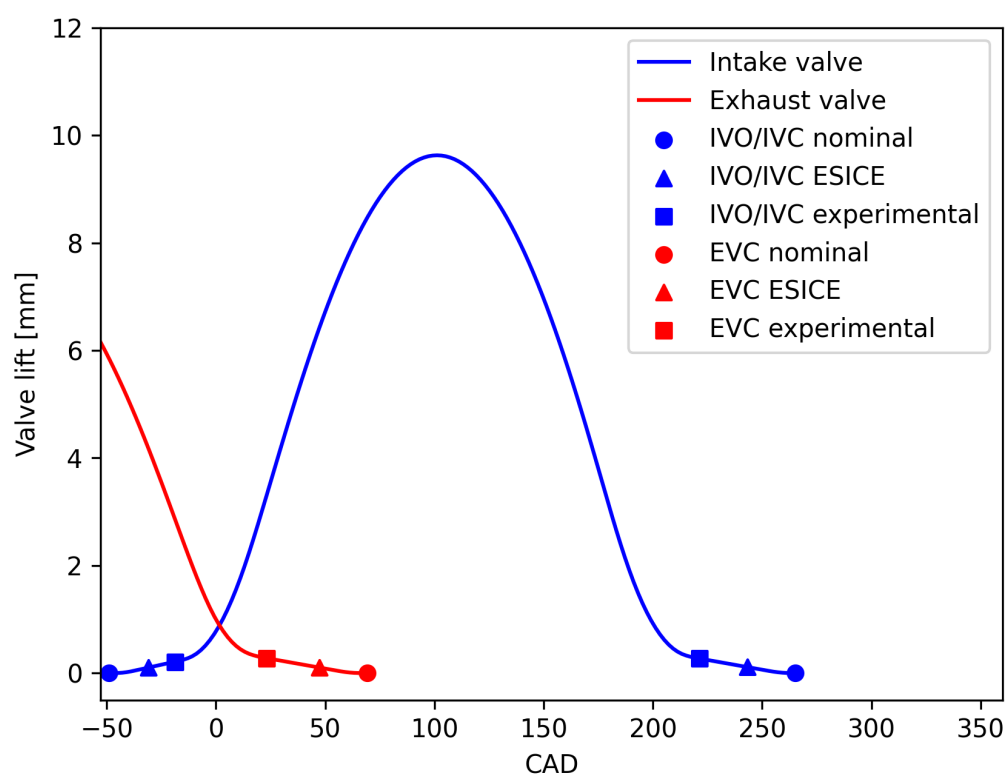


Fig. 3.17 Valve lift profiles with different reference points for the closing/opening stage. The profiles refer to 1500 rpm – 100 Nm operating conditions.

The in-cylinder CFD setup comprised the MARS approach to solve momentum, turbulence and temperature as already seen for the quiescent volume simulations. The density of the fluids was treated by means of the Central Differencing (CD) scheme while turbulence was predicted through the RNG k - ϵ closure approach. The analogy with the quiescent simulations continued with the use of the RANS method as it represents the best trade-off between computational costs and prediction capabilities. In that sense, to increase the model performance during crucial phases of the engine cycle, the time step of the simulations was

dynamically modified between $10\text{e-}5$ and $10\text{e-}6$ s [124, 3]. In fact, the time step was reduced to the minimum threshold during valve movement and fuel injection.

The experimental work, carried out by DYNAMO project partners Loughborough University and Ford Motor Company, and the parallel modelling work covered a wide range of fully warmed, steady-state engine operating conditions, with speeds between 1200 and 3200 rpm and torque between 20 and 114 Nm. For calibration points, engine control strategies in regard to valve timing, SOI, FRP and ST were adjusted during experimental runs to ensure the MBT (Maximum Brake Torque). All the operating conditions were recorded at stoichiometric, theoretical homogeneous, conditions. Figure 3.18 presents the 18 main operating conditions used in this research project on a speed-load space. The red marks indicate the operating conditions where a variable sweep was executed. The sweeps included SOI, FRP and ST. For the FRP sweep the variation of the injection pressure was done from 50 to 200 bar in steps of 50 bar. The SOI sweep ranged between 325 and 180 CAD BTDC, while the ST sweep was done between 15 and -5 CAD BTDC. A total of 34 operating conditions were investigated and details are provided in Table 3.6. Even if a dataset with 34 points seems large from the perspective of similar CFD analysis [60], the operating space was designed by the consortium partners with no attempt to follow a consistent statistical experimental design perspective. As a result, the sparsity of data indicates a bias on the 2000 rpm condition. Ideally, a 34-point Halton sequence [134] could have increased the level of information provided by the design space.

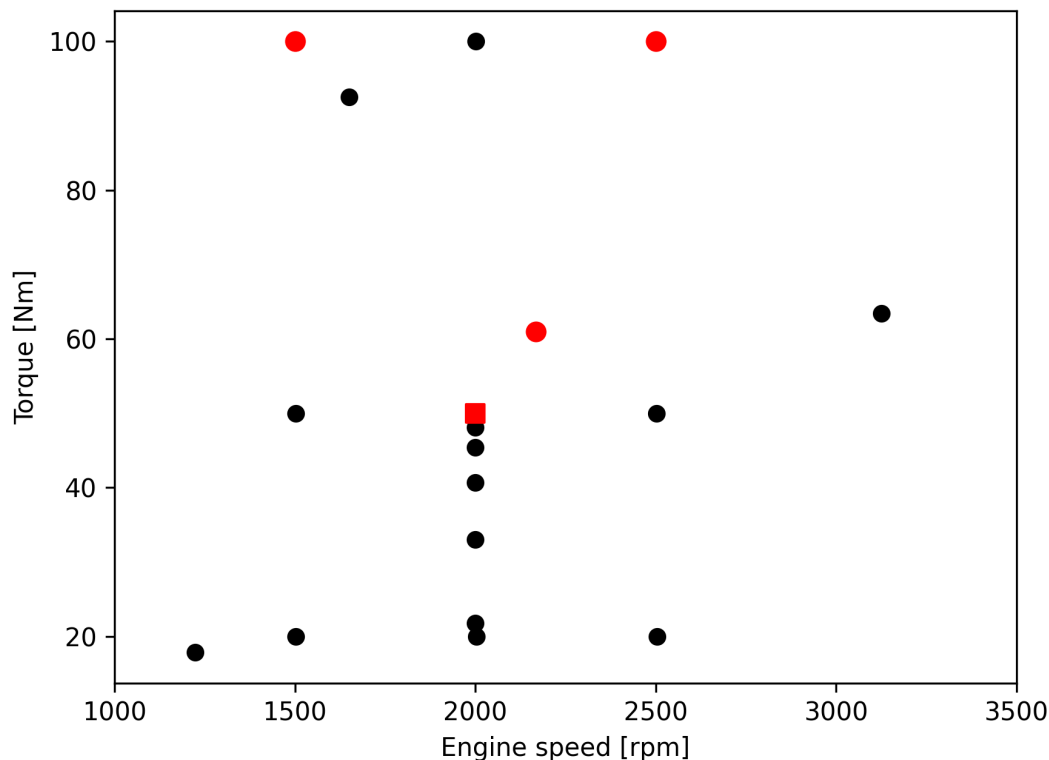


Fig. 3.18 Engine operating conditions available for this study were provided by the consortium partners. The red dots indicate conditions where a FRP sweep is available. The squared marker is the operating condition where a FRP/SOI/ST sweep was performed [2].

As the aim was to carry out a statistical regression analysis on mixture characteristics, a wide range of mixture quality features was obtained from CFD results at different times/locations before the combustion event.

Mixture preparation describes the process of direct fuel injection, fuel vapourisation and consequent mixing with in-cylinder air charge [28]. The experimental quantification of mixture characteristics is difficult. CFD simulations can be exploited to evaluate the quality of the mixture for each cell of the 3D domain. One of the most used indicators of mixture homogeneity is the UI [28]. In this work, the index has been quantified through the calculation of the volume-based UI of the equivalence ratio:

$$UI_{\varphi} = 1 - \left[\frac{1}{V_{tot}} \int \frac{|\varphi - \varphi_{aver}|}{2\varphi_{aver}} dV \right] \quad (3.18)$$

In this equation, the integral is evaluated considering all the cells in the computational domain representing the combustion chamber, knowing both the volume and the equivalence

Table 3.6 Engine operating conditions details. If not specified, the engine parameters are set to calibration values. These cannot be disclosed due to confidentiality as requested by Ford UK.

Case Name	Engine Speed [rpm]	Engine Torque [Nm]	MAP [bar]	Mass of fuel [mg/cycle]	Variable sweep
P1	2167	61	0.88	18.5	FRP 50
P2	2167	61	0.88	18.5	FRP 100
P3	2167	61	0.88	18.5	FRP 150
P4	2167	61	0.88	18.5	FRP 200
P5	1500	100	1.16	31	FRP 50
P6	1500	100	1.16	31	FRP 100
P7	1500	100	1.16	31	FRP 150
P8	1500	100	1.16	31	FRP 200
P9	2000	50	0.87	16	SOI 180
P10	2000	50	0.87	16	SOI 205
P11	2000	50	0.87	16	SOI 235
P12	2000	50	0.87	16	SOI 295
P13	2000	50	0.87	16	SOI 325
P14	2000	33	0.86	16	ST 0
P15	2000	45	0.86	16	ST 10
P16	2000	48	0.86	16	ST 15
P17	2000	40	0.86	16	ST 5
P18	2000	21	0.86	16	ST -5
P19	2000	50	0.86	15	FRP 100
P20	2000	50	0.86	15	FRP 150
P21	2000	50	0.86	15	FRP 200
P22	2500	100	1.14	30	FRP 50
P23	2500	100	1.14	30	FRP 100
P24	2500	100	1.14	30	FRP 150
P25	2500	100	1.14	30	FRP 200
P26	1200	18	0.53	10	-
P27	1650	92	1.07	29	-
P28	3125	63	0.85	19	-
P29	2000	100	1.14	30	-
P30	2500	50	0.83	15	-
P31	1500	20	0.54	10	-
P32	1500	50	0.90	16	-
P33	2000	20	0.50	11	-
P34	2500	20	0.50	10	-

ratio ϕ of each cell. UI is normalised by the total volume of the domain and hence is defined between 0 and 1. The latter represents an ideally perfect homogeneous mixture between air and fuel. Since Star-CD did not include any subroutines to automatically calculate the UI, the calculations were performed offline using the discretised quantity of volume and equivalence ratio [28].

Based on the author's previous experience [28, 3], other mixture properties can be used to define a feature database that can support a detailed statistical regression analysis. The main features are (if not specified the feature was calculated automatically by the software):

- Mixing time, Δt_{mix} [s] – Time interval between the EOI and ST [28].

$$\Delta t_{mix} = t_{ST} - t_{EOI} \quad (3.19)$$

where t is the time converted from the CAD using the specific engine speed (rpm). This function was calculated offline.

- Main tumble coefficient, Y_{origin} [dimensionless] - Rotational motion with an axis normal to the symmetry axis of the cylinder and passing through the centre of the cylinder [124].
- Liquid Film mass, LF_{mass} [kg] - Mass of the liquid portion of the injected fuel deposited on the cylinder walls.
- Liquid Film thickness, LF_{thick} [m] - Thickness of the LF distributed across the whole in-cylinder domain.
- Liquid Spray, LS [kg] - Mass of the liquid droplets of the injected fuel evaluated between SOI and EOI. This function was calculated offline.
- Equivalence ratio, ϕ [dimensionless] – Inverse of the air-to-fuel ratio over the stoichiometric value.
- M^+ [kg] – Sum of the fuel mass within the cell domain with an equivalence ratio above or equal to a certain threshold (x). This function was calculated offline [3].

$$M_x^+ = \sum_{vol} FuelMass_{\phi \geq x} \quad (3.20)$$

Since each of the mixture properties was defined in regard to a discretised 3D domain during an engine cycle, the precise location inside the combustion chamber and other details

considered to evaluate the feature can be modified. For Example, for UI, M^+ and ϕ the mean, maximum, minimum, standard deviation and COV values were evaluated and inserted in the final database. Moreover, location-based properties were introduced to capture, for example, fuel-enriched pockets [28, 3]. Following this methodology, this study counted a total of 100 mixture-related features. Among them, two main groups can be distinguished: one for the liquid fuel parameters and one for gas-phase mixture characteristics. The latter group included features calculated over five zones: whole cylinder, region 0, region 1 (cylindrical annulus), region 2 (cylindrical annulus) and a small spark plug (SP) cylindrical region of 5 mm radius, as shown in Figure 3.19. The aim was to reveal the connection between region-specific mixture quality and PN formation.

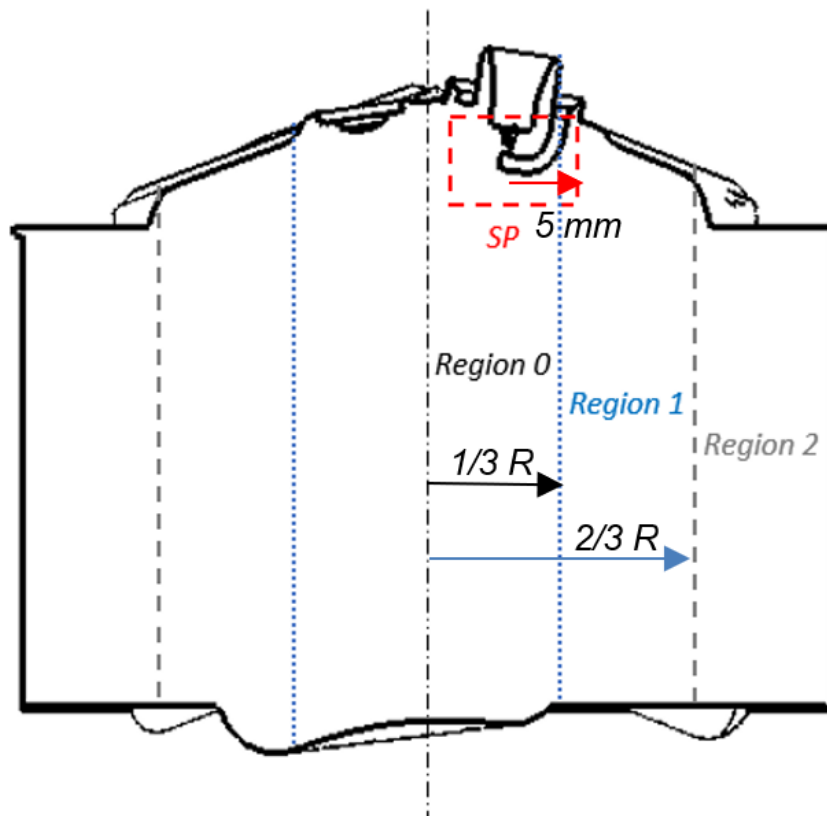


Fig. 3.19 Cross-section of the CFD model representing the combustion chamber. The three regions inside the chamber (concentric to the cylinder's symmetrical axis) are shown plus the cylindrical region that envelops the spark plug [2].

The distinction between liquid and evaporated parameters comes from the analysis of the fuel injection process as presented in Figure 3.20. It can be seen how while fuel evaporation begins at SOI and continues throughout the injection, the liquid spray has a peak at around

the EOI with some fuel deposit on the wall for the highest FRP. As clarified in the following sections, the regression analysis provided the following four most relevant variables from the initial 100-strong features list²:

1. Maximum Liquid Spray, LS_{max} [kg] – Maximum mass of the liquid portion of the injected fuel, which takes place at the EOI.
2. Maximum Film thickness, $LF_{Thickmax}$ [m] – Maximum thickness of the LF distribution across the whole combustion chamber at ST.
3. $M_{1.1SP}^+ = \sum_{SPvol} FuelMass_{\phi \geq 1.1}$ - Computes the mass of evaporated fuel within computational cells showing equivalence ratio $\phi \geq 1.1$ at ST, in region SP.
4. $\phi_{mean-reg2}$ - Mean equivalence ratio at ST computed in region 2.

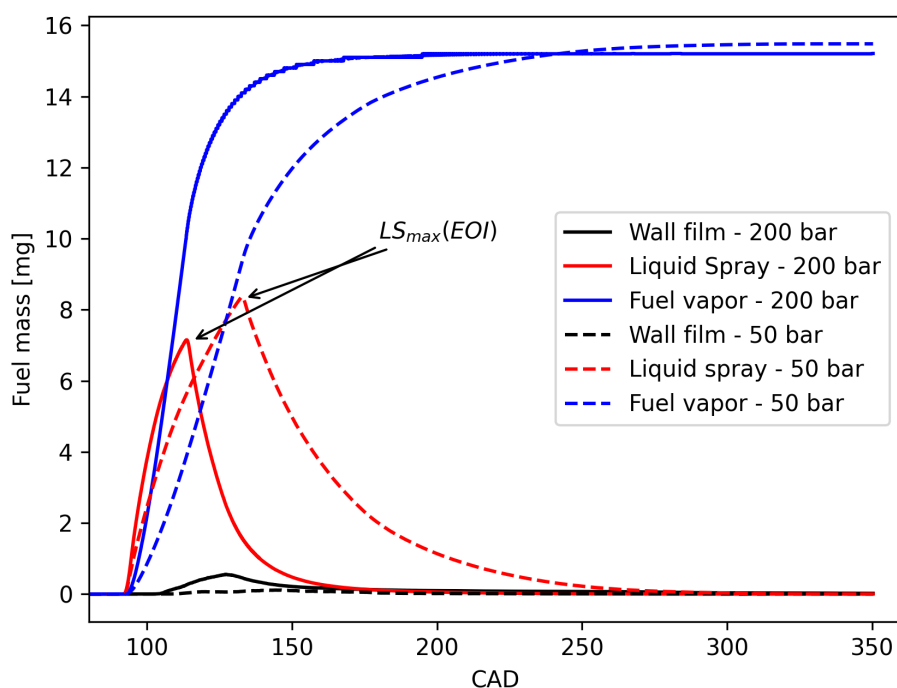


Fig. 3.20 Numerical representation (CFD results) of the fuel spray process as a function of CAD. Two different FRP, 50 and 200 bar, are presented for the same operating condition (2167 rpm – 61 Nm) [2].

²The methodology presented in section 3.4, continued in Chapter 4, section 4.3, and the related results presented in Chapter 7, section 7.1 – 7.3, led to a publication [2].

3.5 Fuel Surrogate Model

For mixture purposes, this work proposes a multi-component fuel blend model developed in parallel research work carried out within the EMT at OBU [3]. The fuel mimics the E5 RON95 gasoline used in the experimental campaign. A detailed hydrogen analysis revealed the hydrocarbon content while the distillation curve was obtained through the ISO 3405 method (European Norm EN 2298). The latter provides the upper and lower limits in which the boiling curve should be kept. Table 3.7 provides the mass fraction of the seven components selected to replicate the real fuel blend. The optimisation was carried out following the distillation curve of the experimental counterpart and maintaining a similar percentage of the main chemical groups. As evident from Figure 3.21, the EMT surrogate reproduced well the distillation curve of the real fuel.

Table 3.7 Composition of the EMT surrogate fuel model [3]..

Fuel Species	Nomenclature	Surrogate mass fraction [%]	Chemical HC group
Pentane	C_5H_{12}	5	Paraffines/ Iso-paraffines/ Naphthenes
Hexane	C_6H_{14}	33.3	
Isooctane	C_8H_{18}	16.9	
Dodecane	$C_{12}H_{26}$	2.2	
Toluene	C_7H_8	20.5	Aromatics/
Mesitylene	C_9H_{12}	16.5	Olefines
Ethanol	C_2H_6O	6.1	Oxygenates

To capture the non-isothermal behaviour of the fuel injection, the initial temperature of the fuel was set with an increment of 20 degrees in comparison with the experimental value. In fact, it is reasonable to think that the vicinity between hot walls and injector nozzles, and the cycling of the injection process, produces an increase in liquid temperature.

To accurately reproduce the LF in the 3D domain, the coefficient B_s from 3.15 (please refer to section 3.2 for more details) needs to be above 1 and below the smallest value of the blend components. Following [3], a value of 1.2 was selected for this investigation as the best compromise across all operating conditions investigated and used consistently.

A vapour-liquid equilibrium-state model was adopted to model evaporation from spray droplets and deposited LF; this was modified through the UNIFAC scheme available in STAR-CD to account for the presence of ethanol in the fuel blend [3, 124]. Temperature-dependent thermophysical properties from the NIST tables were used for all gaseous and

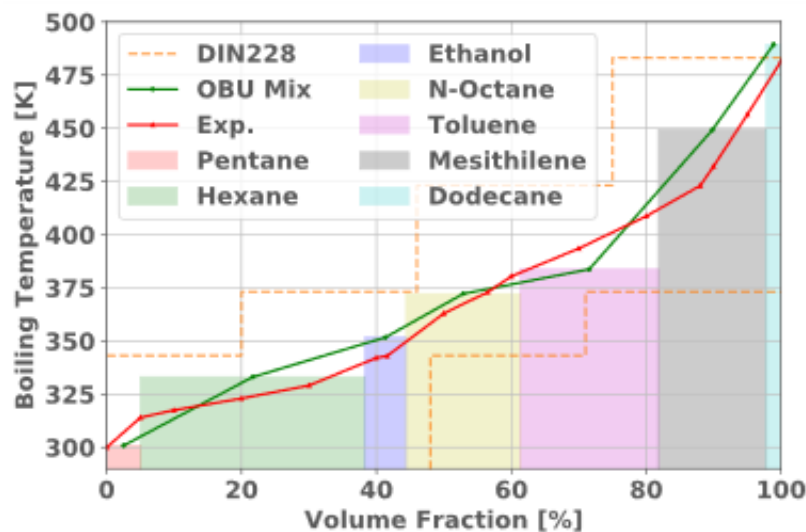


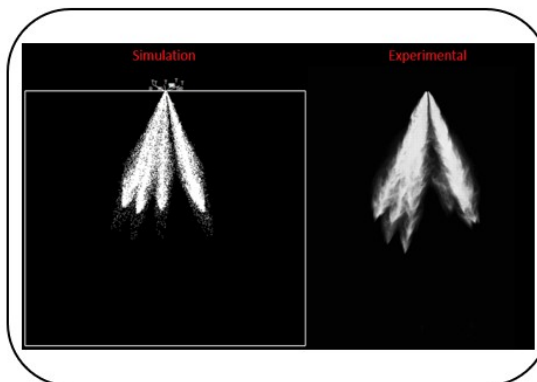
Fig. 3.21 Distillation curve comparison between EMT surrogate (green line) and experimental fuel (red line) [3].

liquid components during the CFD analysis [124]. The wall heat flux was modelled by means of the Angleberger wall function [3, 124, 132].

3.6 Summary of Models Implementation Workflow

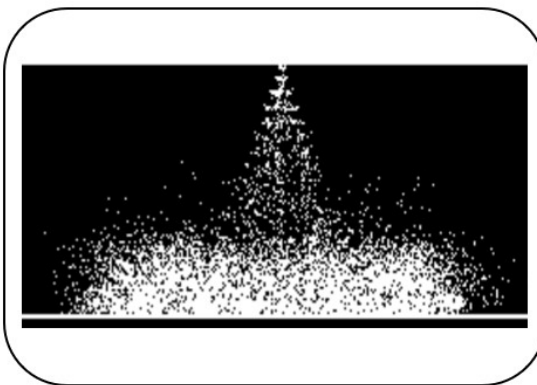
The workflow followed to first calibrate the fuel spray and then implement the related model and sub-models into the combustion chamber domain is presented in Figure 3.22. The quiescent volume was designed to replicate the experimental counterpart and understand the correct orientation of the five holes that constitute the injector. A footprint comparison and the reconstruction of the MFR profiles served as the first step to calibrating the spray characteristics. The spray penetration, the cumulative distribution function that captures the characteristic droplet diameters, and the plume morphology were validated using accurate experimental data. The spray model produced was then tested against hot walls to unveil the connection between fuel thermal/chemical properties and the wall characteristics. The B_s parameter, which connects the Nukuyama temperature with the saturation temperature of the fuel, was tuned to produce a realistic prediction of the liquid deposit. The boiling parameters of the fuel and the related limiting temperatures are then analysed as they constitute the thresholds for the different regimes experienced by droplets impacting a hot surface. The behaviour is connected to the analysis of the liquid deposit on the piston crown and cylinder walls. The quiescent vessel stages served as an initial test of spray characteristics before the implementation of the calibrated/validated models within the engine 3D domain. The

1. Quiescent vessel – spray calibration



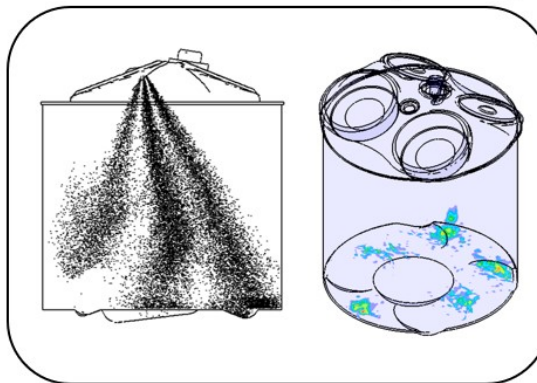
- Reproduction of the experimental spray vessel on a computational fluid domain
- Injector hole dimensions and orientations based on experimental data provided by Ford
- Reproduction of the experimental tests by imposing the same FRPs and background pressure
- Calibration of CFD spray and validation with experimental data through statistical and optimisation approaches: penetration, CDF and morphology calibration
- Evaluation of the best break-up model to reproduce the GDI injector used during the experimental campaign

2. Fuel-wall interactions



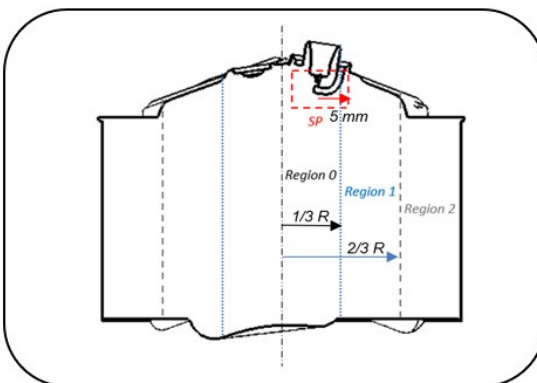
- Spray calibrated in the previous step used to conduct the fuel-wall interaction analysis.
- New computational fluid domain with a hot wall on the bottom. A sweep of wall temperatures was investigated
- Temperature and kinematic analysis. Relation between fuel deposit and wall temperature and how this modifies the impact regime
- Fuel surrogate model developed for mixture phase following the distillation curve of the experimental fuel
- Calibration of the fuel impact through available experiments and literature

3. In-cylinder implementation



- The calibrated fuel spray was used inside the fluid domain that reproduced the combustion chamber of the engine used for the experimental campaign
- In-cylinder mesh sensitivity analysis
- OD/1D boundary model calibration through experimental data
- Trapped air mass calibration
- Investigation of the mixture characteristics at different operating conditions and qualitative comparison with experimental PN emissions. In particular, mixture homogeneity and liquid film location.
- Split injections and qualitative analysis of mixture characteristics

4. Mixture quality indicators



- All the experimental operating conditions reproduce through CFD
- Liquid and gas-phase mixture characteristics identification
- Time/region identification
- Feature engineering to produce regression matrix with 1000 features based on mixture characteristics
- Elastic net regularisation to define a PN surrogate: the model connects CFD-based mixture parameters with experimental PN emissions

Fig. 3.22 Modelling workflow. From the fuel spray to the PN surrogate. In green are the parts developed/supported by colleagues of the EMT within the DYNAMO project.

combustion chamber of a single cylinder was reproduced with hexahedral volume cells and a mesh sensitivity analysis revealed the base mesh size as a starting point for the subsequent mesh refinements. Crank angle-based boundary conditions from 0D/1D models provided accurate intake and exhaust thermodynamic conditions. The performance of trapped air prediction at IVC timing was evaluated together with the crank angle-based in-cylinder pressure up to ST. Then, a fuel surrogate model able to reproduce the real fuel used for the experimental campaign is implemented considering the chemical groups as reference. Finally, mixture parameters are mathematically transformed through a feature engineering approach and used for an Elastic Net regularisation. The final result was a PN surrogate model that correlates CFD-based mixture characteristics with experimental PN emissions.

Chapter 4

Models Calibration and Optimisation

The use of advanced statistical techniques to calibrate the initial droplet distribution and break-up models can increase the model's prediction accuracy. The steps defined in this chapter, propose a novel systematic approach that can be generally used to calibrate phenomenological models. An investigation of the most used model combinations for spray modelling was performed to unveil the advantages and disadvantages of each configuration, and to identify a recommended setup for GDI applications. The calibration of the spray process is essential for the accurate reproduction of in-cylinder mixture characteristics. These have an impact on the PN production and can be used as regressor parameters for surrogate PN models. However, due to the highly non-linear nature of engine-out PN, the definition of such models requires the use of techniques well consolidated within the machine learning framework. First, a multi-independent variable analysis and transformation was performed, and then a regularization process revealed the most effective engine-based regressors to predict experimental PN emissions.

4.1 Factorial Screening of Spray Calibration Constants

As reported in section 3.1, the spray model is created by combining an initial droplet distribution (RR model) and a break-up model (KH-RT or RD). To understand which calibration factor has a major effect on the model response, a factorial screening was conducted. This approach is generally utilised for statistical problems [135]. Firstly, the range of variation of each factor was selected based on available literature [113, 115, 116] and the author's previous experience [28]. These values are presented in Table 4.1. Since X is a reference diameter (see 3.1), the range was consistent with the injector hole diameter and the experimental SMD for all the FRP analysed. The overall workflow for the factorial screening, the model calibration and validation is presented in Figure 4.1. The factorial screening

Table 4.1 Calibration factors range for the droplet initial distribution and break-up models. The values were used to define the factorial screening space [1].

	RR		KH-RT				RD			
Calibration Factor	X [μm]	q	B_0	B_1	C_3	C_t	C_{b1}	C_{b2}	C_{s1}	C_{s2}
Max	100	5	0.61	100	0.4	10	8	3.15	0.55	20
Min	50	1.5	0.59	1.5	0.1	1	1	3.13	0.45	2
Typical	100	2	0.61	40	0.1	1	6	3.14	0.5	20

revealed the most dominant factors on simulated spray characteristics. These factors are utilised for response surface models and the subsequent definition of the objective functions (that represent the error between numerical and experimental values) to be optimised with a nested optimisation. Instead of conducting a computational intense optimisation for all the calibration factors, only the dominant factors were optimised during the calibration process. The optimisation was based on a space-filling principle by means of a Halton sequence [134]. Lastly, a validation process revealed the spray model prediction performance against the experimental counterparts.

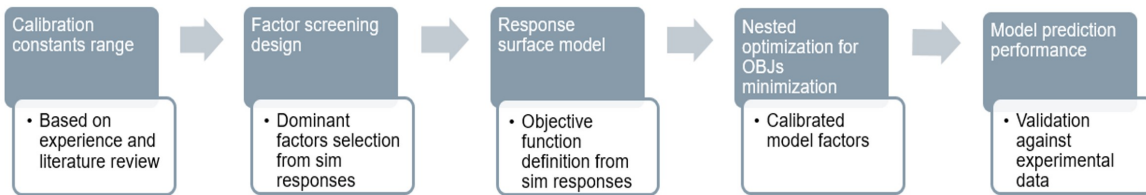


Fig. 4.1 Workflow for the factorial screening, model calibration and prediction performance against experimental data [1].

The analysis was carried out with two model combinations, i.e., RR+RD and RR+KHRT. The aim was to establish which spray model combination is most suitable for GDI applications. The fuel injection selected for the screening phase was 150 bar, as this condition is often utilised in the real experimental points. However, the validation process was performed at 150 and 250 bar to have a more generalised perspective and prove the validity of the proposed methodology.

Regarding the screening process, a matrix with $2^{(6-1)} = 32$ (half-factorial) calibration factor combinations was designed. Hence the same amount of CFD simulations was run to evaluate the response. In this number, the base (i.e., 2) represents the two levels (max and min) of each calibration factor while the index 6 is the number of factors for each model combination (i.e., RR's two factors plus the other four for each break-up model) [136]. It is possible to write the regression equation as:

$$y = b_0 + \sum_{i=1}^6 x_i b_i + \sum_{i=1}^5 \sum_{j=i+1}^6 x_i x_j b_{ij} \quad (4.1)$$

where y is the model response, b_0 is the intercept of the regression, x_i is the factor combinations and b_i is the corresponding coefficients. The higher the coefficients the more effect that factor has on the response. The R^2 was used to quantify the goodness of fit of each regression model.

Following the sparsity of effects principle [136], the responses of a system depend on main effects and low-order interactions among the factors. The half-factorial procedure presented here was hence selected because it is considered a reasonable trade-off between accuracy and computational cost. The calibration factor performances on the CFD simulation responses were investigated in terms of SMD on a plane 50 mm down the nozzle, and spray penetration at 0.8 ms ASOI. The former was selected to align the numerical results with the experimental counterpart. The latter accounts for the spatial and temporal evolution of spray near the maximum penetration.

4.2 Spray Model Calibration and Optimisation

The optimisation process to obtain the calibrated factors required a more complex approach in comparison with the factorial screening defined in Equation 4.1. A 50-point Halton sequence (DoE space) was chosen for the optimisation. Then a surrogate modelling approach was selected to quickly predict the responses between the simulated points of the DoE space. The surrogate model of a simulated model is defined as a meta-model [4]. The meta-model development used a hybrid Radial Basis Function (RBF) polynomial approach within MATLAB MBC toolbox to interpolate the results from the CFD simulations. An overview of the concept is presented in Figure 4.2 where two factors (variable 1 and 2) and a finite number of responses provide the foundation for a continuous space (meta-model) where an indefinite number of responses can be extrapolated [134, 137].

The CFD simulations, performed following the DoE space, provided the penetration and SMD responses, and were used for the definition of the following objective functions:

$$OBJ1 = \frac{1}{t} \int_0^t \left(\frac{p_{num}(\tau) - p_{exp}(\tau)}{p_{exp}(\tau)} \right)^2 d\tau \quad (4.2)$$

$$OBJ2 = \frac{1}{D} \int_0^D \left(\frac{c_{num}(\delta) - c_{exp}(\delta)}{c_{exp}(\delta)} \right)^2 d\delta \quad (4.3)$$

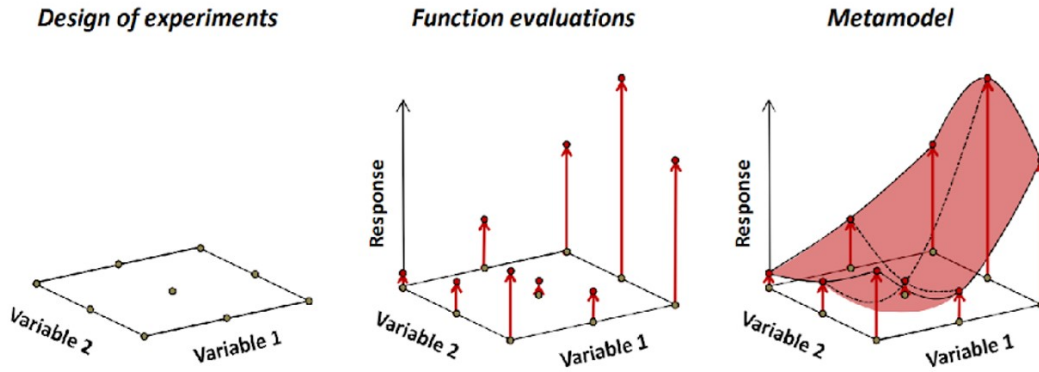


Fig. 4.2 Meta-modelling approach for a response that depends on two design variables [4].

Equation 4.2 and 4.3 were defined as the squared deviation of the numerical values (obtained from the CFD simulations) from the experimental counterpart. Specifically, Equation 4.2 indicates the square error between the instantaneous numerical penetration p_{num} and the experimental equivalent p_{exp} as a function of time τ . Similarly, Equation 4.3 evaluates the squared error between the numerical cumulative curve c_{num} and the experimental c_{exp} of droplet diameter δ . Both curves were evaluated at 50 mm from the nozzle at 0.8 ms ASOI. The use of both penetration and cumulative droplet dimensions to characterise the gasoline spray is aligned with the SAE J2715 recommended practice [121].

For each FRP tested for this analysis (150 and 250), a nested optimisation process was performed with a population of 2000 and 500 interactions. Nested optimization, also known as hierarchical optimization or multi-level optimization, refers to the process of optimizing one optimization problem within the context of another, larger, optimization problem [138]. The advantages of using this approach are the flexibility of nesting sub-problems and the efficiency in findings near-optimal solutions. In fact, OBJ2 was selected as a priority to be optimised and OBJ1 was imposed as a constraint. Since the spray penetration is influenced by the droplet velocity, for a fixed MFR it is reasonable to prioritise the prediction performance of the droplet dimensions and hence OBJ2. The constraint imposed in OBJ1 was a minimum error threshold.

The threshold influenced the solutions of the optimiser in terms of calibrated factors. Consequently, an iterative process was performed to select, for each injection pressure, an OBJ1 threshold to provide the best solutions that follow the variation of the spray characteristics observed experimentally. The analysis of these results enabled, as reported in the result section (section 5.1), to select the model combination RR+RD as the most suitable for modelling sprays in high-pressure GDI applications.

4.3 Regression Techniques

A versatile PN surrogate model is ideally a low-dimension model, i.e., formed by a limited amount of regressor variables (independent variables or features) that correlate the experimental observations with the peculiar in-cylinder quantities. Due to the non-linear nature of the problem, the first step was to analyse what regression technique can perform better providing meaningful results. Multiple regression analysis provides the coefficient of the m features minimizing the sum of the squared error between the predictions and the n observations. The method is called Ordinary Least Squares (OLS) and might yield relatively large coefficients, overfitting of the observations and ultimately a not generalized prediction model [139]. The issues are amplified when $m \gg n$, where m is the number of features and n is the number of data points. The accuracy (or bias) and the spread (or variance) of the estimates might be modified to overcome these problems [139, 140]. The regularization approach introduces a penalty term into the OLS loss function reducing the accuracy of the prediction but providing a more generalized model with a mitigated variance [136]. Ridge regression L [141] applies a bias that increases with the sum of the squared coefficients $\hat{\beta}$:

$$L_{Ridge}(\hat{\beta}) = \sum_{i=1}^n (y_i - x_i' \hat{\beta})^2 + \lambda \sum_{j=1}^m \hat{\beta}_j^2 \quad (4.4)$$

Where y_i is the i -th observation, $x_i' \hat{\beta}$ the i -th prediction and λ is the hyperparameter to be tuned. Ridge regression is not useful for regressor variables selection because it assigns a non-zero coefficient to all the regressor variables to feed into the model. An alternative is the LASSO method [142] which penalizes the loss function with the absolute value of the coefficients $\hat{\beta}$:

$$L_{LASSO}(\hat{\beta}) = \sum_{i=1}^n (y_i - x_i' \hat{\beta})^2 + \lambda \sum_{j=1}^m |\hat{\beta}_j| \quad (4.5)$$

Increasing λ , more coefficients and hence regressor variables are zeroed which is beneficial in terms of model simplicity. However, the method might suffer from being dependent on the particular data set and selecting only one regressor out of correlated groups. The combination of Ridge regression and LASSO penalties provides the EN regularization [139] with the aim of mitigating the disadvantages of both methods:

$$L_{EN}(\hat{\beta}) = \frac{\sum_{i=1}^n (y_i - x_i' \hat{\beta})^2}{2n} + \lambda \left(\frac{1-\alpha}{2} \sum_{j=1}^m \hat{\beta}_j^2 + \alpha \sum_{j=1}^m |\hat{\beta}_j| \right) \quad (4.6)$$

Where α is another hyperparameter set to 0.5 to provide a regularization process between Ridge ($\alpha = 0$) and LASSO ($\alpha = 1$).

Equations 4.4, 4.5 and 4.6 are accessible in MATLAB through a built-in function. A script was designed to investigate the performance of the various regularization approaches and to tune the hyperparameters. A final PN surrogate model was obtained automatically after applying an EN regularization to the regression matrix composed of the selected features. These were designed with a feature engineering approach as described in the next paragraph. The PN surrogate model MATLAB code is presented in Appendix A.

4.4 Feature Engineering and PN surrogate model development

A total of 100 region/time-based, mixture-related, features were selected from CFD simulation results. Each feature was normalized and then mathematically transformed using polynomials of a maximum degree of two, logarithm and exponential function as shown in Table 4.2. The normalization was necessary due to the sparse nature of the features that might yield biased coefficients. Normalization of the inputs greatly improves the interpretability of the model as the units of the β_i are the same as the response metric. A maximum degree of two was applied to each polynomial transformation as it was considered a good trade-off between model generalization and accuracy. The regression matrix was composed of a total of 1000 features (columns) and 40 values (rows, one for each simulation associated with the specific operating condition). An EN regularization was used to filter out the features with relatively low or no direct correlation with experimental PN.

The regularization was performed by imposing a sweep to the hyperparameter λ with a range of variation between 0.001 and 3 [139]. The MATLAB built-in function combines a grid search with a k-fold cross-validation technique [143] to simultaneously select the hyperparameter, λ , and the model coefficients. For each trial value of λ in the grid, a corresponding model was identified using k-fold cross-validation [144, 145]. In this method, the data set is divided into $k = 5$ roughly equal-sized sets. The sampling is performed without replacement, so each data point appears in each set exactly once.

Then 4 sets are used to train the regression model using the alternating direction method of multipliers (ADMM) approach [140] and one set is held back for validation. The mean square error (MSE) is calculated for the validation set. A different set is held back for validation of each of the $k = 5$ iterations. The final MSE is the mean of the $k = 5$ MSE values for each of the held-back data sets. The value of λ , and associated coefficient estimates,

Table 4.2 Mathematical operators are used to transform each feature and construct the regression matrix.

Feature transformation operators
x^2
$\sqrt{x}$
e^x
$\log(1+x)$
$\frac{1}{1+x}$
$\frac{1}{1+x^2}$
$\frac{1}{1+\sqrt{x}}$
$\frac{1}{e^x}$
$\frac{1}{1+\log(1+x)}$

yielding the minimum 5 – fold MSE over all trial λ values was initially chosen as the reference model, which is referred to as *Model – A*. The resultant model had 15 terms, which demonstrates the utility of the grouping effect of the EN. However, the main concern was the relatively low residual degrees of freedom. To further reduce the model dimensionality Bayesian information criteria (BIC) [146, 147] search was undertaken. BIC is a “dimension-consistent” information theoretic measure and is routinely used for model selection in a wide variety of fields. From a Bayesian perspective, BIC arises from a viewpoint of equal prior probability for each candidate model with very vague priors on the parameters given the model. BIC is a ‘the smaller, the better’ measure. The approach was to set aside terms with small regression coefficients one at a time, beginning with the smallest, and compute the BIC value for this model. The resulting model was denoted *Model – B*. If $BIC_{Model-B} < BIC_{Model-A}$ then *Model – B* is treated as the new reference model. The operation was repeated until no further improvement in BIC was achieved. To further compare the models, the Prediction Error Sum of Squares (PRESS) was also utilised [148]. PRESS is a measure of the predictive performance of a regression model. It is used to evaluate how well a model is likely to perform on new, unseen data. The basic idea behind PRESS is to fit the model to all data points except one and then use the model to predict the value of the omitted data point. The difference between the predicted and actual values for the omitted data point is squared, and this process is repeated for each data point. The sum of these squared differences is the PRESS statistic. Lower PRESS values indicate better predictive performance.

Basically, BIC is more focused on model selection by penalizing complexity, while PRESS is more focused on evaluating the predictive performance of a model.

The overall workflow to obtain the proposed PN surrogate model is presented in Figure 4.3. Terms with very low coefficients are excluded from the analysis, on the basis that they do not belong to any major group of features.

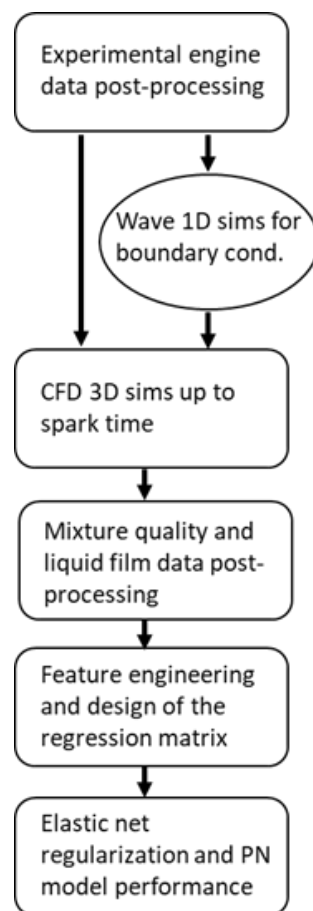


Fig. 4.3 Workflow for the development of the PN surrogate model [2].

Chapter 5

Spray Model Validation Results

In this chapter, the results of the factorial screening analysis applied to the most used breakup models are presented. The dominant factors are then optimised through two objective functions and the complex dependency between model parameters is revealed. The chapter continues with the selection of the best model combination, i.e., the most suitable candidate for an accurate reproduction of the complex phenomena involved in a high-pressure fuel spray. The extended analysis of a wide range of operating conditions indicated how the methodology developed is consistent and able to reproduce the entire engine operating envelope in terms of injection pressures. The calibration was able to capture not only the usual characteristics such as spray penetration and SMD but also the entire droplet size spectrum and plumes' morphology as further evidence that the proposed methodology is robust. The derived contour plots are particularly useful for producing quick and physics-informed model calibration.

The final part of the chapter is still dedicated to quiescent volume analysis but with a specific focus on spray-to-wall interactions. The results are shown with particular emphasis on the relationship between liquid deposits and surface temperature (wall temperature). The correct understanding of this behaviour unlocks the not trivial characterisation of more complex hot surfaces found in a typical combustion chamber, i.e., the piston crown and cylinder walls. Again, the results indicated the consistency of the proposed models, sub-models and the calibration adopted with great correspondence between numerical and experimental trends.

5.1 Factorial Screening and Spray Model Selection

The absolute regression coefficients $|b|$ for the spray penetration and the SMD models, obtained with the RR+RD model combination, are presented in Figure 5.1. The analysis of the R^2 revealed the consistency of both regressions with a value of 0.99 each. Looking at the

effect of the calibration factors on spray penetration (left chart in Figure 5.1), it is clear the dominance of X ($|b| > 10$) followed by q ($|b| > 1$) and their combination Xq ($|b| < 1$). The modification of droplet dimensions with these two parameters has a direct and substantial influence on the distance reached by the droplets from the nozzle during the spray process. Since the MFR (i.e., the droplet initial velocity) is fixed, the major influence on droplet penetration is given by droplet dimensions. Interestingly, the other factors have a minor influence on the penetration ($|b| < 1$) even when associated with the dominating X and q . Comparing the bag and stripping factors, the former seems more influential. This is aligned with similar studies [116, 74].

The dominance of X is repeated by analysing the effect of calibration factors on the SMD (right chart in Figure 5.1). Consistently with the penetration analysis, the bag break-up coefficient C_{b1} ($|b| > 10$) has a major effect in comparison with the stripping counterpart C_{s1} ($|b| < 5$). The combination XC_{b1} results in a dominant impact ($|b| > 10$) on SMD but the effect is lower in comparison with the factors taken individually. The other factors, and in particular the ones related to the stripping mechanism (C_{s1} and C_{s2}) combined with more influential factors, have less ($|b| < 5$) to no impact ($|b| < 1$).

Considering both penetration and SMD analysis, for the RR+RD model combination the factors X and C_{b1} seem the most dominant and hence sufficient to accurately calibrate the spray model characteristics.

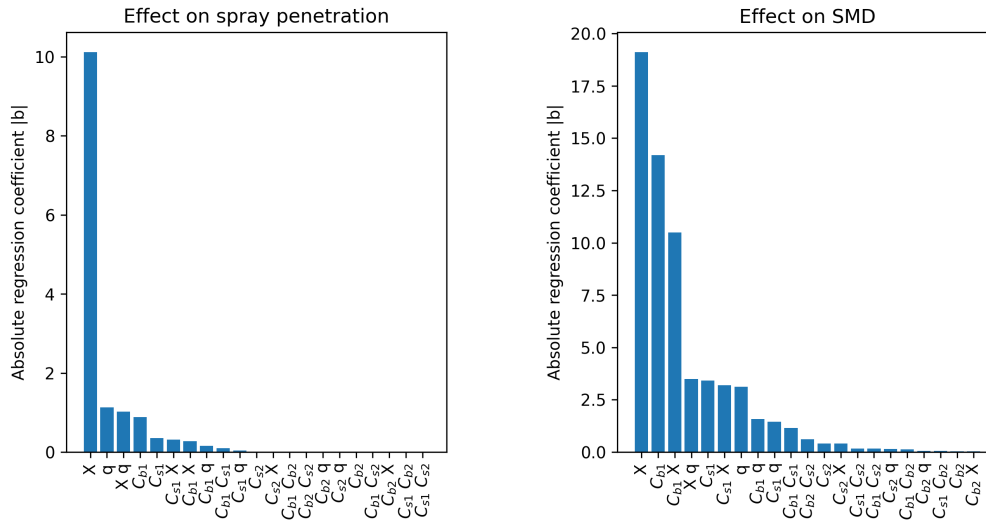


Fig. 5.1 Factorial screening analysis of the calibration factors for the RR+RD model combination as the absolute regression coefficient. The regression model and hence the effect of each factor is obtained for the spray penetration at 0.8 ms ASOI (left) and the SMD at 50 mm down the nozzle (right) [1].

The same analysis proposed for the RR+RD is presented in Figure 5.2 for the RR+KHRT model combination. Regarding the R^2 , both the penetration and the SMD models fitted well with the simulation data with a value of 0.94 and 0.97, respectively. Considering the effect on spray penetration (left chart in Figure 5.2), X ($|b| > 5$) and C_3 ($|b| > 3$) are dominant, followed by the less predominant factors ($1 < |b| < 2$) C_3C_t , C_t , C_3X and C_tX . Since the regression coefficient is almost identical for these combinations, their tuning can result in an equal variation of the modelled spray penetration highlighting the necessity of physically explainable calibration procedures. Other factors and factor combinations are almost irrelevant ($|b| < 1$).

The SMD bar chart (right chart in Figure 5.2) identified the following factors as the most significant ($|b| > 15$) C_3 , X , C_3X , followed by q and C_3q ($|b| > 10$). Just like the previous model combination, the SMD appears to be primarily influenced by the break-up coefficient (C_3 in this case) and the initial droplet distribution controlled by X . The impact of RT coefficients (C_3 and C_t) on SMD is more pronounced than that of KT coefficients (B_0 and B_1), indicating that the model is more responsive to the break-up resulting from droplet deceleration and density rather than aerodynamic forces. Overall, the RR+KHRT combination seems influenced by three factors (X , C_3 and C_t) meaning that the calibration process would be more complex in comparison with the RR+RD combination. However, to simplify the methodology and have an identical DoE approach, the calibration is performed only on X and C_3 .

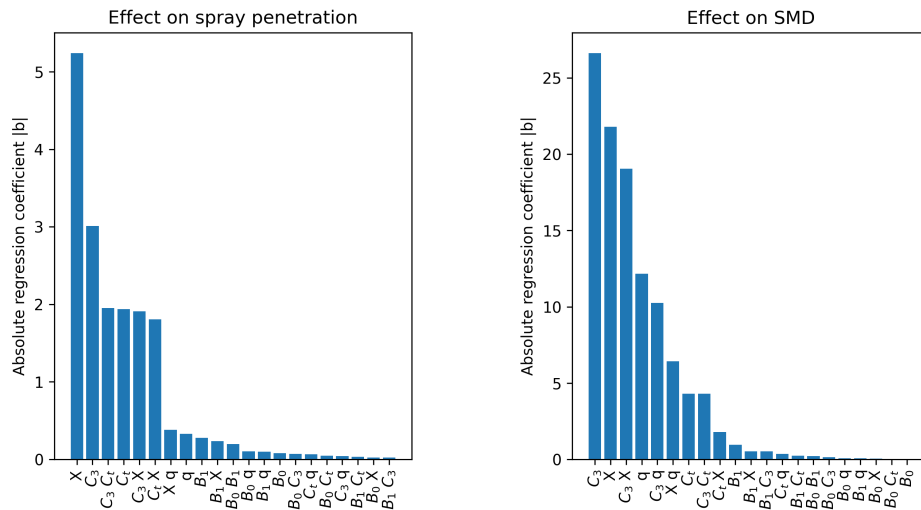


Fig. 5.2 Factorial screening analysis of the calibration factors for the RR+KHRT model combination as the absolute regression coefficient. The regression model and hence the effect of each factor is obtained for the spray penetration at 0.8 ms ASOI (left) and the SMD at 50 mm down the nozzle (right) [1].

Having selected the two dominant factors for each model combination, the next step is to perform an optimisation from a DoE space. The other factors were kept constant and equal to the values reported in Table 4.1 (typical values). The DoE space that provided the factor variation, i.e., the CFD points to be tested, was created with the MATLAB MBC toolbox. The latter was also used to develop the meta-model of the data obtained through CFD simulations. A Halton sequence was selected to generate 46 points scattered on the two factors design space plus 4 points at the corners. This was done to improve the level of information gathered at the extreme of space. The final DoE with a total of 50 points for each model combination is presented in Figure 5.3. Each point was tested with a FRP of 150 and 250 bar. Each simulation for the spray calibration analysis (factorial screening and optimisation) was run on a 96 CPUs cluster and the computational time was 30 minutes meaning a total calibration time of 25 hours for a single injection pressure.

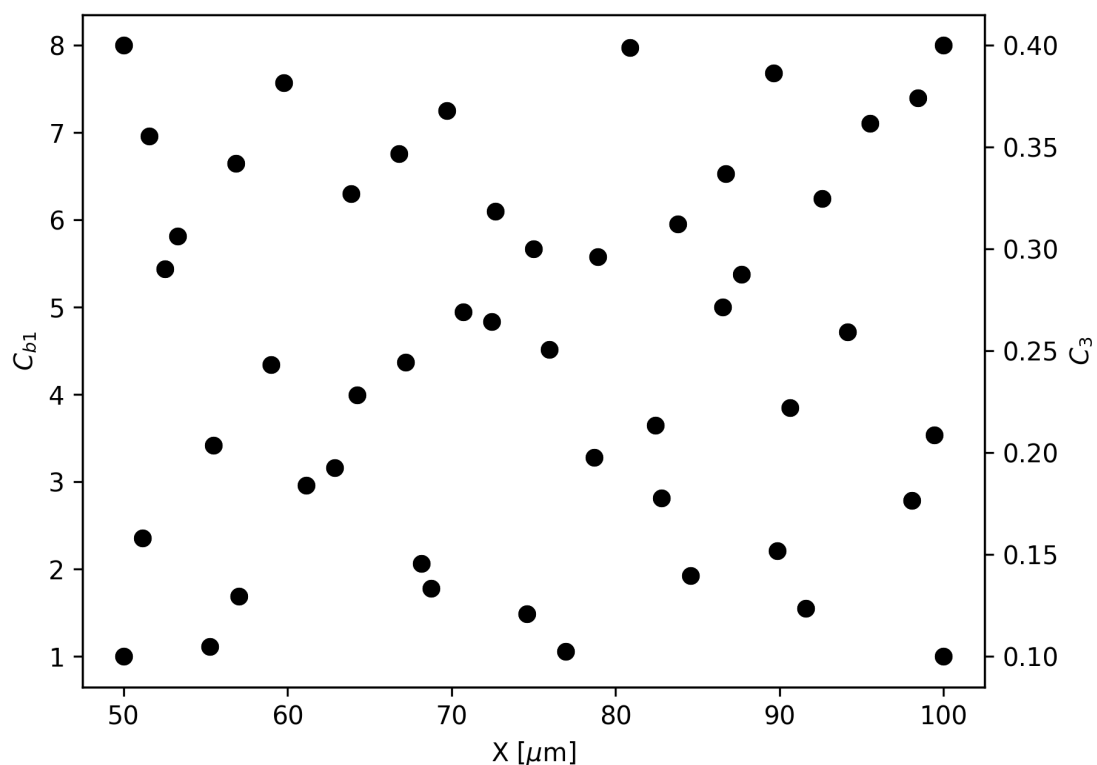


Fig. 5.3 DoE space for the two model combinations, RR+RD with X and C_{b1} ; RR+KHRT with X and C_3 . The design was done with a Halton sequence that comprises 46 points plus 4 placed at the corners of the space. Each of these points represents a CFD simulation to be run for the optimisation process of the spray model [1].

In Figure 5.4 and Figure 5.5 the objective function (Equation 4.2 and 4.3) contour plots, for each model combination, are shown for the 150 and the 250 bar case, respectively. The objectives were normalised to have an easier interpretation. In particular, 0 represents a hypothetical perfect prediction of the experimental data while 1 represents the highest error. Cases with higher error levels were plotted with a narrow range to increase visual interpretability.

Figure 5.4-a presents an area of low penetration error for $90 < X < 100$ and $3 < C_{b1} < 6$ (model combination RR+RD). The maximum error is observed on the left bottom corner where droplet distributions are formed by smaller diameter (i.e., smaller values of X) and the break-up threshold is lower (i.e., lower values of C_{b1}). Setting an initial droplet distribution with a reduced reference diameter (X) and a very low break-up threshold (C_{b1}) produces a simulated spray that abnormally disintegrates and hence is not able to penetrate as the real counterpart.

Looking at OBJ2 in Figure 5.4-b, it is evident an extensive area of an almost perfect match with experimental data. This area spreads for the whole range of X and $C_{b1} > 1.5$ hence the y-axis was truncated at C_{b1} equal to 3. An area of maximum error is present in the bottom right corner of the plot. Similarly to OBJ1, the lowest levels of C_{b1} are responsible for the premature disintegration of the liquid droplets and hence the highest error observed in this analysis.

Figure 5.4-c and Figure 5.4-d illustrate both OBJ1 and OBJ2 for the RR+KHRT at 150 bar injection pressure. OBJ1 (Figure 5.4-c) exhibits an opposing pattern compared to RR+RD, with a maximum error occurring at maximum levels of both X and C_3 . Moreover, a notable region of low error is shown with $C_3 < 0.2$ combined with all X values.

Figure 5.4-d presents a similar pattern in comparison with RR+RD. OBJ2 shows a significant area of low error with $C_3 > 0.12$ and a higher error if C_3 goes below the 0.11 threshold. This has a similar physical explanation initially proposed for the RR+RD case, i.e., lower break-up coefficients are responsible for the unrealistically fast disintegration of the droplets during the simulated spray process.

Increasing the FRP from 150 to 250 bar results in a modification of the OBJ1 pattern while OBJ2 remain similar, as can be seen in Figure 5.5. OBJ1 in Figure 5.5-a has two regions with higher error, at the top right and bottom left corner. The former is a region connected with simulations where bigger droplets (high value of both X and C_{b1}) penetrate unrealistically in the computational domain producing an overestimation in comparison with the experimental data. The area of lower error is moved toward a lower diameter ($75 < X < 92$) if compared to the 150 bar case (Figure 5.4-a). An explanation might be the

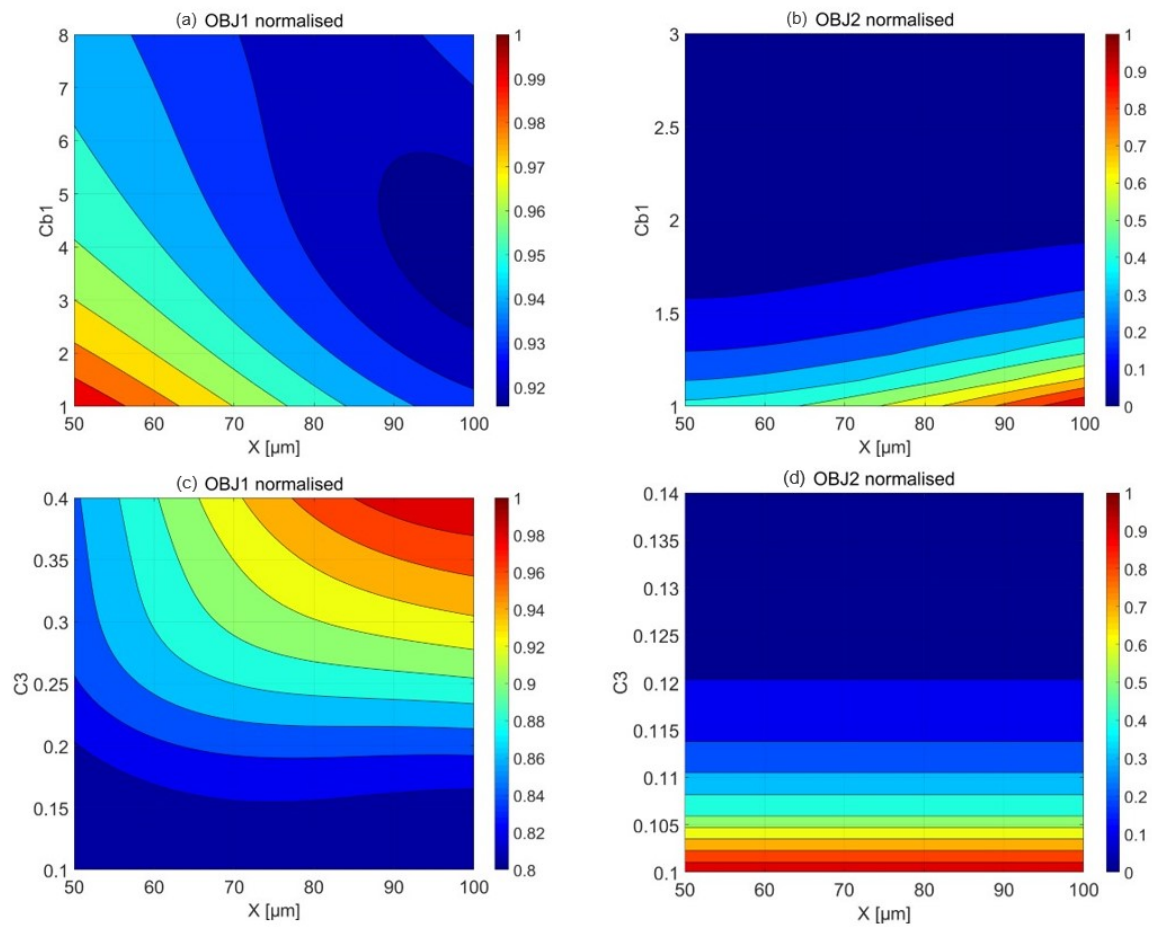


Fig. 5.4 Normalised objective functions from the regression analysis were presented with contour plots at 150 bar injection pressure. RR+RD OBJ1 (a), RR+RD OBJ2 (b), RR+KHRT OBJ1 (c) and RR+KHRT OBJ2 (d) are plotted in a 2D space where the axes are the dominant calibration factors and the intensity of the colour is proportional to the level of error [1].

necessity of a more atomised droplet distribution to match the experimental penetration at higher injection velocity (i.e., FRP).

In Figure 5.5-b, the enlarged region exhibiting a low OBJ2 error resembles the one observed in the 150 bar case (Figure 5.4-b). Similarly, the region with the highest error expanded from the bottom with X at low values of C_{b1} .

Figure 5.5-c illustrates the presence of two regions characterized by a low level of error. This demonstrates the potential of achieving accurate spray predictions using different combinations of calibration factors. As a result, the non-linear property of this calibration problem highlights the importance of conducting an advanced optimization process. Similarly to the 150 bar case, Figure 5.5-d provides evidence of a significant correlation between OBJ2 and C_3 .

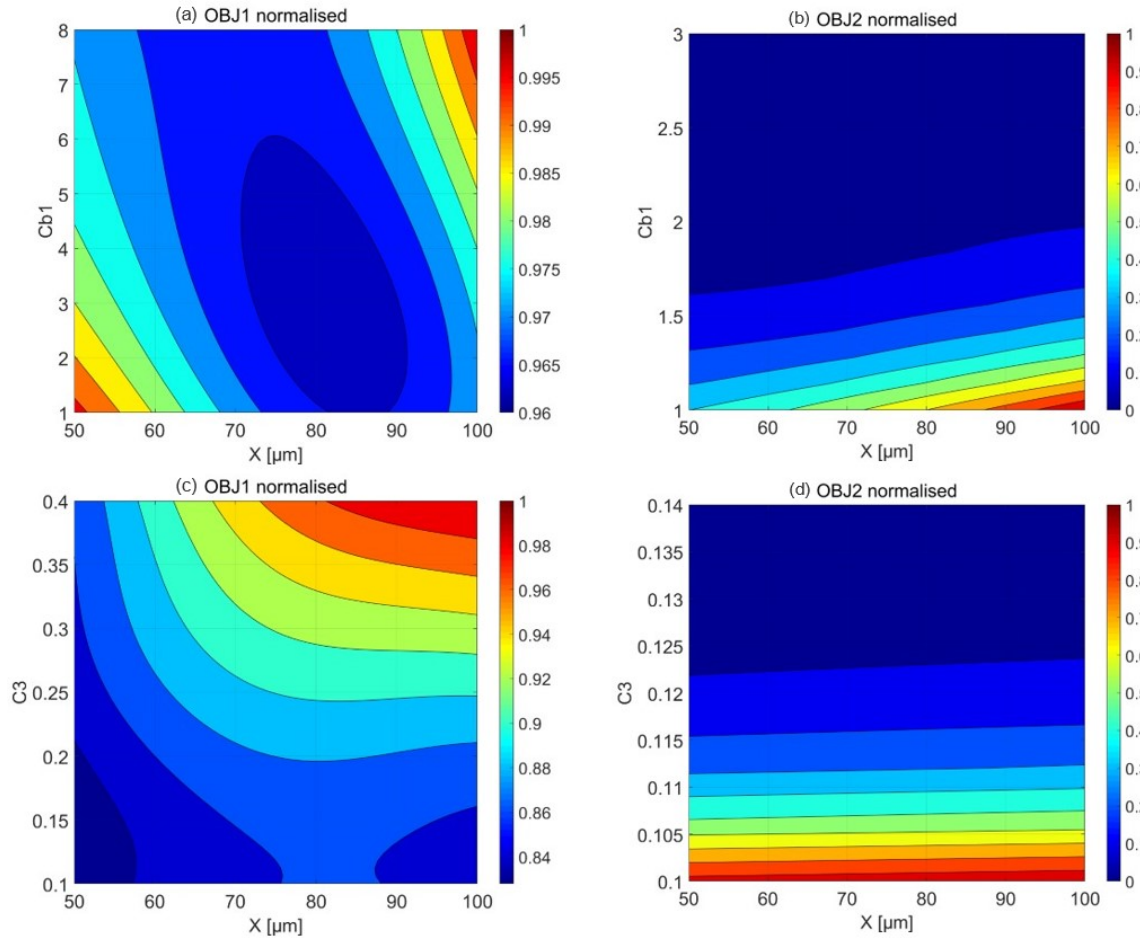


Fig. 5.5 Normalised objective functions from the regression analysis were presented with contour plots at 250 bar injection pressure. RR+RD OBJ1 (a), RR+RD OBJ2 (b), RR+KHRT OBJ1 (c) and RR+KHRT OBJ2 (d) are plotted in a 2D space where the axes are the dominant calibration factors, and the intensity of the colour is proportional to the level of error [1].

Table 5.1 Calibrated factors for both model combinations (RR+RD and RR+KHRT) at 150 and 250 bar [1].

RR+RD	X [μm]	C_{b1}
150 bar	64.1103	5.6391
250 bar	57.0222	5.6367
RR+KHRT	X [μm]	C_3
150 bar	69.1922	0.2214
250 bar	50.0268	0.2126

A nested optimisation was performed with the surrogate models representing the objective functions. The process revealed the optimal values for the dominant calibration factors at each injection pressure (150 and 250 bar) and for each model combination, as presented in Table 5.1. Interestingly, the optimisation algorithm found an optimised X that decreases with injection pressure for both model combinations. This physically plausible characteristic is aligned with experimental evidence as the atomisation and hence droplet dimensions reduce with higher injection pressures [117].

The numerical results from CFD simulations and the comparisons with the experimental counterparts are presented in Figure 5.6, 5.7, 5.8. The spray tip penetration (Figure 5.6), the cumulative distribution functions (Figure 5.7) and the characteristic droplet dimensions on a plane 50 mm down the nozzle (Figure 5.8) are presented for two injection pressures (150 and 250 bar) and for both model combinations (RR+RD and RR+KHRT).

Looking at the penetration prediction performance in Figure 5.6, clearly the RR+RD model outperforms the RR+KHRT as this generally over-predicts the real data from 0.25 ms and beyond. At the same time range, the RR+RD shows a good agreement with the experiments.

However, both models underestimate the ballistic region of the spray up to 0.2 ms. The error might be related to an overprediction of the discharge coefficient, the averaged MFR profiles used in the simulations and errors related to the solver [114]. It is evident how the predicted initial velocity is lower than experimental even if the total mass injected and the opening and closing ramps are identical to the real counterpart. This error is diminished for the other pressures tested, as it is shown in the following section. The general over-prediction near the maximum penetration might be due to a higher concentration of liquid in the proximity of the plumes' tip that inhibits the modelled evaporation [57].

In Figure 5.7 the cumulative distribution function is predicted with the lowest level of error by the RD model. As per the penetration analysis, the KH-RT shows an abnormal

deviation in comparison with the sigmoid experimental trend. In particular, for droplet diameters around $10\ \mu m$ and above $20\ \mu m$.

The three characteristic droplet diameters are obtained from the cumulative distribution function and plotted in Figure 5.8. In particular, the SMD is the most used diameter when validating fuel spray models for GDI applications [3]. Consistently with the other plots, the RD model outperforms the KH-RT which generally overestimates each diameter. As a result of this analysis, the RR+RD model combination was chosen as the best for fuel spray modelling for GDI applications.

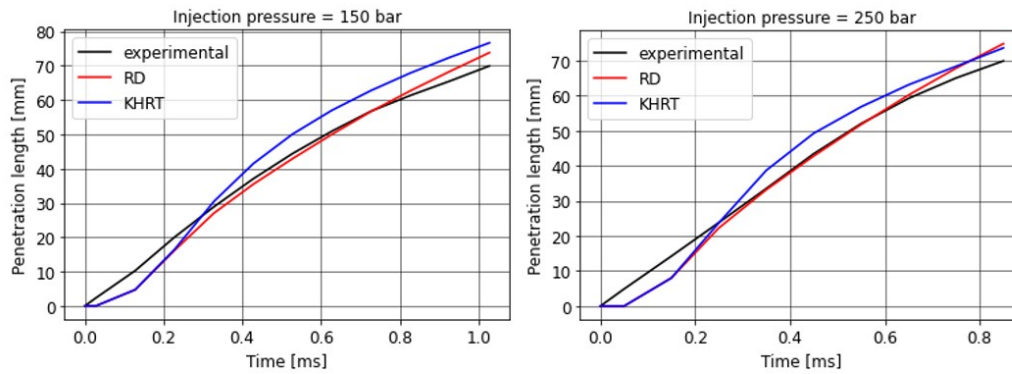


Fig. 5.6 Spray model validation in terms of penetration for the two break-up models, RD and KH-RT. The analysis is done at FRP 150 (left) and 250 (right) bar [1].

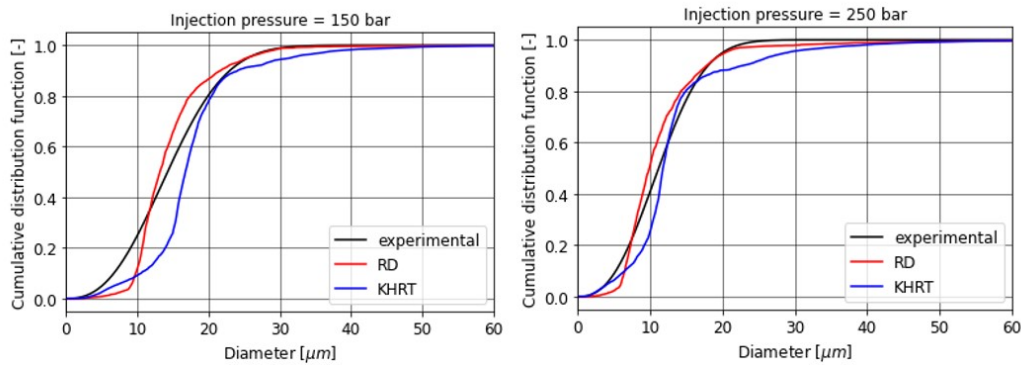


Fig. 5.7 Spray model validation in terms of cumulative distribution for the two break-up models, RD and KH-RT. The analysis is done at FRP 150 (left) and 250 (right) bar on a plane 50 mm down the nozzle [1].

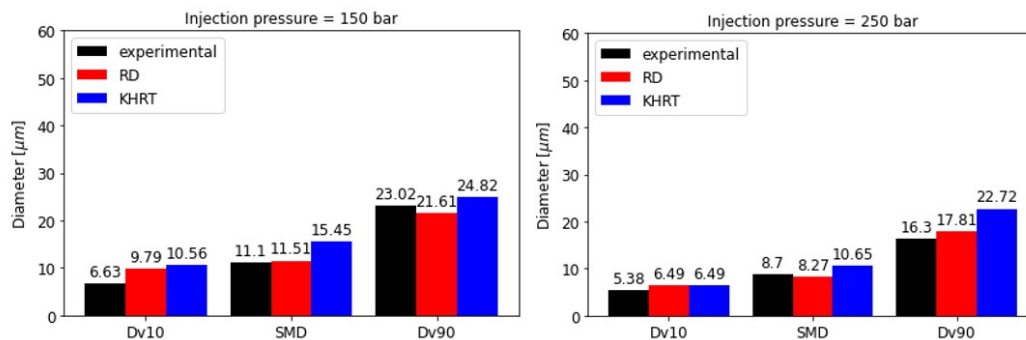


Fig. 5.8 Spray model validation in terms of characteristic droplet diameters, D_{v10} , SMD and D_{v90} , for the two break-up models, RD and KH-RT. The analysis is done at FRP 150 (left) and 250 (right) bar on a plane 50 mm down the nozzle [1].

5.2 Meta-Modelling of Spray Characteristics

The meta-model of spray simulation responses in terms of penetration at 0.5 ms ASOI and SMD on a plane 50 mm down the nozzle are presented in Figure 5.9. The analysis shows similar results for the two FRPs tested, i.e., 150 and 250 bar. Figure 5.9-a presents a maximum penetration variation of over 15% across the whole $X - C_{b1}$ plane. As expected, the spray penetrates more when formed by bigger droplets, i.e., higher values of both X and C_{b1} . Interestingly, the penetration seems unaffected for $C_{b1} < 2$. An area of minimum penetration is formed for $75 < X < 100$ and $C_{b1} < 1.5$. In Figure 5.9-b the strong correlation between C_{b1} and SMD is consistent with the results obtained for OBJ2 (Figure 5.4-b). In particular, the SMD on a plane down the nozzle can be tuned to a specific dimension by C_{b1} and it is basically independent from X . Moreover, the SMD increases by three times within the range of the calibration constants analysed. At 250 bar, the maximum penetration variation is 11% as shown in Figure 5.9-c. A region of minimum penetration is obtained for $75 < X < 100$ and $C_{b1} < 2$. Consistently with the 150 bar case, the maximum penetration is obtained at maximum X and C_{b1} . The SMD in Figure 5.9-d is quadrupled within the calibration factor range and the maximum level is reduced by 60% if compared to the 150 bar case (from 13 to 8 μm).

The overall analysis can inform the initial stage of a spray calibration and, most importantly, visualise the effect of calibration factors on spray model characteristics.

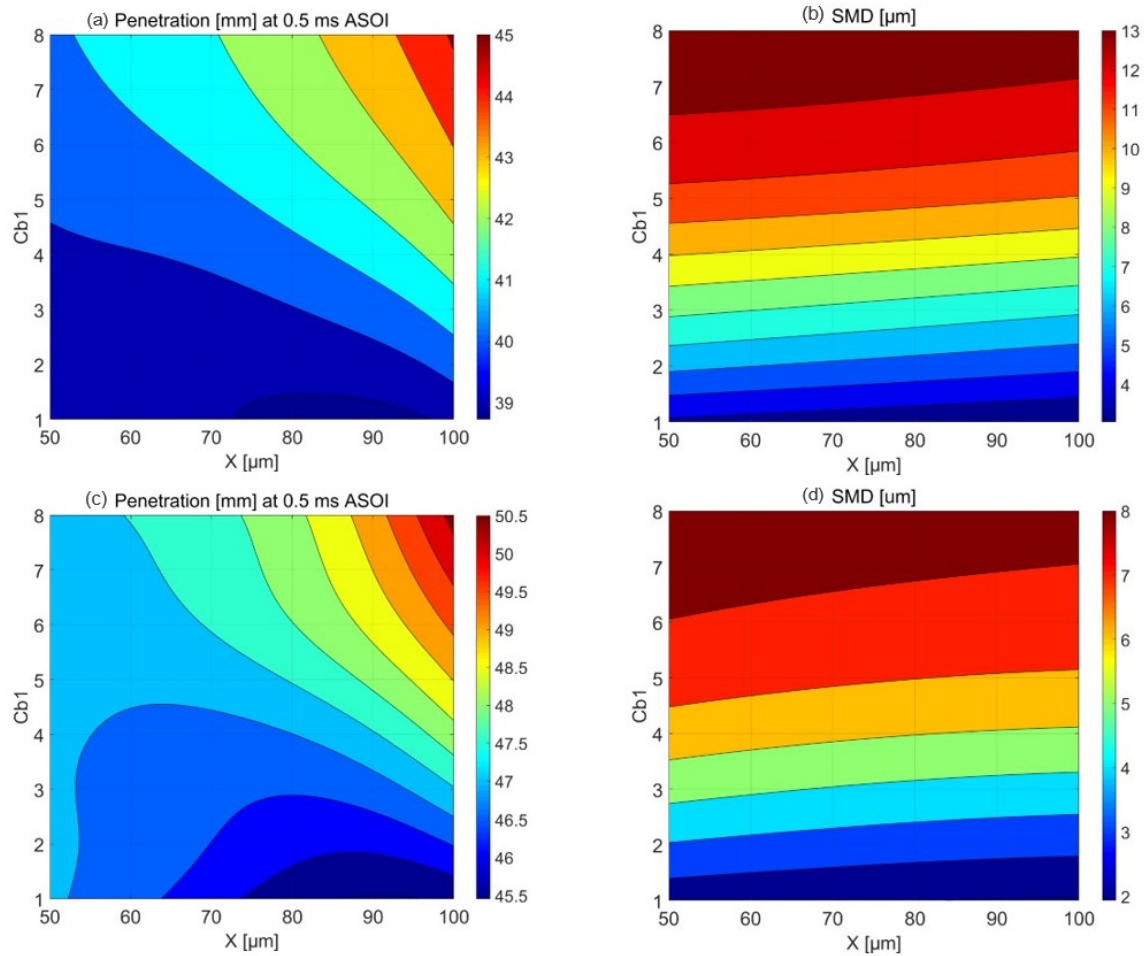


Fig. 5.9 Modelled spray characteristics as a function of dominant calibration factors: a) spray penetration at 0.5 ms ASOI and b) SMD at 50 mm down the injector at 150 bar; c) spray penetration at 0.5 ms ASOI and d) SMD at 50 mm down the injector at 250 bar [1].

5.3 Calibration Methodology Extended to Other Injection Pressures

The optimisation process was extended to the other available injection pressures, i.e., 50, 100 and 200 bar. A validation of the optimised X values, function of the FRP, against the equivalent experimental values reconstructed 50 mm down the nozzle, is presented in Figure 5.10. The values are normalised to focus on the trend variation. It is evident a good level of alignment between the numerical and the experimental data, with a slight deviation from 200 bar and beyond. It is plausible that a higher FRPs the X quantities imposed at

the nozzle (simulation) need to produce slightly bigger droplet dimensions to match the experimental SMD data 50 mm down the nozzle.

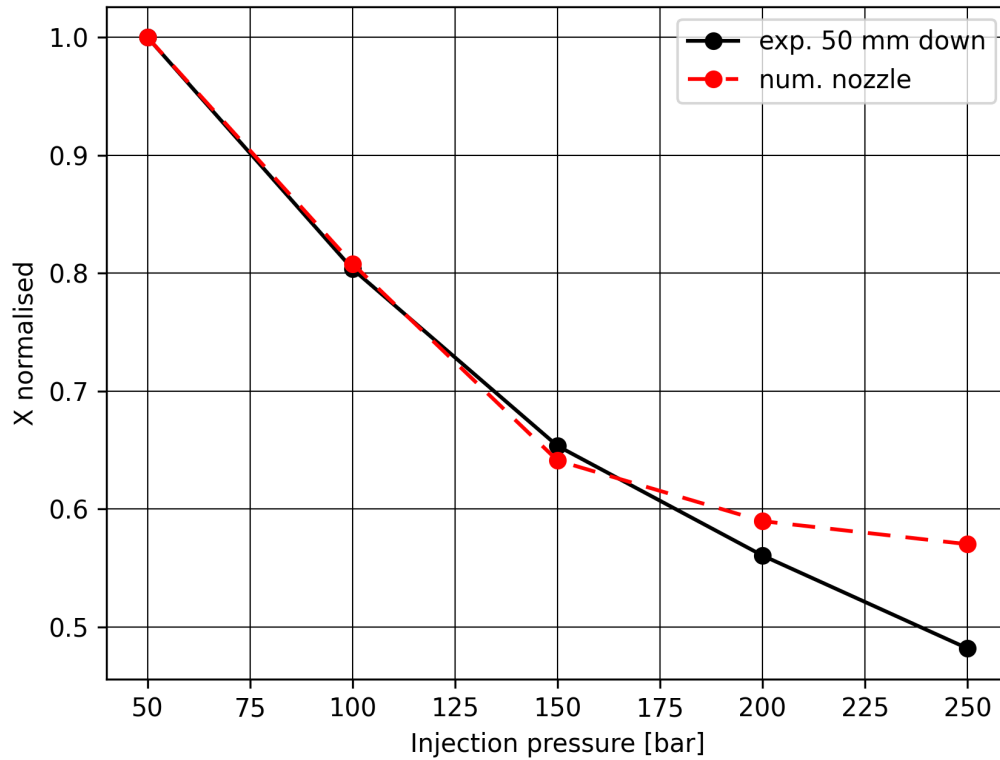


Fig. 5.10 X values are normalised as a function of FRP. The numerical quantities are the ones obtained from the optimisation process and hence imposed at the nozzle; the experimental are reconstructed from the experimental SMD obtained on a plane 50 mm down the nozzle [1].

The validation of the spray model extended to the other FRPs is presented in Figure 5.11. The left column refers to the 50 bar condition, the central to the 100 bar and the right column to the 200 bar condition. As before, the validation is performed against the experimental counterpart of spray penetrations (first row), cumulative distribution functions (central row) and characteristic droplet diameters (bottom row).

In Figure 5.11-a, b and c, a good level of prediction performance is shown by the model. Numerical results replicate almost perfectly the liquid penetration for the 50 bar case (Figure 5.11-a), with a slight under-prediction on the ballistic area (0 – 0.2 ms). The 100 bar case (Figure 5.11-b) increases this under-prediction phenomenon that seems instead reversed and moved toward the limit of the measurement window for the 200 bar case (Figure 5.11-c).

The cumulative distribution function for the 50 bar case (Figure 5.11-d) was well predicted up to the SMD diameter (corresponding to 32% of the distribution, D_{32}). Above this threshold, a constant under-estimation is presented for droplet diameters between 15 and 40 μm . The phenomenon is underlined in Figure 5.11-g where an under-estimation of 38% is shown for D_{v90} . The reason for this incongruity might be the non-linear relation between FRP and atomisation specifically for bigger droplet dimensions hence the inability of the optimiser to capture it. In fact, increasing the FRP by 50 bar, from 50 to 100, the decrease in D_{v90} was around 30% and hence of similar entity when increasing the FRP from 100 to 200 bar. On the contrary, SMD and D_{v10} have a smoother variation with FRP. This aspect is further analysed in the following section where a morphology validation is proposed.

The 100 and the 200 bar cases, shown in Figure 5.11-e and h and Figure 5.11-f and i respectively, have similar under-estimation issues but improve noticeably the accuracy.

Overall, the optimisation and consequent validation were considered sufficient for the reproduction of the real fuel spray and were generally more accurate than similar studies [57, 119].

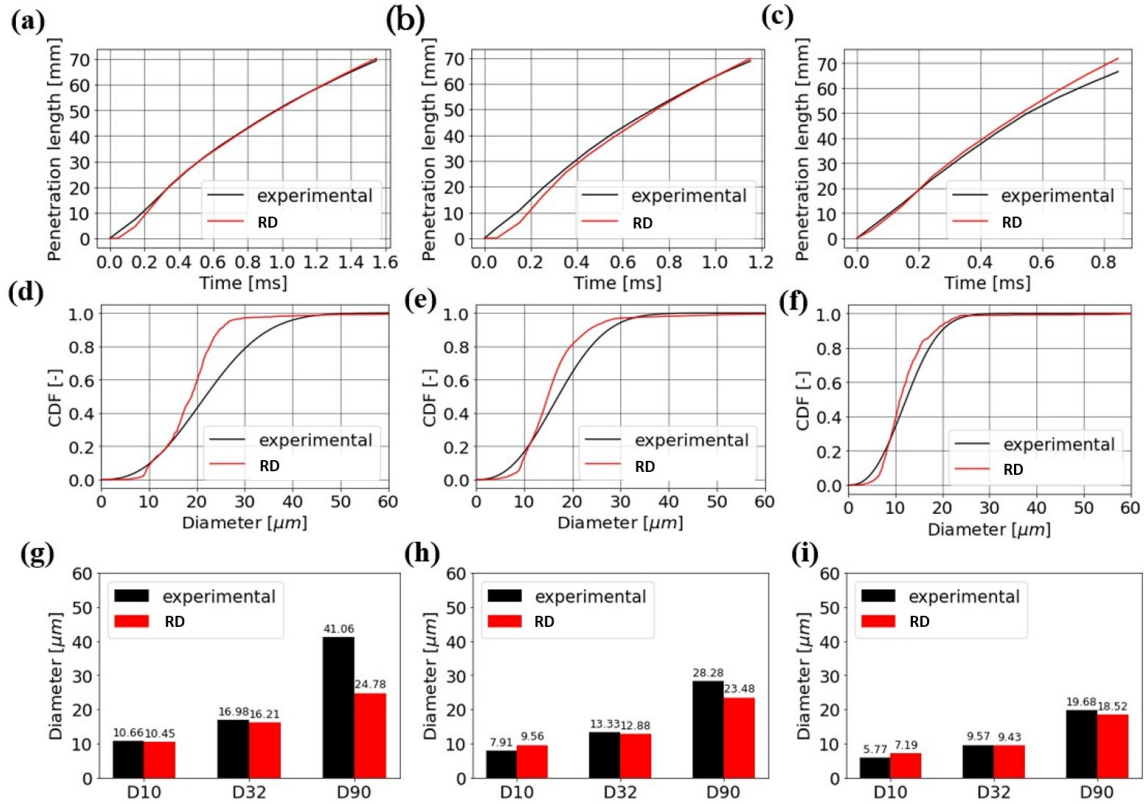


Fig. 5.11 Calibrated fuel spray model compared with experimental results in terms of penetration at a) 50, b) 100 and c) 200 bar; in terms of cumulative distribution function (CDF) 50 mm down the injector location at d) 50, e) 100 and f) 200 bar; and in terms of Dv_{10} , SMD and Dv_{90} at g) 50, h) 100 and i) 200 bar [1].

The optimised calibration factors for all the FRPs are plotted in Figure 5.12 and tabulated in Table 5.2. The other factors (q , C_{b2} , C_{s1} and C_{s2}) were kept constant and equal to the typical values presented in Table 4.1. The reduction of X with the injection pressure is aligned with the expected physical behaviour, i.e., a reduction of droplet diameters due to more intense atomisation [117]. The trend suggests that the reduction is stronger between 50 and 150, and then almost levels off up to 250 bar. In the same range, the C_{b1} increases linearly up to 150 bar and then stays around 5 up to 250 bar. The increase of the break-up threshold is necessary to compensate for the effect of velocity (function of FRP) on droplet atomisation. However, the reduction at 200 bar is unclear and will be investigated in future works. The relation found between calibration factors and FRPs is injector-specific. However, the mathematical fitting curves that can be extrapolated from Figure 5.12 can serve as an initial step for spray model calibration related to similar injectors.”

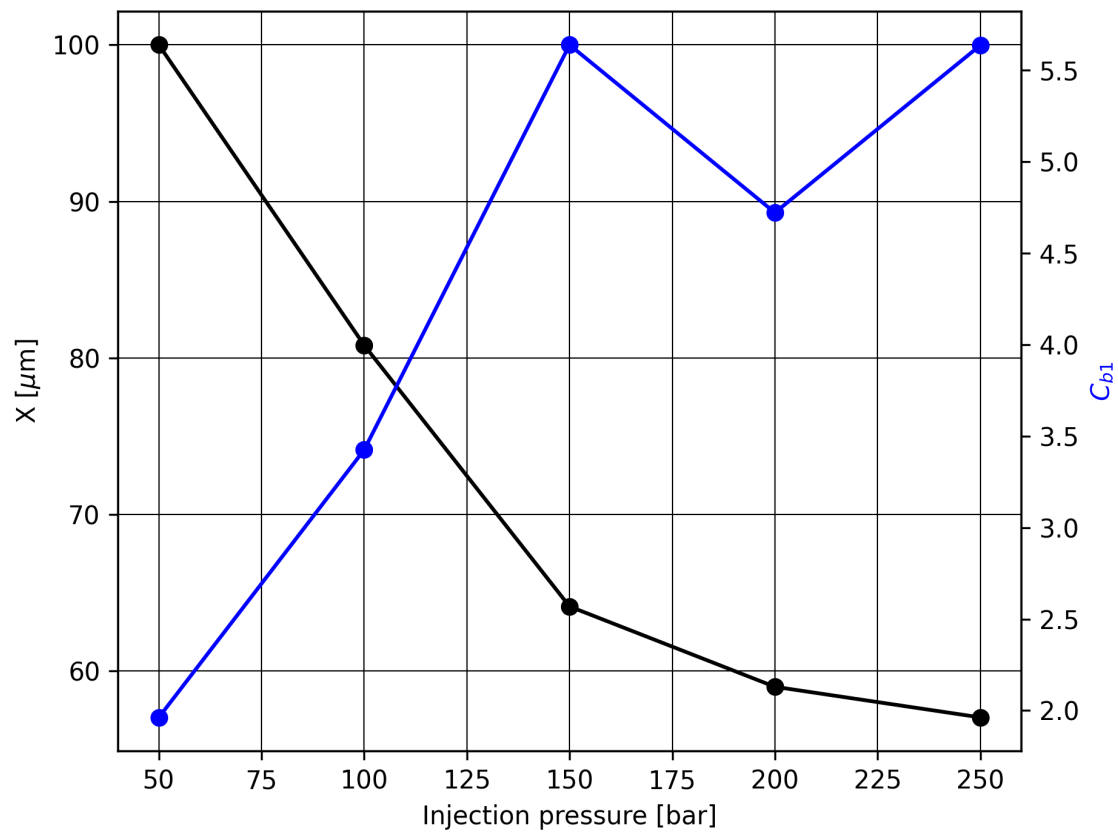


Fig. 5.12 Calibrated dominant factors for the RR+RD model combination as a function of the fuel rail pressure [1].

Table 5.2 Tabulated calibrated factors for the RR+RD model combination as a function of the fuel rail pressure [1].

FRP [bar]	$X [\mu m]$	C_{b1}
50	99.9996	1.9627
100	80.8061	3.4253
150	64.1103	5.6391
200	58.9774	4.7221
250	57.0222	5.6367

5.4 Spray Morphology Analysis

A morphology comparison of the spray using the CFD-based (coloured) and the experimental (grey) images is presented in Figure 5.13. Two viewpoints are shown for the 250 bar case at 0.8 ms ASOI to capture the full extension of the spray just before reaching the limit of the experimental measuring window (70 mm). Each plume of the numerical spray has a different colour, and the droplets are represented by dimension. It is worth noting that the numerical spray images represent the liquid phase, while the experimental images refer to both liquid and vapour. As a result, the experimental appears more jagged compared to the numerical counterpart due to two main factors: 1. The fleeting threshold between vapour and liquid is not clearly defined in the experimental images [113, 57, 101]; 2. The RANS numerical framework averaged and simplified the turbulence small scale [149]. Nevertheless, the good agreement between numerical and experimental results is evident, with the model able to capture well the plume morphology, the overall cone angle of the spray and the penetration.

The regions of experimental spray with higher vapour concentration, at the boundary of each plume, were reproduced with smaller droplets in comparison with the big clusters introduced at the nozzle exit. Moreover, each plume is well distinguished due to the wide hole configuration of this specific injector.

As indicated in [1], from the droplet dimension analysis, four characteristics regions can be defined:

1. Near-field: The typical liquid ligaments at the nozzle exit [112, 36] are simplified by imposing an atomized spray formed by clusters of big droplets with a maximum diameter $D_d = 100 \mu m$. Smaller droplets also exist in this region, as evidenced by a initial SMD of $26.5 \mu m$ obtained imposing the calibrated constant factors. These small droplets reproduce the rapid phase change of the fuel droplets and consequently the primary atomization mechanism.
2. Plume bulk: The secondary break-up due to pressure instability and the shearing process [113, 128] produces a large variety of diameters with evidence of big droplets that tend to persist in the proximity of the central region of the plumes. As explained in the next paragraph, several droplets in this region show a stagnation behaviour, i.e., almost zero momentum.
3. Plume interface: The air entrainment and generally the interaction between the gas-liquid phases promotes rapid evaporation of the fuel. Turbulent phenomena were noticeable experimentally and fish-bone structures were evident for most external

plumes. The behaviour was reproduced with a scattered distribution of small droplets showing evidence of a strong evaporation rate [36, 150].

4. Plume tip: This region is usually characterized by a higher concentration of fuel vapour and a fully developed secondary break-up [57]. The clusters of highly disintegrated droplets ($D_d < 10 \mu m$) mimic the combined effect of turbulent motion and drag force, as well as the longest residence time (0.8 ms) of the liquid injected.

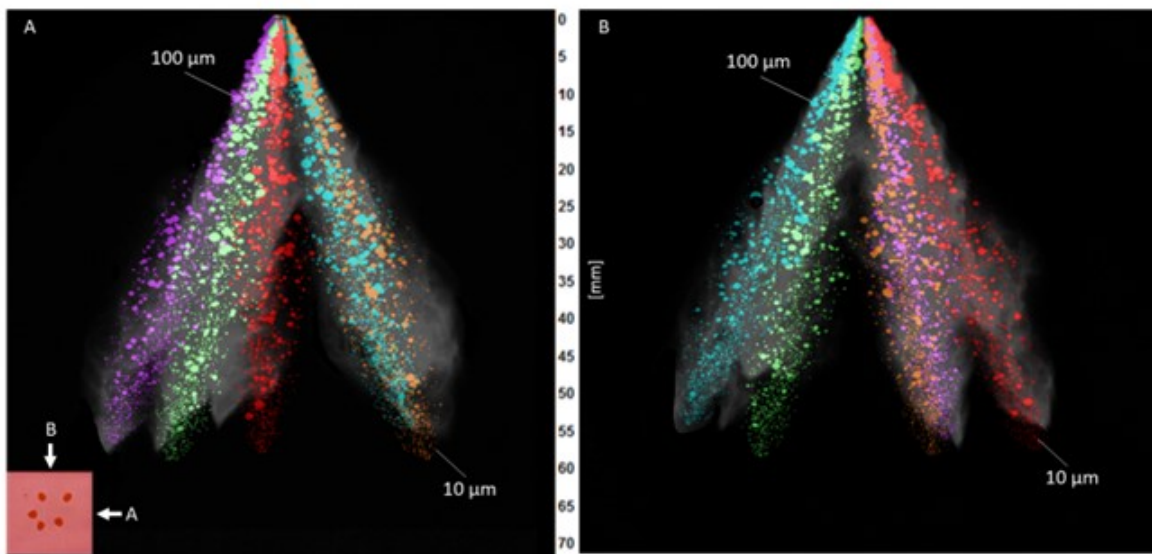


Fig. 5.13 Morphology validation of the CFD-based spray (coloured) super-imposed over the experimental counterpart (grey). Images were obtained at FRP 250 bar and 0.8 ms ASOI. Two viewpoints are presented, A and B, following the available experimental spray dataset. The experimental spray footprint is shown at the left bottom corner to clarify the viewpoints [1].

The mid-range velocity magnitude of the spray model plotted against the SMD is presented in Figure 5.14. This velocity is obtained by averaging the instantaneous value between the maximum and minimum values. This is a common practice as it aims to provide a representative measure of the velocity, especially in situations where there are significant fluctuations in the flow. On the graph, each point represents an injection pressure. Moreover, on each point, the corresponding CFD-based images are presented by instantaneous velocity.

In the proposed pressure range, from 50 to 250 bar, the velocity magnitude and SMD variations are 113% and -50% respectively. While the variation seems almost linear, the largest velocity increment and SMD reduction are registered between 50 and 100 bar. In contrast, between 200 and 250 bar the variations are minimal. This behaviour can inform

the design of optimised injectors because highlight the balance between droplet velocity and dimensions [58]. In fact, if increasing the velocity might result in more LF deposits on the piston crown, on the other hand enhanced atomisation is necessary to obtain a well-homogenised air-fuel mixture [128, 58, 151].

Regarding the spray images for each injection pressure, the area near the nozzle is where the droplets reach the maximum speed. Similar behaviours are presented in each image. The speed decreases quickly after around 15 mm and continues to diminish toward the plumes' tips. Interestingly, a stagnation effect (velocity near zero) is present around the plumes' bulk area due to a combined effect of air entrainment/recirculation and drag forces.

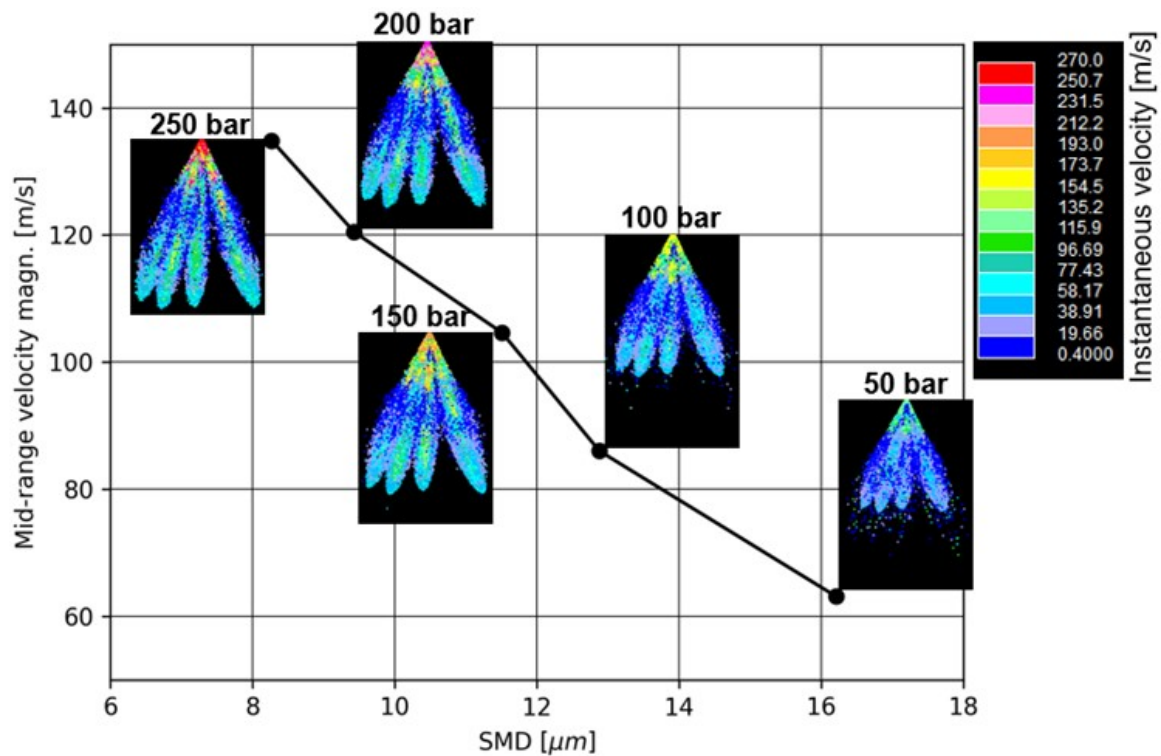


Fig. 5.14 Numerical mid-range velocity magnitude versus the SMD for injection pressures between 50 and 250 bar. For each point, a CFD-based image of the spray is plotted as a function of the instantaneous velocity [1].

5.5 Vessel Analysis of Fuel-to-Wall Interactions

Fuel-to-wall interactions and fuel deposit vaporization depend on thermo-kinetic factors as presented in Chapter 3 (section 3.2). When a fuel deposit is formed, the lifetime of liquid

pools is a direct consequence of the variation of the heat flux between the hot wall and the liquid [5, 130].

Figure 5.15 shows the normalized isooctane liquid deposit lifetime and the numerical heat flux q_w from the hot wall to the liquid as a function of the wall temperature $T_{wall} \geq T_{sat}$. Experimental values of the droplet lifetime on a hot surface were taken from [5]. The liquid lifetime trend was obtained by analysing the footprint of the spray plumes injected at high velocity against the bottom hot wall of the modelled vessel. The footprint images were taken at 1 ms ASOI hence 0.61 ms after EOI to allow the complete fuel deposition and the partial film evaporation. In [5], an experimental droplet life trend was obtained by recording the full evaporation time of a single droplet gently deposited on a hot plate. The heat flux was modelled as a function of fuel characteristics and ambient conditions during the injection process. Despite the substantial difference between the two life tests, especially in terms of quantity of the liquid involved and droplet velocity, it may be noticed how the two life curves follow a similar trend up to $T_N + 20$, i.e., 415 K. The heat flux determines the life trends as follows:

- *Nucleate boiling* ($T_{sat} < T_{wall} < T_N$): at $T_{wall} = T_{sat}$ the relatively high amount of liquid deposit ($T^* < 0$) experiences a slow evaporation rate due to the almost null heat exchange. Increasing the wall temperature, the formation of vapour bubbles at the boundary layer between liquid and wall has a double effect: 1. increase of the drywall fraction; 2. absorption of the increased heat flux. However, the phenomena are light in this regime resulting in a drastic reduction of the liquid life due to the increased heat flux. Both life curves reach a minimum at $T_{wall} = T_L$.
- *Transition boiling* ($T_N < T_{wall} < T_L$): above T_N the formation of bigger bubbles and the further increase of the drywall fraction in the proximity of the liquid deposit increase the dimension of the vapour layer. As a result, heat flux decreases enhancing liquid life up to $T_w = T_N + 20$. Moreover, the relatively high wall temperature influenced the impact regime of the liquid ($T^* > 0$) and consequently, the amount of deposit was reduced in comparison with lower temperatures. Approaching $T_{wall} \approx 445K$ film life and drop life differed due to the nature of the tests and the distinction between LF and single droplet within the numerical model. The amount of film deposit continues to decrease with increasing wall temperature and even if the heat flux is reduced, the resulting life is lower. The single droplet instead is increasingly protected by the vapour bubbles and hence its life is increased.
- *Film boiling* ($T_{wall} > T_L$): at $T_{wall} = T_L$ no LF was formed because of the Leidenfrost effect that influenced the impingement behaviour of the droplets (rebound). As a result,

LF life is zero from $T_{wall} = T_L$ and above. The amount of heat flux is negligible. In the experimental counterpart, the vapour cushion formed between the droplet and wall dissipated the vast majority of the heat resulting in the highest drop life.

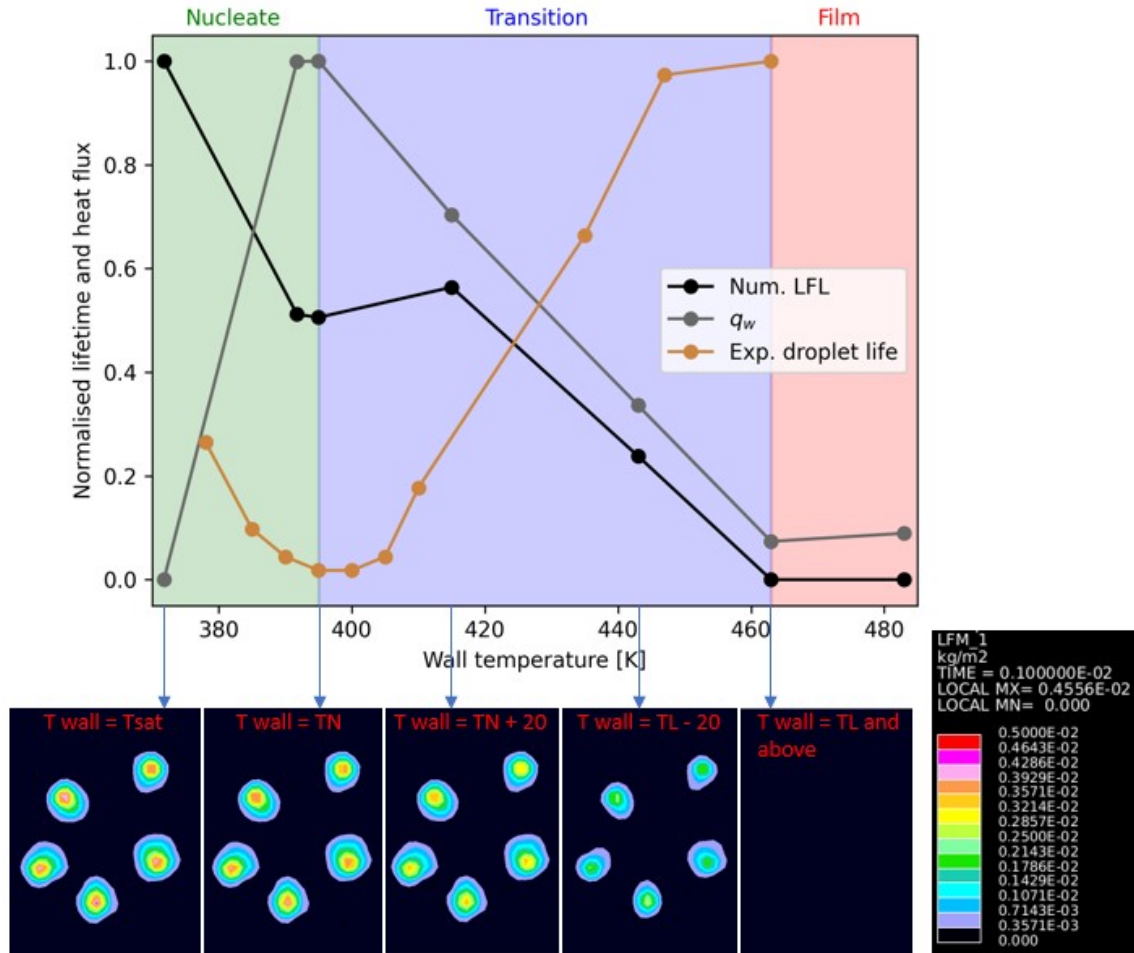


Fig. 5.15 The normalised LF lifetime for a high-pressure fuel spray (black line) impacting on a hot wall as a function of the wall temperature. In the images below the graph the liquid footprints and their tendency to deteriorate for higher temperatures. The heat flux (grey line) reconstructed from Equation 3.17 is reported. For comparison, the droplet lifetime (gold line) from the Stanglmaier experiment [5].

The comparison between numerical fuel droplets, vapour and film mass as a function of wall temperature is shown in Figure 5.16. Across the wall temperature sweep, the amount of fuel vapour is almost identical while droplets and LF are inversely proportional. The balance among the three quantities is similar up to T_N , i.e., 395 K, because the operating conditions fell into the fuel deposition impingement region ($T^* < 0$). The balance in percentage compared with the total fuel injected is 50% fuel drops, 16% fuel vapour and 33% fuel

film. Above $T_{wall} = T_N$, the impingement behaviour produces by the hotter wall increases the number of droplets fluctuating after the first impact with the wall and consequently the amount of LF mass is reduced ($T^* > 0$). At $T_{wall} = T_L$ and above the balance is 84% fuel drops and 16% fuel vapour due to the Leidenfrost effect that creates a vapour cushion between fuel droplets and the hot wall. The phenomenon is crucial for GDI engine application because the increased quantity of free droplets, if not vaporized before ST, might have an impact on mixture preparation and in turn on engine-out emissions [60]. In particular during stratified charge operations, due to the limited time between EOI and ST, the residual droplets may suffer direct carbonization during the combustion process, with a consequent increase in PM emissions [79].

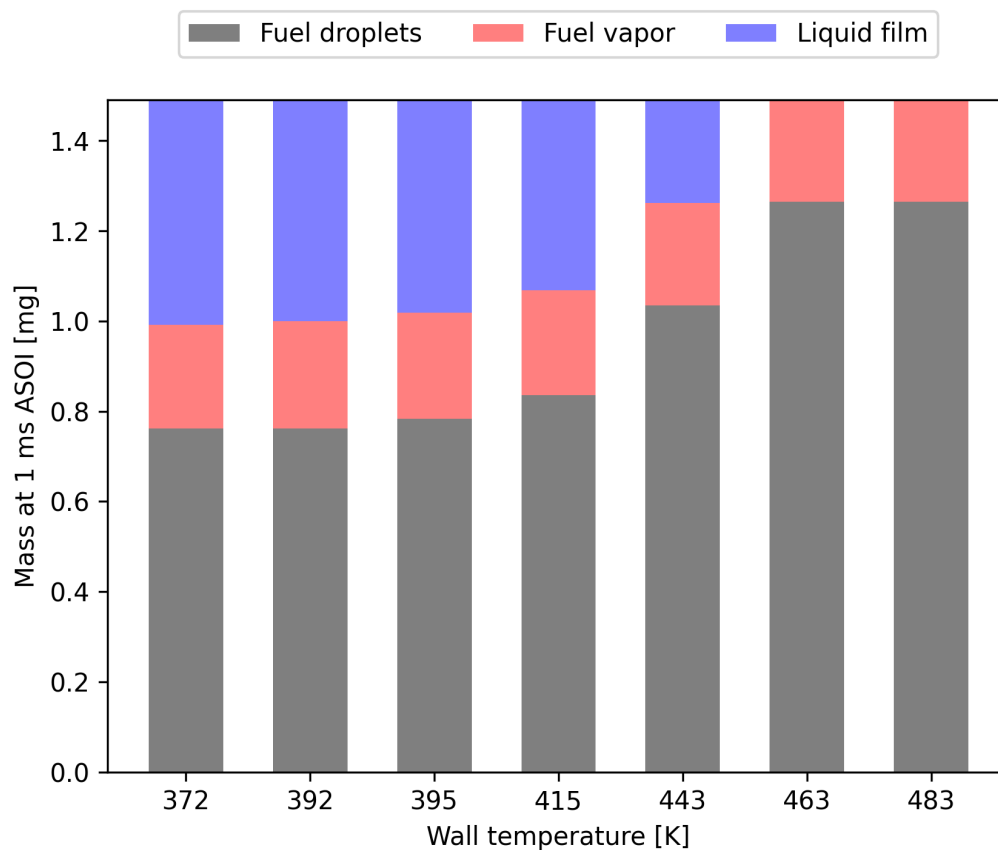


Fig. 5.16 Fuel shares among droplets, vapor and film as a function of the wall temperature.

To further validate the LF model, Figure 5.17 shows a comparison between experimental and CFD values for two FRP (150 and 300 bar), highlighting the consistency of the model in reproducing fuel retained on a hot surface. The analysis was performed by a member of the Engine Modelling Team and the results are presented in [3]. At the lowest temperature tested, the fuel deposit was 38% of the total injected. The number reduced significantly to

6% and almost zero for 140 and 180 °C, respectively. Once passed the boiling temperature threshold of the fuel (for isooctane, 99.4 °C) the reduction of fuel deposit is driven by an increased evaporation rate. The deterioration of liquid deposits mitigates the pool fire phenomena and a possible source of soot emissions [3, 101]. However, the creation of sub-stoichiometric regions in proximity to the hot wall might compromise the charge homogeneity with detrimental effects on engine-out emissions. Similar to the previous injection pressure, the 300 bar case presents a decreasing trend with increasing temperature but with an overall reduction of the liquid retained due to enhanced atomisation and evaporation prior to the impact of the fuel on the surface.

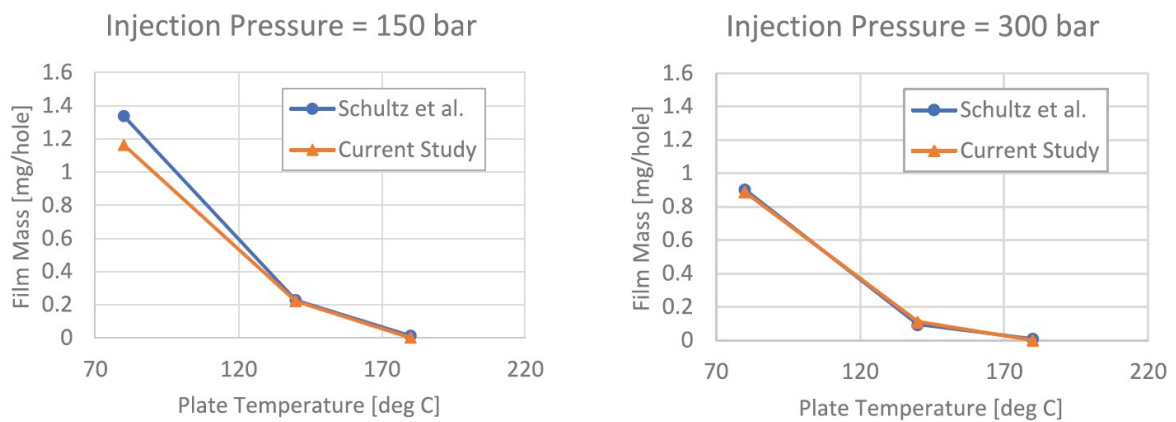


Fig. 5.17 LF mass comparison between the current study and experimental measurements [6] at 150 and 300 bar injection pressure [3].

Chapter 6

In-Cylinder Mixture Analysis Results

In this chapter, a detailed analysis of the mixture characteristics is presented with a particular focus on LF and the influence of piston temperature. As it will be revealed, the latter can be controlled to mitigate the engine's tendency to liquid deposit and accumulation.

First, a simplified LF analysis for isooctane was performed proving the physical behaviour of the model and how wall temperatures have a direct effect on the mixture preparation process. Then three engine operating conditions were investigated using an accurate surrogate fuel model. For each point, engine variable sweeps (FRP and SOI) aimed to uncover the interconnection between LF, mixture indicators and PN emissions¹. The chapter continues with an analysis of piston cooling due to the direct injection of fuel. The other cooling mechanism due to PCJ is then explored given the experimental evidence of PN level reduction with higher piston temperature. Temperatures for LF minimisation and full disappearance are provided.

The last section of the chapter presents an analysis of split injection strategies for three operating conditions. While no experimental data were available for split injections, the analysis gives reliable indications on how to improve mixture indicators and mitigate liquid deposits.

6.1 Liquid Film Analysis - Isooctane

The operating condition 2000 rpm – 50 Nm, using isooctane as fuel, was selected to carry out a simplified analysis of the LF deposit on the piston crown during the engine cycle up to ST. This part-load point was the most tested during the project, both experimentally and numerically, and hence, from a statistical perspective, it was the best choice to reveal if the

¹The result presented in section 6.2 led to a publication [3].

data obtained were plausible. The initial use of isooctane instead of the surrogate fuel was dictated by the necessity to have an easy-to-solve, single-component fuel to reveal, at low computational cost, if the combustion chamber mesh was producing a plausible evolution of the liquid spray and deposits. A highly volatile fuel, with higher concentrations of isooctane might follow the presented trends. Figure 6.1 indicates the crank angle resolved LF evolution (Figure 6.1-a) and the corresponding LF life (LFL) (Figure 6.1-b) for 7 piston temperatures selected within the limiting temperature of isooctane, i.e., T_{sat} (365.2 K), T_N (387.7 K) and T_L (455.7 K). In Figure 6.1-a the highest peak of the LF corresponds, as expected, to the temperature of the piston equal to T_{sat} .

Once the film is deposited, it takes longer to evaporate completely because of the highest quantity of liquid involved and the relatively cooler temperature of the walls. Increasing the piston temperature up to T_N , the peak linearly decreases by 65% from 0.8 to 0.28 mg. An additional rise of 20 K revealed a reasonable increment (39%, from 0.28 to 0.39 mg) of the liquid deposit because of heat flux reduction. Above $T_N + 20K$ the reduction of the peak of LF is consistent with full disappearance at T_L . Following a physical behaviour, in the film boiling regime, the fuel deposition is inhibited by the Leidenfrost effect and the highest evaporation rate. Interestingly, no trace of the LF is retained at ST indicating how the isooctane is too volatile to replicate complex multi-component behaviours. Figure 6.1-b revealed how LFL and the heat flux were inversely proportional up to T_N . LFL is maximum (90 CAD duration) for wall temperature equal to T_{sat} and then it decreases to 27 CAD at T_N . LFL increases from 27 CAD to 34 CAD at $T_N + 20K$ due to heat flux reduction. From T_N the heat flux steadily decreased from its peak, 250 kW/m^2 , to 20 kW/m^2 where the Leidenfrost effect mitigates the liquid deposit and creates a vapour insulation between the piston and the liquid droplets. Increasing the wall temperature above the T_L does not produce any evident changes in terms of both LFL and heat flux.

To better explain the previous LF results, Figure 6.2-a shows the maximum mass of LF (LF peak) on the piston crown as a function of the temperature. It can be noticed the linear reduction up to 387.75 K (T_N), the slight increase at 407.75 K ($T_N + 20K$) and the severe reduction entering the transition and film boiling regime. Figure 6.2-b, for the same temperatures, shows the UI and the $M_{1,2}^+$ at ST. While for most of the temperatures the UI > 0.955, i.e., the combustion chamber was operating at high mixture homogeneity, the only noticeable reduction was during the slight increase of LF and LFL at 407.75 K. A reason might be the combination of the higher liquid deposit formed at this temperature that creates a delay of the total evaporation and the formation of localised sub-stoichiometric pockets in the region near the piston. However, UI might not be the best candidate to describe the mixture distribution as it is not able to capture the localised mixture inhomogeneity. For

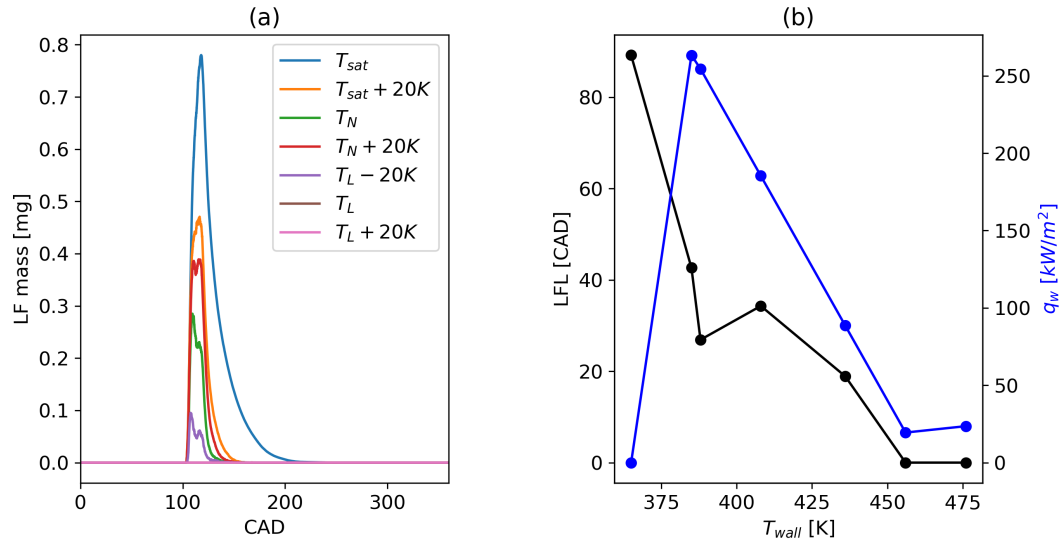


Fig. 6.1 LF mass as a function of CAD at different piston temperatures selected considering the limiting temperatures of the isooctane (a); LFL and heat flux as a function of the same temperatures (b).

this reason $M_{1,2}^+$ is analysed in parallel with UI. It can be noticed how $M_{1,2}^+$ provides a more linear variation when changing the piston temperature. As expected, the maximum value is obtained at the maximum temperature due to the Leidenfrost effect and hence the persistence of sub-stoichiometric pockets.

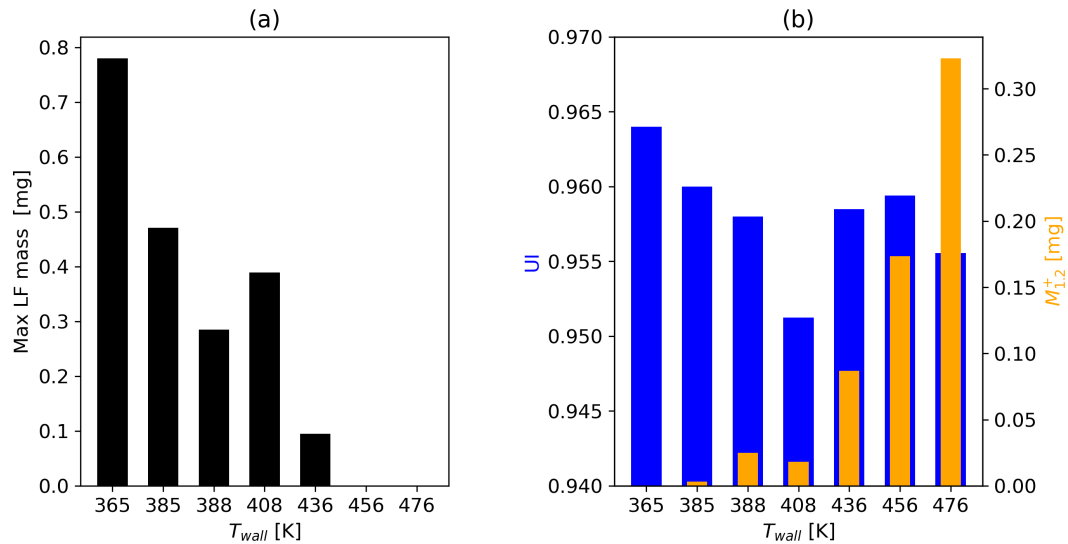


Fig. 6.2 Maximum LF mass at different piston temperatures selected considering the limiting temperatures of the isooctane (a); UI and $M_{1,2}^+$ for the same cases (b).

Figure 6.3 shows the in-cylinder images of droplets (top row) and LF (bottom row) at EOI considering the same piston and wall temperatures analysed so far. At T_{sat} the highest level of LF is produced with a footprint dictated by the injector geometry. Increasing the temperature until $(T_L - 20K)$ produced an expected reduction of LF and the start of the Leidenfrost effect with a thicker cloud of droplets in the proximity of the wall. When the piston temperature approached T_L the droplets rebounded on hot walls or suddenly evaporated. The cloud of free droplets was remarkable at T_L in comparison with the adhesion experienced by the fuel at T_{sat} . The region of LF deposition is also of great importance when trying to understand emission formation. It can be noticed how at T_{sat} a portion of the LF was formed on cylinder walls. Since all the LF disappeared at ST, this creates sub-stoichiometric regions and compromises the mixture homogeneity.

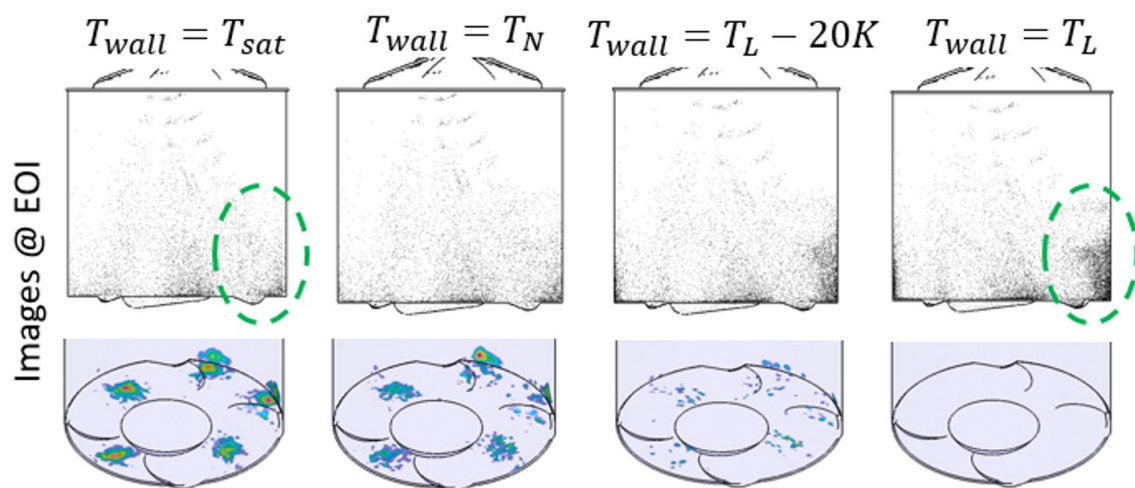


Fig. 6.3 In-cylinder images of the fuel droplets (top row) and LF (bottom row) at EOI. The piston temperatures were selected considering the limiting temperatures of the isooctane. In green circles the evidence of fuel droplets adhering to the cylinder walls at T_{sat} and the rebound experienced at T_L .

6.2 Mixture Characterisation and Liquid Deposition - Surrogate Fuel

SOI and FRP are among the most influential engine parameters to control the mixture process. The effects of SOI and FRP variation on mixture characteristics and correlations with engine-out PN are discussed in this section. Simulations were performed using the surrogate fuel describe in Chapter 3 (section 3.5). For clarity and brevity, one operating condition (2000

rpm, 50 Nm) was selected with three SOI settings: the calibration SOI (P21, calibration SOI and FRP 200 bar), an early SOI (P10) and a late SOI (P13). Calibration SOI value cannot be disclosed due to confidentiality as instructed by Ford UK. Regarding the FRP sweep, two operating conditions were selected to account for the variations introduced with different engine brake torques. The points investigated were P1-P4 mid-load conditions (2167 rpm, 61 Nm) and the high load P22-P25 (2500, 100 Nm). Please refer to Table 3.6 for more details regarding these points.

SOI sweep. Figure 6.4 offers a comprehensive representation of LF evolution during the intake/compression stroke (a), as a function of SOI (b), the resulting mixture indicators (c) and the experimental PN emissions (d). The vicinity between the piston and the injector produces the highest liquid deposit for the early SOI (Figure 6.4-a), LF that is retained in relatively great quantity (3% of the fuel injected) up to ST (Figure 6.4-b). As expected, the late SOI produces the lowest level of LF peak due to the reduced impact between the fuel spray and piston surface. The amount retained up to ST was less than 1%. The evaporation of the liquid deposit is faster for the calibration SOI due to the hotter piston temperature, in comparison to the early SOI where the cooling effect of the piston inhibits the evaporation, creating bigger deposits. For the calibration SOI, only 0.4% of the fuel injected was retained as LF at ST. Consistent with the LF analysis, the study of mixture indicators UI and M^+ reveals how the time for mixture preparation plays an important role in enhancing the mixture homogeneity. Figure 6.4-c shows how the late SOI, i.e., reduced mixture preparation time, has the worst UI (92%) and M^+ (3.2 mg). At calibration SOI, the mixture characteristics improve consistently with a UI > 95% and less than 0.8 mg of cells with $\phi > 1.2$. Interestingly, even if the calibration case is theoretically indicated as a stoichiometric, homogeneous mixture at ST, the model suggested how part of the fuel does not participate in the evaporation/mixing process and the equivalence ratio is less than ideal. Fuel-rich chamber pockets, represented by fuel-rich cell clusters in the computational domain, almost disappear for the early injection case, which presented both an almost zero M^+ and UI of 98%. The combined information of liquid deposit and mixture homogeneity can be connected to the experimental PN emissions. In Figure 6.4-d the PN levels suggest how PN emissions are driven more by LF than mixture homogeneity. In fact, despite the best levels of UI and M^+ , the early SOI shows the highest PN level of $5.5 \times 10^5 \text{ \#/cm}^3$ due to a massive fuel impact on the piston crown. With a calibration SOI, the level of PN decreases by one order of magnitude down to $1.1 \times 10^4 \text{ \#/cm}^3$, which is the lowest as expected. Effectively, any change from the baseline SOI would lead to an abnormal mechanism for mixture preparation (late SOI) or LF retention (early SOI), and in turn to much higher levels of PN.

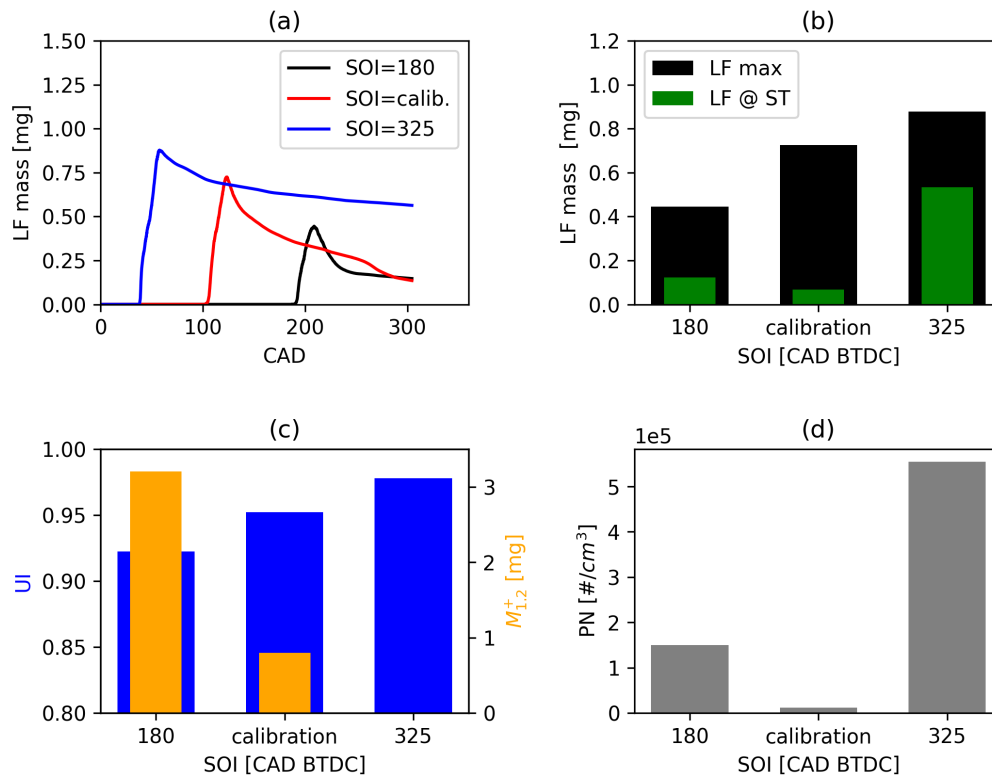


Fig. 6.4 Mixture analysis for the SOI sweep (P10, P13 and P21) in terms of crank angle resolved LF (a), LF as a function of SOI (b), mixture indicators as a function of SOI (c) and corresponding PN experimental emissions (d).

To better understand the mechanisms that lead to liquid retention and lack of homogeneity, in-cylinder images are presented in Figure 6.5 [3]. The author of these images, as well as Figure 6.7 and Figure 6.9, is the first name in [3], a member of the EMT. The study was conducted as a team effort and confirmed the mixture inhomogeneity effects analysed in this research project. The first row displays the distribution of spray liquid droplets at 10 CAD ASOI for the three cases. The second row reports the equivalence ratio distribution on a symmetrical plane mid-way through the compression stroke (90 CAD BTDC) and the last two rows show the equivalence ratio and LF thickness at ST, respectively.

For the calibration case, even if the injection process takes place during the intake stroke and hence while the piston was moving away from the cylinder head, the spray-to-wall interaction is responsible for a substantial fuel deposition. The rapid evaporation of the deposit, in combination with the free droplets' evaporation and the clockwise tumble motion, creates a highly rich region (red colour, $\phi > 4.6$) during the compression stroke. At the ST instant, even if the mixture distribution and homogeneity are improved, some areas with $\phi > 1.2$ persist demonstrating how engine calibration points cannot reach an ideal air-fuel distribution. Looking at the location of these highly rich regions, it seems that they corresponded to the location of the liquid deposit retained up to ST. This is physically reasonable as the evaporation of the LF creates sub-stoichiometric pockets next to the evaporation surfaces. For SOI 180 CAD BTDC, the spray plumes are at a reasonable distance from the piston and this mitigates the formation of LF on the piston's central area. However, two spots of liquid deposit were observed in the proximity of the liner/crevice as a result of the insufficient time available for droplets to fully evaporate and the squish motion of the charge toward the exhaust valves. The consequence of a limited mixture preparation time is noticeable looking at the equivalence ratio at 90 CAD BTDC where an extensive region of the chamber was at $\phi > 4.6$. The abnormal mixture process and the consequently richer regions persist up to ST where the evaporated fuel is mal-distributed, with central lean regions ($\phi < 0.8$) and a richer mixture concentrating toward the walls. As depicted in previous plots (Figure 6.4-a-b), the spray impingement is substantial for the early SOI case and the subsequent droplets' rebound and evaporation create a central, sub-stoichiometric region during compression. The richer charge pockets are then squeezed towards the walls by the piston motion and distributed on the two opposite sides of the chamber between the intake and exhaust valves. The overall mixture was slightly lean in the central, near-spark plug region. The piston cooling effect of the spray impingement, discussed below, promotes the formation of thicker LF in the piston bowl. The excessive liquid deposits and their location in the proximity of the spark plug are deemed responsible for the PN peak observed experimentally (Figure 6.4-d).

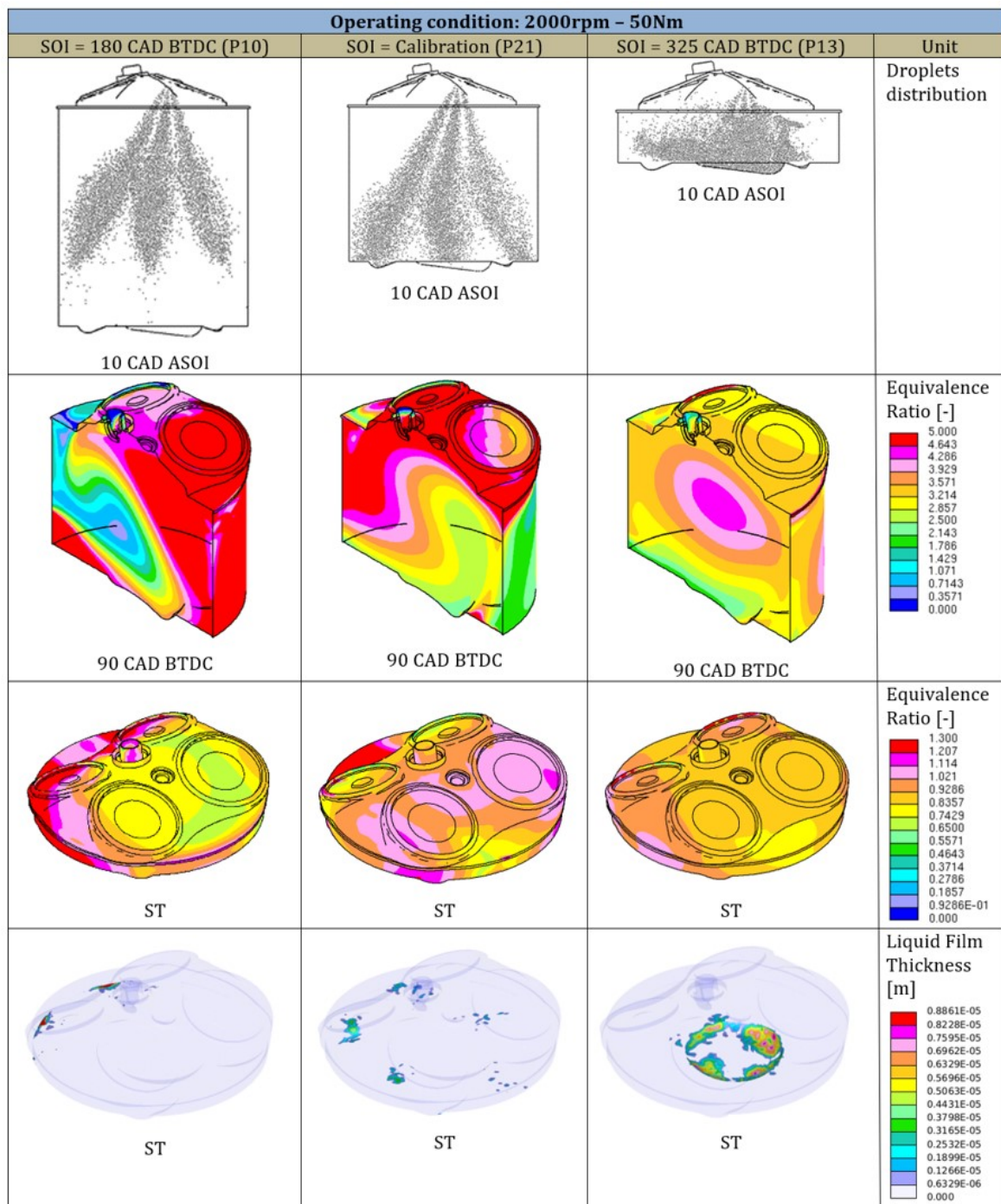


Fig. 6.5 Images of spray, equivalence ratio distribution and LF thickness distribution at various cycle locations, for 2000 rpm – 50 Nm operating condition. The column on the left refers to late SOI (180CAD BTDC, P10); the central column refers to baseline SOI (P21); the column on the right refers to early SOI (325 CAD BTDC, P13) [3].

FRP sweep. The engine operating conditions P1-P4 (2167 rpm, 61 Nm, mid-load case) and P22-P25 (2500 rpm, 100 Nm, high-load case), were selected from the available experimental database. The latter included FRP data between 50 and 200 bar.

FRP sweep, mid-load case. Figure 6.6 shows the crank angle resolved LF for all the FRPs (Figure 6.6-a), the LF peak quantities (Figure 6.6-b), the mixture homogeneity indicators (Fig. 72-c) and experimental PN (Figure 6.6-d) as a function of the FRP. Figure 6.6-a shows how the peak of the liquid deposit is proportional to the FRP. LF trends are similar for FRP50 and FRP100 with the first peak at around 15 CAD ASOI and a second peak at EOI (maximum peak). After the first peak, the combination of lower droplets' velocity, dictated by the relatively low FRP, and the piston moving away from the injector reduces the rate at which the liquid fuel accumulates on the walls. As a confirmation of the weaker atomisation for lower FRP, the SMD at 30 CAD ASOI was $16.6 \mu\text{m}$ at 50 bar and $6.88 \mu\text{m}$ at 200 bar. On the other hand, for the higher FPRs (150 – 200 bar), the wider fuel impingement due to greater plumes' penetration creates a single LF peak at EOI. Then the LF declines due to the joint effect of hot wall surfaces (hence evaporation) and interactions with the surrounding gas-phase motion. The decline of LF is similar for all the FRPs with a knee in the proximity of the last part of the compression stroke. This is related to the inertia of the piston, decelerating towards TDC, and the consequent stripping phenomena of liquid from wet regions [3]. The phenomenon is more pronounced at higher injection pressure because of the greater quantity of liquid involved.

To better quantify the LF as a function of FRP, Figure 6.6-b shows the maximum value of LF and the quantity retained at ST for the same operating conditions. It is clear that higher FRP brings disadvantages in terms of spray impingement, with 0.55 mg of maximum deposit (3% of the total fuel injected) at the highest pressure. The liquid retained at ST is less than 1% of the total fuel injected for the lower pressure cases (50 and 100 bar), almost 1% at 150 and more than 1% at 200 bar. While LF plays an important role in determining the emission behaviour, it cannot be directly correlated to PN without a combined analysis of mixture homogeneity indicators. As for the previous SOI sweep study, the UI and M^+ indicators were investigated as a function of injection pressure and the results are reported in Figure 6.6-c.

For FRP 50 bar, the mixture inhomogeneity is driven by relatively low spray atomisation that produced big and slow droplets. This case produces a relatively low UI and consequently a higher level of M^+ , with values $<93\%$ and 3.3 mg, respectively. Even a small reduction in UI can be associated with a large variation in PN emissions [28]. Indeed, a parallel analysis of PN in Figure 6.6-d suggests how even if the 50 bar case has the lowest liquid deposit retention, the inhomogeneity of the mixture is the main cause of the highest level of PN recorded within the FRP sweep analysis, i.e. $8 \times 10^4 \text{ \#}/\text{cm}^3$. At 100 bar, the mixture

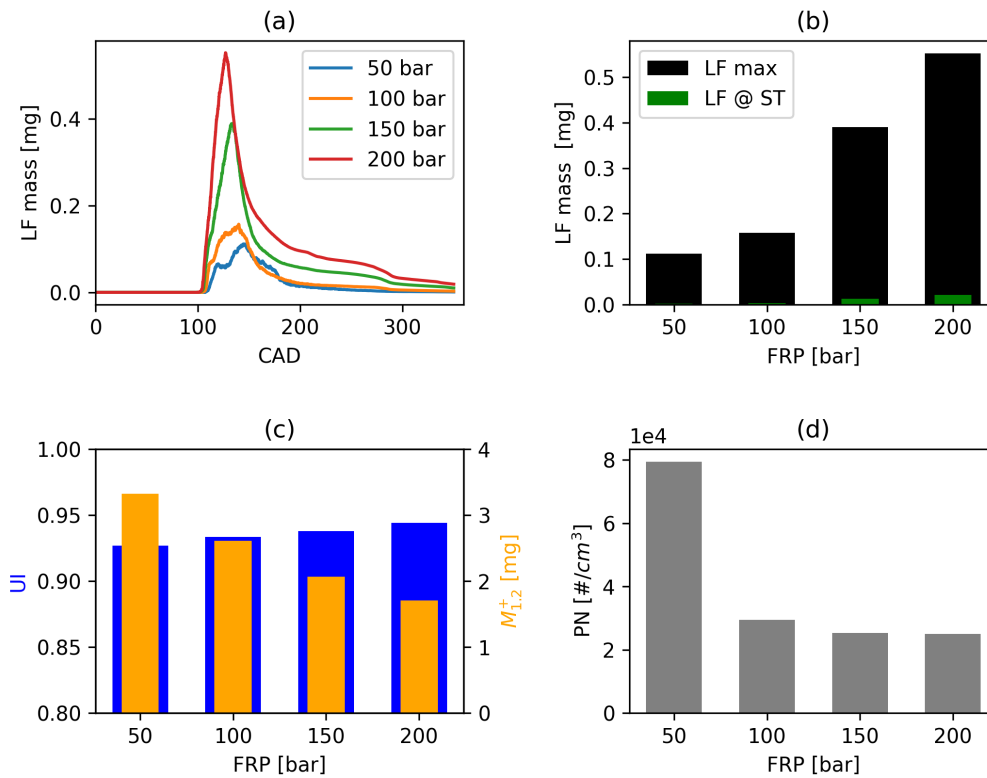


Fig. 6.6 Mixture analysis for the FRP sweep (P1, P2, P3 and P4), operating condition 2167 rpm – 61 NM, in terms of crank angle resolved LF (a), LF as a function of FRP (b), mixture indicators as a function of FRP (c) and corresponding PN experimental emissions (d).

indicators improve with $UI > 93\%$ and M^+ at 2.6 mg, meaning that less than 15% of the fuel injected is retained as vapour in fuel-rich pockets ($\phi > 1.2$). Consequently, PN reduced to $3 \times 10^4 \text{ \#}/\text{cm}^3$ and the decrease was consistent through all other pressures. In fact, from 150 bar to 200, UI steadily increases above 93% while M^+ levelled off at around 2 mg (11% of the total mass injected).

The details of the mixture distribution and the LF location are presented by means of CFD images in Figure 6.7. The figure shows spray images (top row), equivalence ratio distribution (middle two rows) and LF thickness (bottom row) for all the injection pressures investigated. The stronger atomisation produced by higher FRP increases both the fuel atomisation and spread for the 200 bar cases. In fact, considering the instant 30 CAD ASOI, the 200 bar case has a cloud of droplets on the left side of the image that does not appear for the lower injection pressure.

The equivalence ratio distribution improves as FRP increases. At 90 CAD BTDC (compression stroke) the mixture distribution was slightly more stratified for the 50 bar case. The extra-lean central region ($\phi < 0.7$) gradually disappears increasing the injection pressure. At ST, the 50 bar case shows two fuel-rich regions ($\phi > 1.2$); one in the proximity of the exhaust valves and another along the dome near the injector location. The equivalence ratio of this second region gradually decreases with injection pressure. In fact, at 200 bar an almost stoichiometric mixture is obtained in the vicinity of the injector and spark plug. The fuel-rich region in proximity of the exhaust valves (squish region) seems almost unaffected by the FRP variation as a result of the interactions between the spray plumes and the bulk flow motion of the chamber that pushes the fuel droplets toward the exhaust side.

The LF thickness and the spread of the pools increase with increasing FRP. The peculiar footprint with five clusters noticeable at 200 bar is obviously related to the injector geometry but also to the fact that the points were investigated using the baseline/calibration SOI timing. Different SOI would have produced different footprints as evident referring back to the early injection setting (see Figure 6.5, SOI = 325 CAD BTDC). Very small amounts of LF are retained before combustion, with the maximum quantity registered at 200 bar due to stronger spray penetration and fuel-piston interactions.

FRP sweep, high-load case. In Figure 6.8-a the crank angle resolved LF up to ST is presented for the injection pressures 50 bar – 200 bar. Similarly to the mid-load case, the peak of LF is proportional to the FRP. On the contrary, the higher injection pressures (150 and 200 bar) show two peaks (one soon after the SOI and a second at the EOI). This is related to a combination of higher fuel quantity injected and the phasing of the SOI specific to this operating condition. Figure 6.8-b shows the maximum peak of LF during the cycle and the liquid retention at ST as a function of the FRPs. More than 0.5 mg of fuel accumulates on the

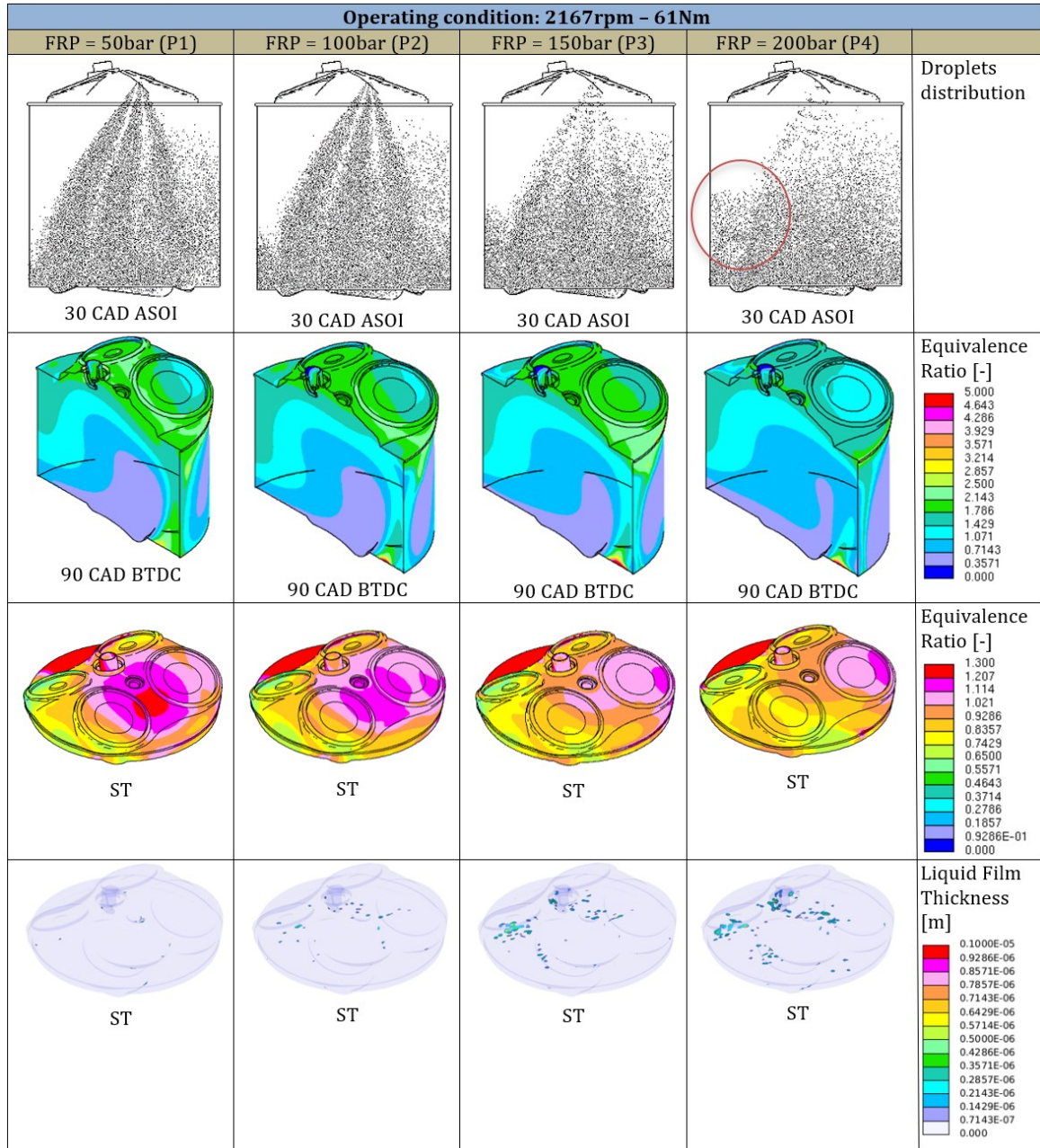


Fig. 6.7 Images of spray, equivalence ratio distribution and LF thickness distribution at various cycle locations, for the 2167 – 51 Nm operating condition. From the left column to the right, the FRP is increased from 50 bar (P1) up to 200 bar (P4). [3]

piston crown for the 200 bar case but all this quantity evaporates before ST. This behaviour is consistent when looking at the lower FRPs. Interestingly, the 100 bar case produced the greatest amount of deposit at ST even if this quantity is well below the 0.1 mg threshold. Consistently with the previous load, both mixture indicators (UI and M^+) improve with FRPs, as shown in Figure 6.8-c. In particular, the UI stabilises at around 0.95 from 150 bar and above, while the M^+ is below the 3 mg threshold. The worst mixture was recorded for the 50 bar case, with a UI < 0.94 and a M^+ at almost 4 mg. The mixture indicators are well aligned with the experimental PN emission trends. As evident in Figure 6.8-d, the level of PN decreases from $3.8 \times 10^6 \text{ \#}/\text{cm}^3$ at 50 bar to $1.5 \times 10^6 \text{ \#}/\text{cm}^3$ at 200 bar.

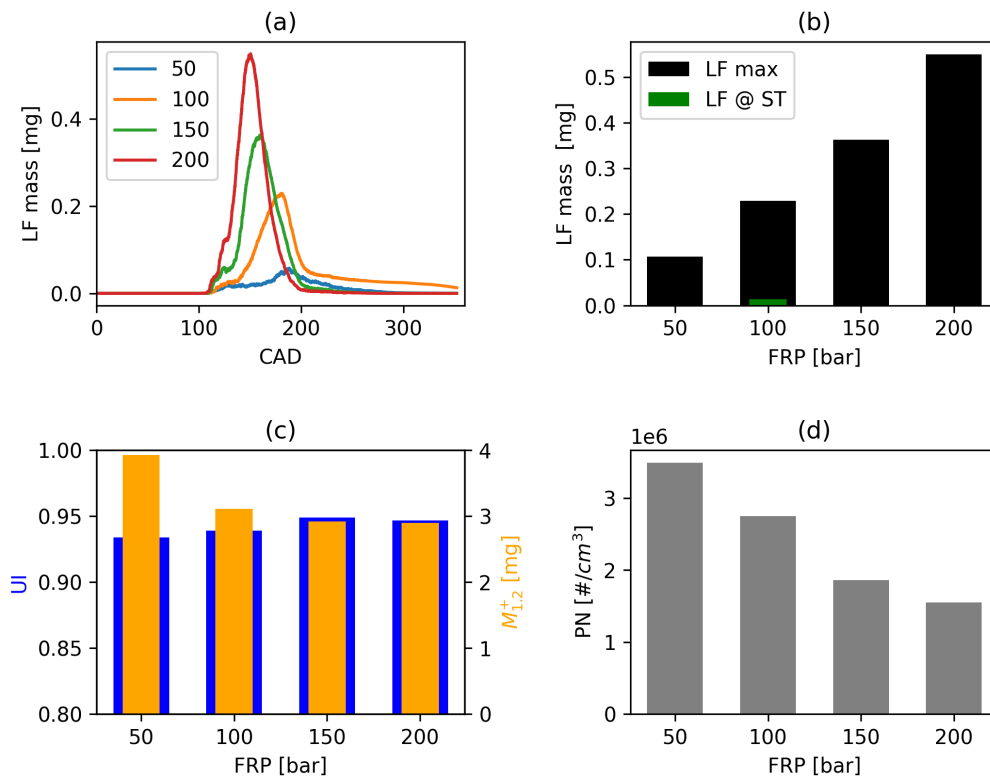


Fig. 6.8 Mixture analysis for the FRP sweep (P2, P23, P24 and P25), operating condition 2500 rpm – 100 NM, in terms of crank angle resolved LF (a), LF as a function of FRP (b), mixture indicators as a function of FRP (c) and corresponding PN experimental emissions (d).

Figure 6.9 presents the in-cylinder images in terms of droplet distribution (top row), equivalence ratio (two rows in the middle) and LF thickness at ST (bottom row). The droplet distribution is quite similar for all the injection pressures. The lowest pressure case, 50 bar,

had the slowest plume penetration and this is noticeable with one of the plumes not able to reach the piston surface. This was correlated to the overall tumble motion that generated a flow field able to contrast the liquid penetration in that region. While the injector holes are tuned to produce the same MFR (at a fixed pressure and mass injected), the weaker momentum of the plumes at 50 bar and the bulk-plume interactions in that region produce a stall of the droplets. To support this, a vector scene is added. It is evident the antilock-wise bulk motion that prevented the full propagation of the far left plume. This phenomenon is evident also at 100 bar and disappears at 150 and 200 bar due to a stronger droplet penetration/momentum.

In contrast with the previous mid-load case, this high-load case does not produce any major improvement in mixture homogeneity increasing the FRP from 150 to 200 bar. A fuel-rich region ($\phi > 1.2$) persists near the exhaust valves/squish region. While the charge is stratified in proximity to the injector, the values are almost stoichiometric ($\phi = 1$). This is evident at 200 bar injection pressure, where the stoichiometric area expands toward the second intake valve. The higher load translates into the maximum piston temperature and consequently a fast fuel deposit evaporation. Almost none of the fuel deposited on the piston crown is retained at ST. While the strong evaporation facilitates the disappearance of the LF before the combustion event, the limited mixing time and the higher amount of fuel injected are responsible for the great amount of PN measured during experimental tests ($\text{PN} \approx 1\text{e}6 \text{ \#}/\text{cm}^3$). This behaviour is consistent throughout all the injection pressures.

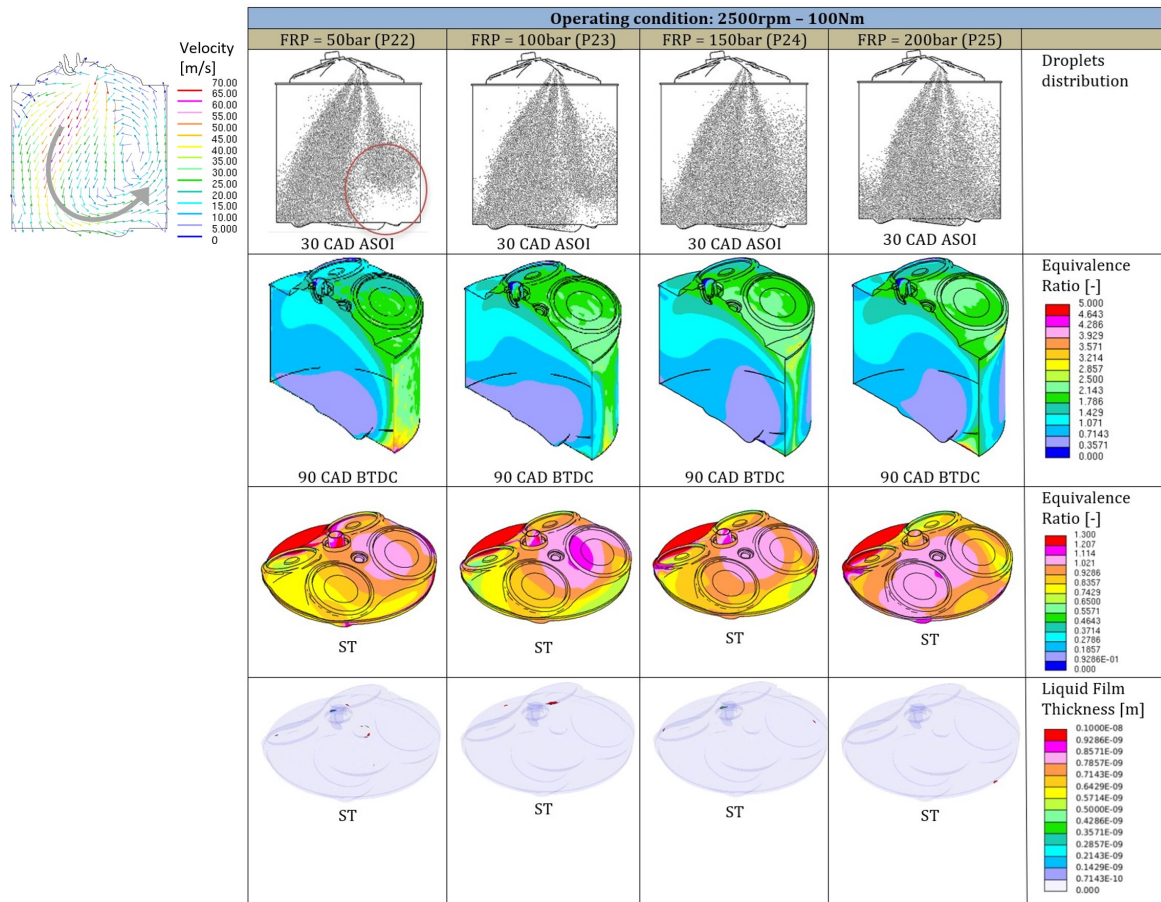


Fig. 6.9 Images of spray, equivalence ratio distribution and LF thickness distribution at various cycle locations, for the 2500 – 100 Nm operating condition. From the left column to the right, the FRP is increased from 50 bar (P22) up to 200 bar (P25). [3]

6.3 Piston cooling effect

As the fuel spray impacts on the piston crown, it produces a cooling effect. This paragraph quantifies the momentary fall in temperature that might be associated with an accumulation of LF if considering multiple engine cycles [152, 107].

The dependency between the cooling of the piston surface and the selected engine control parameters, FRP and SOI, is presented in Figure 6.10. The operating condition investigated were P9, P21 and P13, i.e, 2000 rpm, 50 Nm of torque at three levels of SOI (early, calibration and late) and 200 bar of injection pressure. Using the parametric nature of the CFD simulations, the same points were analysed reducing the injection pressure to 50 bar. The aim was to evaluate how a reduced fuel impact intensity on the piston crown affects the cooling effect. For all the simulations the fuel temperature at injection was 348 K as per

the experimental counterpart. The piston temperature was set to 480 K as reported in similar studies [3].

On average, because of the spray-to-wall interactions, the piston temperature decreases by more than 2 K at 200 bar and below this threshold for the 50 bar case, as reported in Figure 6.10-a. As expected, retarding the SOI timing mitigates the intensity of the liquid impact, reducing in turn the drop in temperature experienced by the piston. While the overall surface temperature did not seem particularly affected by the injection process, the localised effect at the plumes' footprints generated reductions in excess of 20 K as indicated in Figure 6.10-b. Interestingly, the late SOI case (180 CAD BTDC) had an increased localised drop in temperature in comparison with the calibration SOI point due to the location of the wetted area near the cylinder walls as shown in Figure 6.11. On the contrary, in the case of early injection timing, the area of spray impact is concentrated on the piston bowl. For the case of calibration SOI timing, the areas with localised cooling corresponded more precisely to the plumes' footprint. This was due to the location of the piston during the injection process for the specific SOI.

If LF mass retained at ST is sufficiently large (≥ 1 mg), it may survive through the engine cycle, especially if supported by lower piston temperatures, e.g., at early SOI and/or low engine load conditions [3]. This might cause an accumulation of liquid deposits in time, raising PN due to the phenomenon of pool fire. As discussed above, the process also influences the mixture homogeneity by creating regions of air-fuel mal-distribution in the proximity of the deposits. For these reasons, the modelling of the cooling effect is essential for a correct representation of the spray and mixture preparation process. Following this investigation, as mentioned in the methodology section, to capture the effects of spray impingement, the piston surface temperature was reduced linearly between calibration SOI timing and early SOI timing, with a reduction of 30 K for $\text{SOI} > 300$ CAD BTDC.

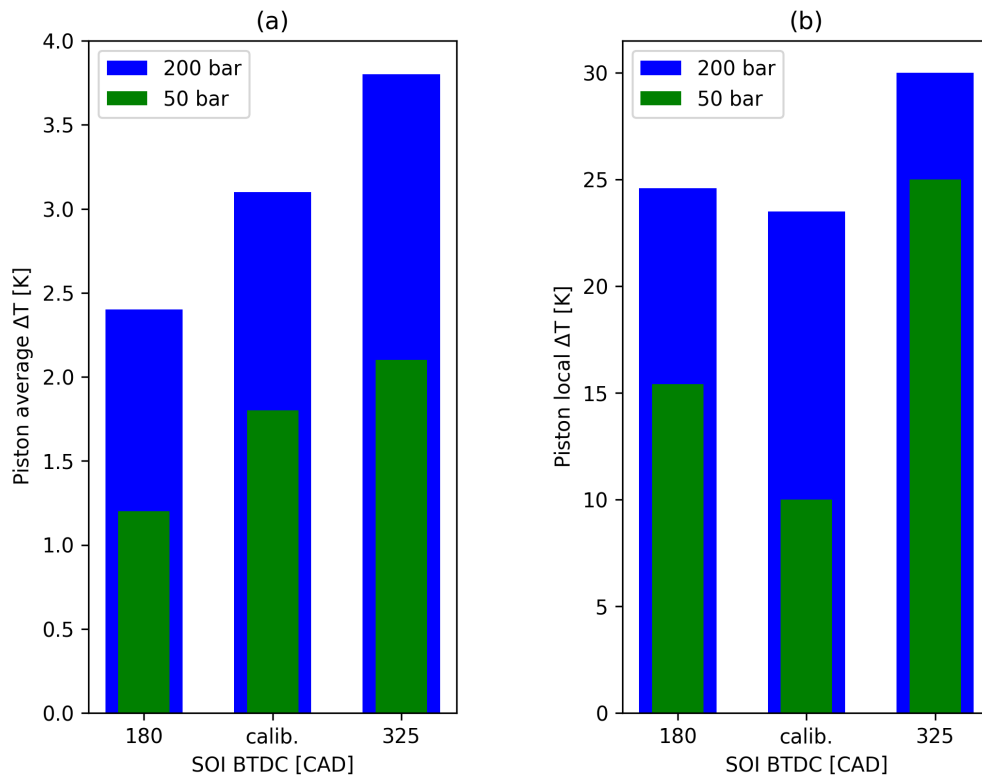


Fig. 6.10 The cooling effect experienced by the piston due to spray-to-wall interactions is presented for the 2000 rpm – 50 Nm operating condition for different combinations of SOI and FRP. The average temperature drop (a) refers to the entire piston surface; the localized temperature drop (b) considers the regions interested in droplets' impact.

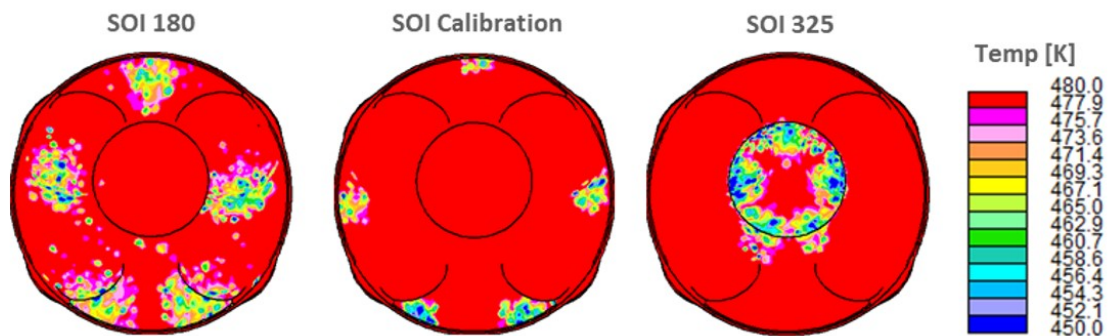


Fig. 6.11 CFD images of the piston surface temperature at EOI for three levels of SOI, 200 bar injection pressure, and 2000 rpm - 50 Nm operating condition. SOI is expressed in CAD BTDC.

6.4 Piston Limiting Temperatures

The cooling effect produced by the fuel spray over the piston crown might initiate an accumulation of liquid deposit that eventually burns releasing higher levels of PN, as mentioned in the previous paragraph. Moreover, the specific PCJ strategy might cool the piston bottom surface, aggravating the phenomena. The combustion of the accumulated liquid fuel, i.e., pool fire, for the operating condition 3000 rpm – 85 Nm is shown in Figure 6.12-a. For more details on the experimental borescope videos please refer to [3]. The experimental image was provided by DynAMO project partner Loughborough University. The flame is generated toward the end of combustion (MFB90) in the piston bowl location. The digital model of the same operating condition in Figure 6.12-b clarifies how the piston bowl is the location where a higher quantity of LF is accumulated at ST. The abnormal combustion process not only introduces cycle-to-cycle instabilities but also generates more PN.

Using the digital model capabilities, a parametric study was conducted to understand at which temperature the piston should be kept to remove any LF retention at ST. The idea was developed by a member of the EMT and here is briefly described using the results obtained by the author. Figure 6.13 shows three operating conditions from Table 3.6 and the extra point 3000 rpm – 85 Nm. The points were selected to see how this piston limiting temperatures change in respect of engine speed and load. Increasing both speed and load (P31, P21 and P25) the piston temperature must be increased to produce a full evaporation of any LF left at ST. Despite the higher bulk flow intensity at a higher speed, the full evaporation of LF seems more effective by increasing the piston temperature. At P31 (low speed and load) a piston temperature of 500 K is necessary to remove any fuel liquid deposit and this temperature increased by 10 K for the higher speed-load (P25). The slight reduction of this temperature seen at 3000 rpm – 85 Nm clarifies how the temperature is more affected by the engine load (hence fuel injected) rather than speed.

Ideally, all the liquid deposits should evaporate completely and on time for an appropriate mixture homogenisation. If the piston temperature is consistently kept above 510 K, LF should fully evaporate before combustion at all operating conditions presented in this analysis. The proposed concept might also explain the high surge in PN emissions typically measured during transient operation [152, 107]. In fact, during acceleration or cold starts the sudden cooling of the piston crown (from fuel spray) and bottom (from PCJ) boosts the accumulation of liquid deposits. Even if this limiting piston temperature is engine/fuel-specific, the methodology is robust and can be used for informed decisions when developing piston coating and/or emissions strategies. To have a complete framework of the proposed concept, further investigation should be carried out in terms of engine efficiency, reliability and piston costs. Future works will focus on the analysis of these crucial factors.

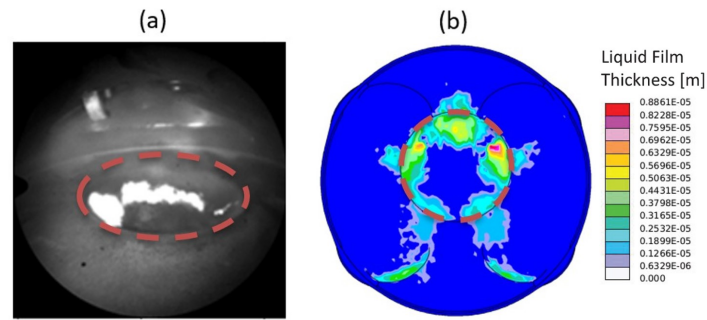


Fig. 6.12 In-cylinder experimental image from borescope videos of the combustion process at MFB90 (a) and the corresponding CFD image (top view of the piston) of liquid film at ST (b) [3]. Operating condition 3000 rpm – 85 Nm.

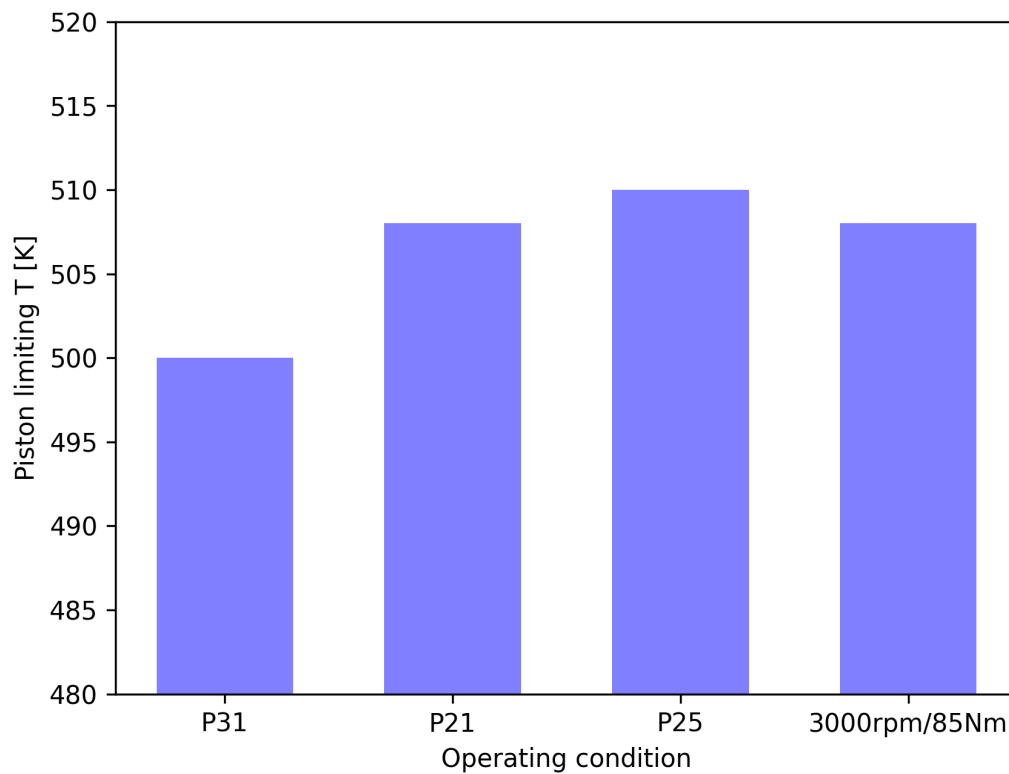


Fig. 6.13 Extrapolated limiting piston temperatures for LF full evaporation (0 mg) at ST; P31 (1500 rpm – 20 Nm), P21 (2000 rpm – 50 Nm) and P25 (2500 – 100 Nm). The 3000 rpm – 85 Nm was investigated because experimental images from borescope videos were available for this operating condition.

6.5 The Benefit of the Split Injection Strategy

To exert the full potential of the model, injection strategies targeted at improving the mixture preparation process were investigated. The analysis aimed to quantify the advantages of split injection in terms of LF retention at ST and mixture homogeneity indicators (UI and M^+). Even if no experimental data were available on the use of split injections, the numerical investigation served to outline the potential effects of delivering the fuel in separate pulses, firstly reducing spray penetration and, in turn, wall impingement and secondly enhancing the mixture homogeneity. Table 13 shows the details of the P4 operating condition selected for this analysis. The MFRs for the operating condition are presented in Figure 6.14. Slip injections are produced by dividing the total injection pulse width and assigning a specific quantity of fuel for each pulse. For this analysis, the same amount of fuel was injected for each pulse. The injection strategies were 1 injection (reference case), 2 injections and 3 injections. The pulse width separations were imposed at 1200 μs following similar studies [153]. For the single injection case, the overall injection duration was 22 CAD. With the 2 and 3 injections the overall duration was 40 and 57 CAD, respectively. The overall fuel injected was identical for all the cases (18.5 mg).

Table 6.1 Engine operating conditions for split injection investigation.

Point	Engine Speed [rpm]	Engine Load [Nm]	Fuel Injected [mg]	FRP [bar]
P4	2167	61	18.5	200

In Figure 6.15-a the LF evolution over the engine cycle as a function of CAD is reported for the three injection strategies. While the single injection case shows a maximum peak of LF of more than 0.5 mg, the split injection strategies reduced this peak by more than half, down to 0.2 mg. It is noticeable how the 2-injection strategy has two LF peaks and the 3-injection strategy has three. The delay between each pulse allows the piston to move away from the nozzles reducing the spray-to-wall interactions. Also, the reduced pulse width introduced by the split injection translates into a substantial decrease in spray penetration. The analysis of LF as a function of the number of injections shown in Figure 6.15-a confirms the advantages of splitting the injection phase. Similar levels of LF are predicted for all the injection strategies, with liquid fuel retention at ST below the 0.1 mg threshold.

In Figure 6.15-c, the reference case (single injection) shows the worst mixture parameters with $UI < 0.95$ and $M^+ > 1.5$ mg. These parameters improve with the two-split injection and even further with the three-split one, where UI is above 0.97 and no cell is found with $\phi > 1.2$ (i.e., $M^+ = 0$). Indeed, a three-split injection strategy for P2 would most likely translate into a large reduction in PN emissions.

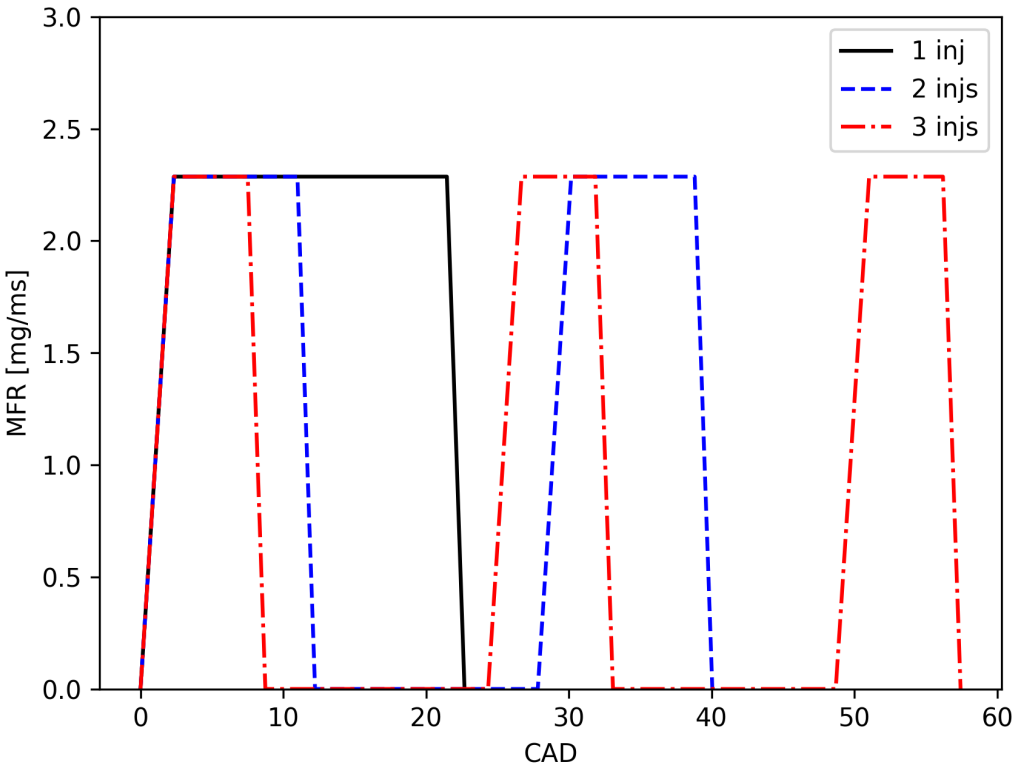


Fig. 6.14 MFR profiles for P4. The black line represents the single injection, the blue is for the double and the red line indicates the three injections.

The location of the liquid deposits at ST for the three injection strategies is presented in Figure 6.16. Even if a similar quantity of LF at ST is predicted for all the cases, again the 3-injection strategy seems the best in reducing the spray-to-wall interactions.

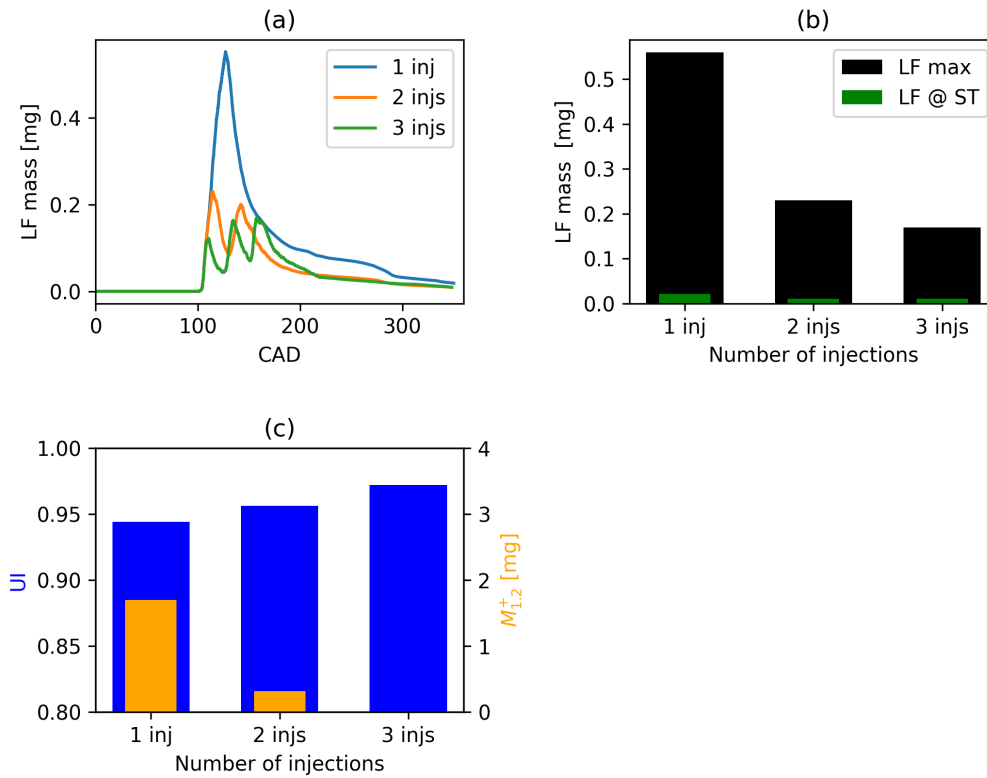


Fig. 6.15 Crank angle resolved LF (a), LF as a function of the number of splits (b) and the corresponding mixture indicators (c) for P4 operating conditions. No experimental data were available for the PN levels obtained with split injection strategies.

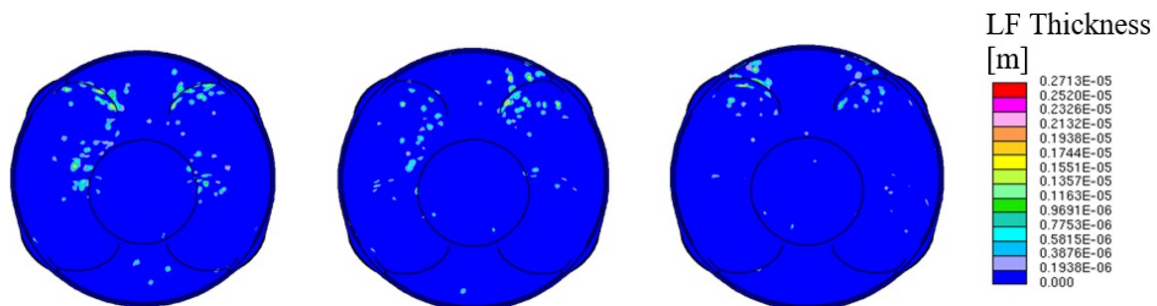


Fig. 6.16 LF on the piston crown for single injection (left), double injection (middle) and three injections (right) at ST. P4 operating condition.

Chapter 7

PN Surrogate Model

The development of a novel PN surrogate model based on mixture characteristics is presented in this chapter. The model is developed through extensive CFD analysis and considers a range of part-load operating conditions and single-variable sweeps where control parameters such as SOI and FRP are varied in isolation. The test points used in this piece of work are summarised in Table 3.6 (Chapter 3). An EN regression technique was used to identify the relevant relationships between experimental engine-out PN emission levels and modelled pre-combustion air-fuel mixture quality indicators. Within limits, engine sooting tendencies can be reliably predicted without reliance on combustion characteristics, which are complex to measure and predict through modelling techniques.

The chapter begins by presenting the cascade model approach utilised to obtain a PN surrogate model from a vector containing one hundred CFD-based quantities. Then the performance of models obtained through EN regression is evaluated against relevant statistical indicators. Once the best model combination is selected, the prediction capabilities are evaluated through a comparison with the experimental counterpart. Finally, the model features are analysed by observing their behaviour for relevant engine operating conditions and through the single-variable sweep of SOI and FRP.

7.1 Cascade Model

The cascaded PN surrogate model layout is presented in Figure 7.1. PN can be expressed as a function of mixture indicators (features) extrapolated from the CFD analysis as discussed in sections 3.4 and 4.4. The x matrix is formed by a total of 100 region/time-based, mixture-related, features selected from CFD simulation results. Each feature was normalized and then mathematically transformed using polynomials of a maximum degree of two, logarithm and exponential function as shown in Table 4.2 in section 4.4. As a result, the number of

regressors was much larger than the number of data points (34 points, indicated in Table 3.6). An EN regression approach [139] identified the values of the coefficient related to each factor and this resulted in a chart where the most influential were selected. A total of four mixture indicators (surrogate input feature models) were sufficient to predict the experimental PN.

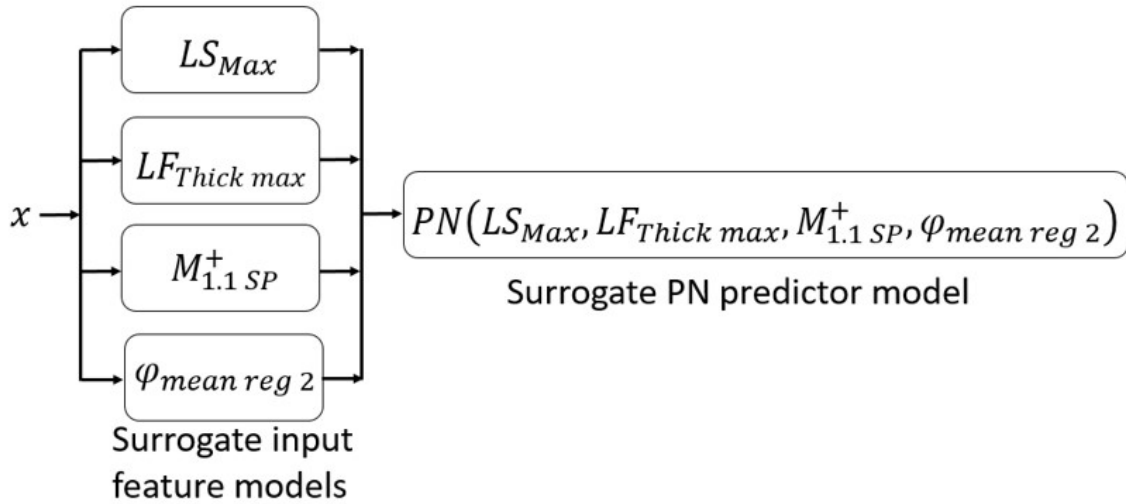


Fig. 7.1 The PN surrogate model was obtained through a cascaded approach. The regression matrix x is formed by CFD-based mixture quality indicators. The EN regularisation approach extrapolated the most dominant features to predict the PN and hence provided the resulting equation [2].

7.2 Model Prediction Performance

The regression analysis utilised the experimental PN quantities and CFD mixture features based on all 34 points from Table 3.6 in section 4.4. The variation of MSE as a function of the hyper-parameter λ (please see section 4.4 for more details) is presented in Figure 7.2. The error increases with λ meaning that when the number of features selected by the regression decreases an underfitting problem arises and compromises the prediction performance. As evident from the plot, MSE becomes almost independent for $\lambda > 1.6$. A minimum error of $\text{MSE} = 0.24652$ is found for $\lambda = 0.053454$. This model is called *Model – A* and is formed by 15 features plus an intercept. Analysing the features and the coefficients of *Model – A* it is possible to establish that the most important in determining the experimental PN are mathematical transformations of LS_{max} , $LF_{Thickmax}$, $M_{1.1SP}^+$ and $\phi_{mean-reg2}$.

These features were used to form a new, simpler, regression matrix that then was analysed with an EN approach and led to a new PN model called *Model – B*. Both PN surrogate

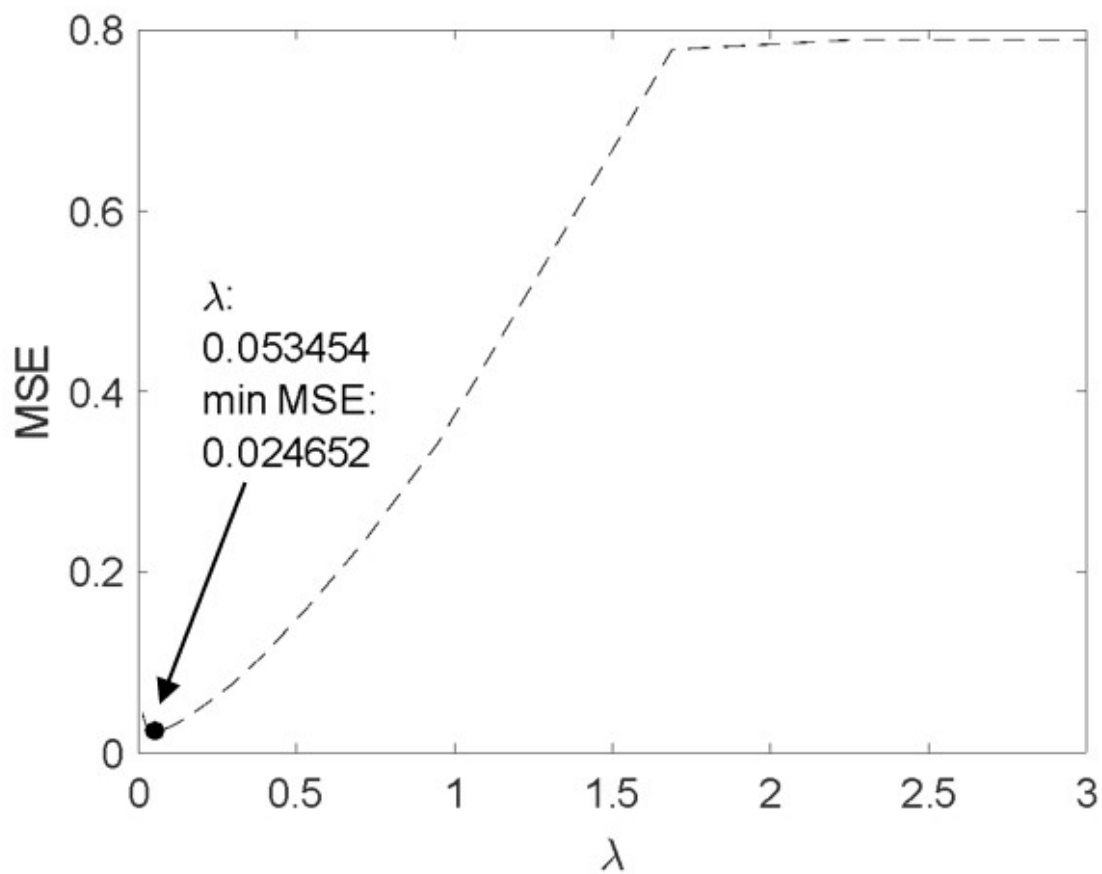


Fig. 7.2 MSE versus the hyper-parameter λ . Each point of the plot corresponds to a PN model with a number of features that decrease with λ . A global minimum is found that corresponds to a model with the minimum error [2].

models, *A* and *B*, were compared in terms of performance using well-consolidated statistical indicators [146, 147]. The results are presented in Table 7.1. *Model – B* outperformed *Model – A* in terms of prediction performance (lower MSE), simplicity (fewer features selected) and generalisation (higher absolute BIC and PRESS). The features of *Model – B* and the related mathematical transformations and coefficients are reported in Table 7.2. The features and coefficients of *Model – A* are not shown for brevity. Each absolute coefficient represents the weight of the specific feature and hence it is possible to understand which is the most influential on the PN response. Remarkably, the sign and transformation follow a physical behaviour meaning that the EN regularisation was able automatically not only to predict accurately the real quantities but also the complexity of the physics involved and interactions among several phenomena.

Analysing the features, it is well-known the direct effect of LF deposits on PN emissions [107] and hence the model capture this by means of the $LF_{Thickmax}$ with a reciprocal function and a negative coefficient.

LS_{max} appears four times as a regressor, with different mathematical transformations and coefficients, highlighting the following crucial aspects: 1. the PN problem is highly nonlinear; 2. the quantity of mass injected and how this is atomised has a direct impact on PN; and 3. the rapidity at which the injected fuel droplets vaporise by means of the charge and turbulence motion influence the mixture formation and hence the PN emissions similarly to [60, 28].

The $M_{1.1SP}^+$ indicates the uniformity of the mixture in the proximity of the SP. The transformation, as per the $LF_{Thickmax}$, is a reciprocal function with a negative coefficient and highlights how richer pockets near the electrode before the combustion process are directly connected to PN [28].

The last factor in importance is the $\phi_{mean-reg2}$, i.e., the equivalence ratio in the periphery of the combustion chamber. The associated transformation is a quadratic function. This region of the combustion chamber is usually associated with a lack of uniformity of the mixture in turn connected to the vicinity of cold cylinder walls and lack of oxygen. The combined effect of these factors has hence a direct effect on PN.

The *Model – B* accurate prediction of the experimental data is presented in Figure 7.3. All the experimental PN points are predicted within the 10% relative error threshold, with the vast majority predicted within the 5% boundary.

Table 7.1 *Model – A* and *Model – B* statistical performance. Both models are obtained with an Elastic Net regularisation approach that searched within a regression matrix for the most dominant features [2].

Model	# Features	BIC	PRESS	MSE
A	15	-44.1461	0.4757	0.0247
B	7	-78.2243	0.4698	0.0181

Table 7.2 *Model – B* features ordered in descending order of the absolute weight. [2].

Original Feature	Transformation	Coefficient Value
$LF_{Thickmax}$	$\frac{1}{1+\sqrt{x}}$	-0.9202
LS_{max}	x^2	0.7349
LS_{max}	$\frac{1}{1+x^2}$	-0.6088
LS_{max}	e^x	0.4645
$M_{1.1SP}^+$	$\frac{1}{1+\sqrt{x}}$	-0.3630
LS_{max}	x	0.2151
$\phi_{mean-reg2}$	x^2	0.1725

Since the PN surrogate model provided a solid prediction of the experimental PN through CFD-based mixture characteristics, the most logical step forward was trying to connect these characteristics with easy-to-access engine parameters (such as engine speed, FRP, SOI, ST etc.). This second step was explored by a member of the EMT in collaboration with the author of this thesis, for more information please refer to [2]. Initially, the same EN approach was followed for the development of these easy-to-use sub-models, but the surrogate extrapolated were inaccurate. Consequently, a hybrid methodology was developed that included the use of generalised radial basis functions (GRBF) [2] with a kernel function. PN model features were designed as a function of engine speed, load, injection characteristics, ST and piston temperature. This analysis has highlighted the inherent limitations of the original experimental dataset, which was not formalized from a statistical perspective. A properly planned design of experiments is necessary to capture the highly non-linear behaviour of engine physics accurately.

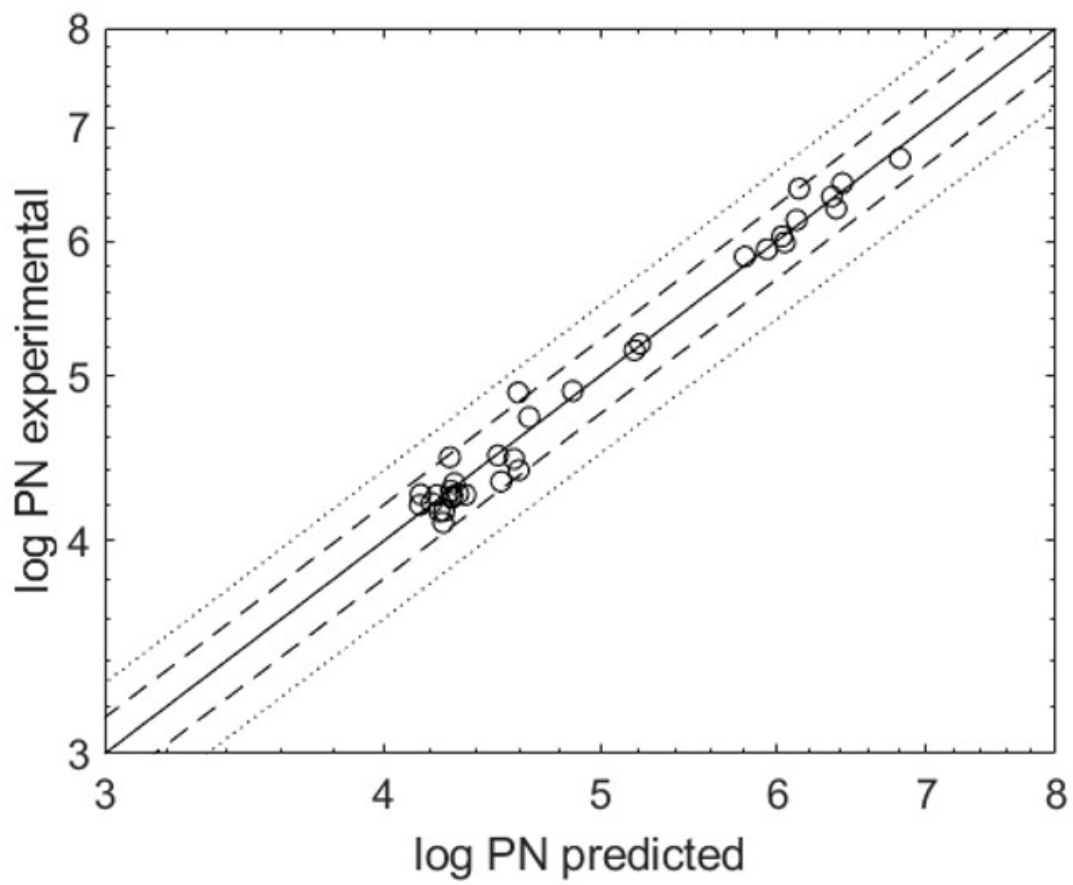


Fig. 7.3 PN surrogate model (Model B) prediction of the experimental PN data. Dashed and dotted lines indicate 5% and 10% relative error, respectively [2].

7.3 Regressor Analysis with Engine Parameters

To better understand how the four features that compose the PN surrogate model change in relation to engine parameters, Figure 7.4 presents the normalised features as a function of SOI (left plot), FRP (central plot) and considering three indicative calibration points (right plot). In particular, the SOI sweep refers to the points P9-P12 (please refer to Table 3.6), the FRP sweep to P5-P8, and the three calibration points to P32, P4 and P25. These three points were selected to cover the operating range from low speed/load to high speed/load. The CFD images presented at the bottom of Figure 7.4 indicate the equivalence ratio and the LF thickness for the points P32 and P25. Only these two points are shown for brevity. In the plots, the linear trends between the points are just an assumption to improve interpretability. True values between points might be different due to the system's nonlinearity.

Generally, the mixture quality improves as the SOI is shifted earlier in the intake stroke. Looking at LS_{max} the decrease above 240 CAD BTDC is related to the augmentation of the impingement of the spray on the piston crown with a consequence increase of droplet rebound that might inhibit the evaporation.

The maximum LF thickness trend indicates that LF persists up to ST for SOI ranging between 180 and 240 CAD BTDC. The highest thickness is registered at 205 CAD BTDC for a combined effect of piston distance from the nozzle and evaporation time. For earlier SOI (SOI > 240 CAD BTDC), the evaporation time exceeds a virtual threshold for which all the liquid deposit is evaporated before the ST [3].

It is evident how the late SOI 180 CAD BTDC produces the worst mixture quality with three out of four features having their maximum. In fact, the $M_{1,1SP}^+$ for SOI 180 indicates the presence of richer fuel pockets ($\phi > 1.1$) as a result of a not sufficient mixture time. When the SOI is moved earlier in the intake stroke, the fuel mal-distribution decreases and consequently the richer fuel pockets disappear ($M_{1,1SP}^+ = 0$).

The level of mean equivalence ratio in region 2 of the combustion chamber (please refer to Figure 3.19) slightly decreases with SOI. This is again related to the relative position of the piston during injection meaning that when the SOI occurs with the piston far away from the nozzle (late SOI) the fuel distribution move toward the periphery; when the SOI occurs with the piston near the nozzle the impingement and subsequent deposit of liquid in the proximity of the piston bowl creates a leaner area in the periphery [3].

Looking at the central plot of Figure 7.4, it is evident that both LS_{max} and $M_{1,1SP}^+$ decrease with the injection pressure because of better fuel atomisation. This produces a better mixture that reaches the optimum for the 200 bar case. In terms of LF deposit, the maximum thickness is reduced between 50 and 150 bar, then increases again most likely as a result of the increased spray penetration and hence impact associated with high FRP [3]. Lastly,

the equivalence ratio slightly increases with the FRP. As previously described, when the spray velocity and hence penetration are increased the chance of having spray splash and/or rebound rises. Consequently, a larger quantity of fuel is carried by the charge bulk motion from the impact area to the periphery of the combustion chamber.

The last plot on the right of Figure 7.4 refers to three calibration points at increasing engine speed and load. Among these points, the SOI would be very similar (mid-way through the intake stroke), and so would the FRP. LS_{max} , $M_{1,1SP}^+$ and $LF_{Thickmax}$ generally increase, bias towards the greater mass of fuel injected associated with higher engine load, which is the dominant effect. The trend of $LF_{Thickmax}$, combined with the CFD images show a peculiar behaviour – the mass of LF originally deposited and retained by ST, decreases as speed and load increase mostly due to the increase of piston temperature; nevertheless, the higher centrifugal forces associated with higher engine speed (and the shorter physical time for evaporation/mixing) facilitates the establishment of thick LF deposits on the crevice regions. This has been associated with heavy PM formation in the literature [3, 80, 95]. The distribution of ϕ from the CFD images reveals a generally not homogeneous mixture, with greater richness in the proximity of the SP for the highest speed-load condition (P25).

Even if a limited experimental dataset was available, not originally designed for the development of this specific PN surrogate model, the results are promising. The approach adopted can be generalised to other engine designs and can inform the development of refined engine controls aiming for emission minimisation.

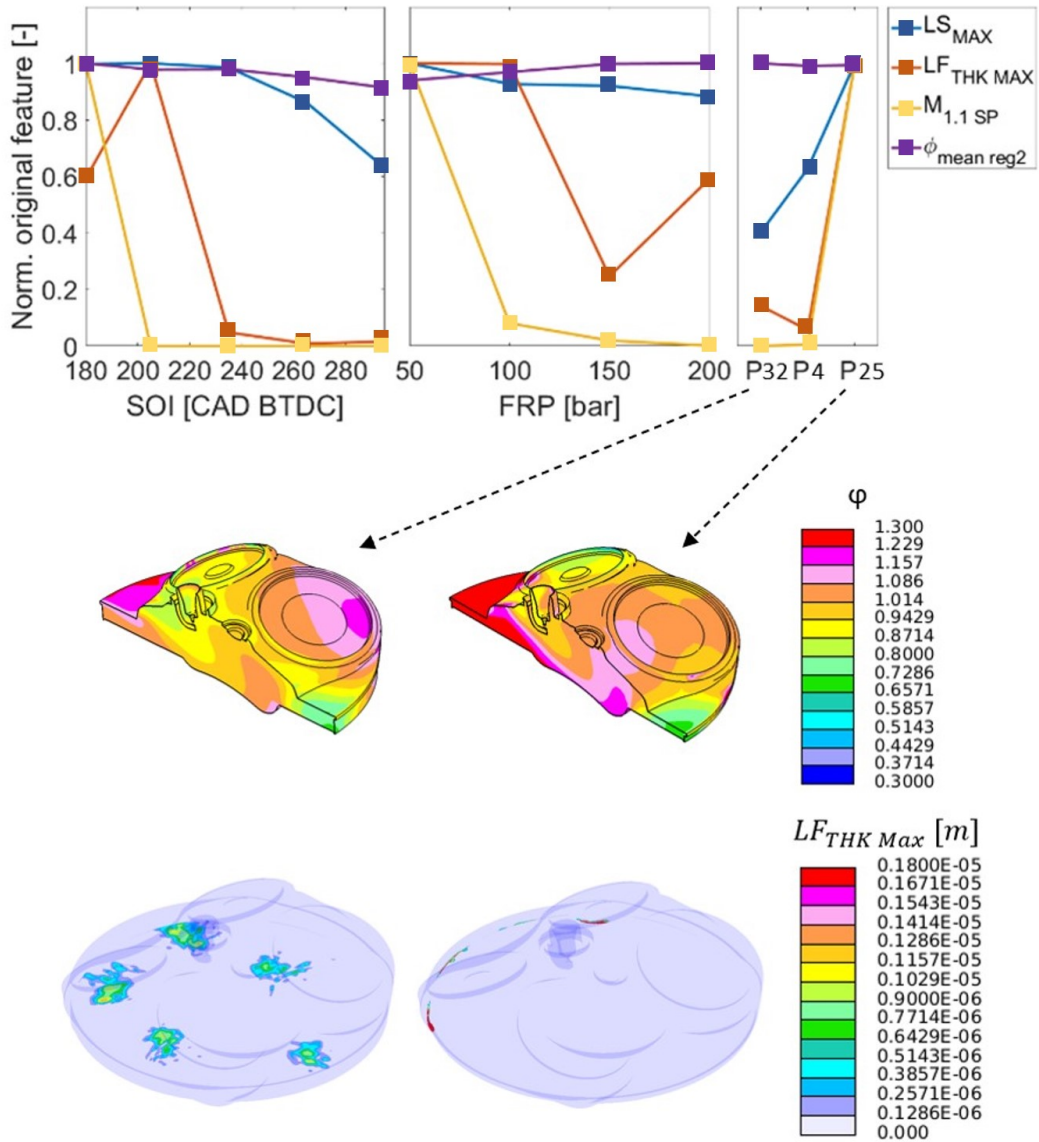


Fig. 7.4 PN surrogate model normalised features for SOI sweep (2000 rpm – 50 Nm, P9-P12), FRP sweep (1500 rpm – 100 Nm, P5-P8) and three calibration points (P32 1500 rpm – 50 Nm, P4 2167 rpm – 61 Nm, P25 2500 rpm – 100 Nm). The CFD-based images are obtained at ST for the equivalence ratio distribution (top) and LF thickness (bottom), and refer to P32 (left column) and P25 (right column) [2].

To further explore the PN surrogate capabilities, the feature values obtained with the split injection cases (please refer to section 6.5) were used to predict the PN levels. The values are reported in Table 7.3 and PN was calculated with the transformations and coefficients from Table 7.2. Overall the mixture indicators improved going from one single injection (1 inj) to two injections (2 injs). As a result, the predicted PN level was reduced by two orders

Table 7.3 Feature values of Point 4 base case (1 inj) and the split injection strategies (2 injs and 3 injs). The predicted PN values are calculated with the transformations and coefficients from Table 7.2.

Feature	1 inj	2 injs	3 injs
$LF_{Thickmax}[\mu m]$	1.5393	0.8231	0.6367
$LS_{max}[mg]$	10.7324	6.3533	5.3862
$M_{1.1SP}^+[mg]$	2.26e-05	9.04e-06	7.89e-06
$\phi_{mean-reg2}[-]$	0.9878	0.3422	0.2876
$PN[\#/cm^3]$	2.14e+04	2.97e+02	1.23e+02

of magnitude. A further improvement was obtained with three injections (3 injs) where the PN was predicted with a 60 % reduction in comparison with the two injections case. While no experimental data were available for the PN obtained with split injection strategies, the analysis indicates the potential of split injections to reduce PN levels.

Chapter 8

Conclusions

A PN surrogate model was developed using CFD-based mixture characteristics obtained from a state-of-the-art engine combustion chamber. Starting from the high-pressure fuel spray calibration, the methodology involved a factorial screening design to identify the most influential factors and optimise them to minimize two objective functions related to spray penetration and droplet diameters. The calibrated spray model accurately represented the real system, encompassing penetration, droplet dimensions, and plume morphology. Subsequently, a LF analysis, in combination with mixture indicators, provided qualitative insights into the correlation with available experimental PN data. However, due to non-linearities in the trends, a more refined methodology was needed. Consequently, an EN regularization approach was adopted to determine both features and coefficients, ensuring a robust correlation with experimental PN behaviour. The resulting surrogate model successfully connected pre-combustion mixture characteristics with experimental PN outcomes. The challenges and expenses associated with measuring in-cylinder parameters led Ford, the industrial lead in the DYNAMO project, to seek alternative methodologies for developing a user-friendly surrogate model that could offer valuable insights for precise engine calibration. The approach proposed in this thesis involves the utilization of tailored, calibrated CFD models. The novelty lies in leveraging a relatively extensive set of engine operating conditions to formulate an equation linking PN with pre-combustion characteristics.

Conclusions are divided into four subsections. The first relates to fuel spray model calibration and best practices drawn from the corresponding analysis. Particular emphasis was placed on the best model combination to accurately predict the break-up process from a modern high-pressure injector as well as the thermal characterisation of spray-to-wall interactions. The second subsection regards the conclusions from the mixture investigation analysis. A clear indication of the connection between mixture indicators, LF behaviour and experimental PN levels is presented. Moreover, it is highlighted how the piston temperature

and ad-hoc injection strategies can mitigate liquid retention and how this translates into better emission performance.

In the third section, the main outcomes from the PN surrogate model are presented. The novel surrogate model was able to predict, with a great level of accuracy, experimental engine-out PN levels relying only on pre-combustion in-cylinder mixture parameters. Moreover, the generality of the approaches adopted and how these can help the engine community are discussed.

Finally, suggestions for future work are presented starting from the limitations encountered during this research project.

8.1 Spray Model Calibration Conclusions

The fuel spray from a modern GDI injector was modelled by means of a 3D CFD code. The aim was to first identify the best model combination to predict the spray characteristics accurately and second to develop a fast calibration procedure able to produce physically reasonable calibrated factors. The model was developed by imposing an RR mono-modal distribution to the parcels of droplets that entered the computational domain and then disintegrated following a break-up model. Two break-up models were investigated, KH-RT and RD, to understand which one was the most suitable for GDI applications. For each model combination, a half-factorial screening was performed to select the most dominant calibration factors. The effect was measured against the fuel spray penetration and SMD. Then, a space-filling, 50 points, DoE was developed with the dominant factors. Each point was a factor combination to be simulated by means of the CFD code. Lastly, the CFD results were utilized to define objective functions that represented the prediction error of the model, subsequently minimised by means of a nested optimisation approach. The analysis highlighted how the RR+RD outperformed the RR+KHRT.

This statistical and optimisation approach can be used for the accurate calibration of other phenomenological models as it consistently reveals dominant factors, the influence that they have on model responses, and sets of optimal factors.

The 3D domain utilised for the initial calibration was then modified by adding a solid hot plate at the bottom to investigate the influence of the wall temperature on liquid deposits from high-pressure fuel spray. The following main outcomes can be drawn from the investigation:

1. A half-factorial screening revealed how to accurately predict the fuel spray characteristics only two calibration factors are sufficient for both RR+RD and RR+KHRT model combinations. The RR factor was X and referred to the reference diameter

- of the initial droplet distribution. The second factor for both combinations was the break-up coefficient, i.e., C_{b1} and C_3 for RR+RD and RR+KHRT, respectively.
2. The RR+RD model outperformed the RR+KHRT in terms of the prediction performance of a real fuel spray within the FRP range 50-250 bar. In particular, the RR+KHRT overpredicted the spray penetration and the droplet sizes. As a result, the model would have needed a more computationally expensive procedure to match the other model prediction capability.
 3. The analysis of the RR+RD factors, X and C_{b1} , as a function of FRP, revealed how generally the break-up coefficient is directly proportional to the rail pressure to compensate for the higher droplet disintegration rate; on the contrary, the reference diameter X decreased with pressure to account for the droplet atomisation. Moreover, the regression analysis of these factors as a function of spray characteristics and consequent contour plots indicated how both spray penetration and SMD increased with X and C_{b1} . This correlation can inform the initial stage of the calibration procedure because it unveils the order of magnitude of the parameters involved.
 4. A spray morphology analysis revealed that the typical liquid ligaments at the nozzle exit were reproduced by the model with a simplified distribution of large and fast droplets that rapidly break up along each plume. Extremely atomised droplets composed the interface between the bulk of the plume and the surroundings. In this region, a stagnation phenomenon (i.e., velocity almost zero) was observed due to a combined effect of air entrainment/recirculation and drag forces.
 5. The spray model revealed a linear correlation between the average velocity of the droplets and the SMD. The study might inform the development of injection strategies that minimise the LF and maximise the atomisation for better mixture formation.
 6. The wall temperature at the spray impingement location changes the characteristics of the liquid. From T_{sat} to T_L , the amount of fuel vapour was similar while droplets and LF deposits were inversely proportional. At T_N , meaning fuel impingement region, the proportion was around 50%, 20% and 30% for the droplets, vapour and LF, respectively. Above this temperature, the rebound regime prevented the droplets from sticking to the wall. This resulted in a more quantitative of free droplets and consequently a reduction of LF deposit. Lastly, at T_L and above, the proportion was 84% and 16% for the droplets and vapour, respectively. The increase of free droplets might contribute to the emission levels because reduces the uniformity of the mixture.

8.2 Mixture Characteristics and LF Conclusions

Part-load stoichiometric operating conditions from a modern GDI engine were used to define a consistent CFD methodology to accurately predict the mixture process and the behaviour of liquid deposits in relation to PN emissions. Relevant operating conditions were selected featuring parametric variations of piston temperatures, SOI and FRP, initially in combination with a simplified isooctane fuel model, and then with a refined multi-component surrogate fuel blend model able to capture the thermo-chemical properties of the actual fuel used during the experimental campaign. Accurate mixture preparation indicators such as the UI, M^+ and the quantity of LF retained at ST were used to quantify the in-cylinder charge characteristics and its homogeneity. The indicators were combined with CFD images that revealed the relationship between equivalence ratio distribution, LF and engine-out measured PN levels. The following concluding remarks can be drawn from the analysis:

1. Even though the isooctane fuel was not able to reproduce the LF behaviour of the real fuel and fully evaporated before ST for all the temperatures tested, the investigation proved that the model was able to follow physical/meaningful trends dictated by wall properties, liquid properties and the heat flux. At 2000 rpm - 50 Nm, the maximum liquid deposit decreased by 65% when the piston temperature was varied from T_{sat} up to T_N . An additional rise of 20 K showed a consistent increment (39%) of the liquid deposit because of heat flux reduction. A realistic full disappearance of LF was noticed at T_L . In fact, in the film boiling regime, the fuel deposition was inhibited by the Leidenfrost effect and the highest evaporation rate. Clouds of droplets persisted near the walls affecting the rapidity of fuel evaporation and hence reducing the mixture homogeneity.
2. LFL and the heat flux were inversely proportional up to T_N . LFL increased from 27 CAD to 34 CAD at $T_N + 20$ K. From T_N the heat flux steadily decreased from its peak and together with the Leidenfrost effect mitigated the liquid deposit by creating vapour insulation between the piston and the liquid droplets. Increasing T_{wall} above the T_L did not produce any evident changes in terms of both LFL and heat flux.
3. The CFD engine model validation was performed by referring to single variable sweeps of SOI and FRP, consistently with a modern GDI engine operation. At 2000 rpm - 50 Nm, early SOI timing presented favourable mixture indicators. Reacher cells almost disappeared meaning an almost zero M^+ and UI of 98%. Despite this good charge homogeneity, the large LF deposition due to the vicinity of spray plumes and piston led to high PN output, measured experimentally at 7×10^5 #/cc. The analysis

of CFD images revealed how even theoretically homogeneous operating conditions had levels of charge mal-distribution, especially in proximity to the cylinder walls. Another important aspect was the location of the liquid deposit. For early SOI the accumulation of liquid was located inside the piston bowl while for late SOI the liquid deposit was accumulated in the crevice/liner region. The latter condition created a richer mixture near the cylinder walls at ST. As a consequence, the PN level was one order of magnitude higher than the calibration case (base SOI). Overall, the results indicated that both charge inhomogeneity and LF quantity and location are associated with PN emissions, and the relative significance of their impact is influenced by the specific operating condition, wall temperatures and control strategies.

4. In a small-capacity engine, greater injection pressures generate stronger spray-to-wall interactions and more initial LF deposition, but also higher rates of film-to-flow evaporation. At mid-load condition the liquid retained at ST was less than 1% of the total fuel injected at lower pressure cases (50 and 100 bar), raising to 1.2% at 250 bar. The UI increased steadily with FRP while the decrease of M^+ levelled off for the 150 bar case and onward. Despite the higher levels of LF and thanks to favourable mixture indicators, the 200 bar case produced the lowest level of PN. Similarly, at 2500 rpm–100 Nm a very small mass of LF was retained at spark timing for the FRP 200 bar and both UI and M^+ presented the advantages of enhanced atomisation. PN was reduced almost linearly with FRP.
5. The localised piston surface cooling may be one of the reasons for LF retention up to and beyond ST. If LF mass retained at ST is sufficiently large (≥ 1 mg), it may survive through the engine cycle, especially if supported by lower piston temperatures, e.g., early SOI and/or low load conditions. This might cause an accumulation of liquid deposits and raise PN due to pool-fire.
6. Even if no experimental data were available regarding split injection strategies, the numerical investigation pointed out the potential of delivering the fuel in different phases, firstly minimising spray penetration that might result in spray-to-wall impingement, and secondly enhancing the mixture homogeneity. For the operating condition 2167 rpm - 61 Nm, the three-injection strategy halved the maximum LF in comparison with the reference case (one injection) and improved the mixture homogeneity. A three-pulse split injection strategy is likely to translate into large potential reductions in PN emissions.

8.3 PN Surrogate Model Conclusions

Pre-combustion 3D modelling carried out using the fully validated CFD modelling scheme presented in this work, was combined with verified experimental engine out PN measurements to ultimately develop the building blocks of a novel, computationally compact, PN surrogate model. The study covered over 30 engine operating conditions focusing on the part-load space. The three main conclusions are listed below:

1. The PN surrogate model is obtained through a cascade approach where the regressors are selected by an EN regularisation. The experimental PN can be predicted for a relatively large set of operating conditions within the 5% relative error threshold by means of only four mixture indicators. These were evaluated at ST and can be classified in descending order of importance as follows: 1. peak thickness of the LF distribution; 2. peak mass of the liquid portion of the injected fuel; 3. total fuel mass in rich pockets ($\phi > 1.1$) around the plug electrodes; 4. mean equivalence ratio in the periphery of the combustion chamber.
2. Surrogate model framework and methodology can be used or adapted to develop similar surrogates for different engine-related quantities (e.g., PN as a function of combustion parameters or easy-to-access engine variables). This can inform the development of optimised engine control strategies that aim for emission reduction.
3. Even if this novel PN surrogate model was developed by means of a single GDI engine platform, the generality provided by the suggested approach and the commonality of modern GDI engine geometries might result in a good level of PN prediction for different engines and operating conditions.

8.4 Future Works

Based on the limitations encountered during this research project, the following notes can be used as a base for future work that might expand, refine and generalise the original investigation:

- The optimisation process carried out as part of the spray model calibration at an injection pressure of 200 bar, returned an unexpected slight reduction of the calibration factor C_{b1} in comparison with the 150 bar case. A further investigation on C_{b1} between 150 and 250 bar injection pressure should be carried out, including possibly different injectors to unveil the relation between the calibration constant and FRP. The use of

different injectors might reveal similar trends and can serve to further generalise the analysis.

- Even though the superimposition of a droplet initial size distribution at SOI is a well-known procedure among the engine modelling community for GDI sprays, turbulence-induced breakup mechanism and vena contract effects might become dominant mechanisms inside the injector. As a result, the modelling of the internal injector geometry and associated flow should be taken as a future refinement of the present work. Firstly to produce an additional validation of the results obtained in this study, and secondly to better understand the mechanisms that lead to the primary breakup process.
- At the time of writing this thesis, the limitations of the STAR-CD CFD software included the impossibility of changing the B_s calibration constant for the Bai-Onera spray-to-wall interaction model. Ideally, the calibration constant should be time/CAD dependent since the Nukuyama temperature changes with the in-cylinder thermodynamic conditions. Strategies to implement a variable B_s were briefly investigated but the consistent and faster results obtained with a fixed value led to the decision to allocate this task to future work.
- To expand the results of the limiting temperature concept beyond the specific characteristics of the engine-fuel combination used, further investigation should be carried out in terms of engine efficiency, reliability and piston costs. This will provide a complete framework for the proposed concept.
- The experimental engine conditions available to develop the surrogate PN model presented in Chapter 7 have highlighted an inherent limitation of the original experimental test plan, which was not formalized from a statistical perspective. A properly planned design of experiments will be necessary to capture the engine's systematic behaviour more accurately, imparting increased robustness and generality to the resulting surrogate model. Moreover, a validation exercise might be conducted using data from different engine platforms, and an extension of the approach for the development of models of other pollutant species. These refinements might improve the model generalisation and facilitate the derivation of sub-models that accurately connect the relevant mixture parameters to easy-to-access engine parameters (e.g., engine speed, FRP and SOI).

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Appendix A

PN Surrogate Model - MATLAB Code

The MATLAB code to obtain the PN surrogate model is as follow:

```
% Loading the matrix with IVs and the DV.
% Please adjust the numbers of column
% corresponding to the total IVs in the csv file. Make
% sure the name of the IVs in
% the csv are resonable (no space or special characters).

data = readtable('PNbigFilt3.csv'); % loading data set

y = log10(data.PN); % DV logPN (Dependent Variable)
obsers = size(y,1); % number of observations

x = data(:,19:118); % IVs selected (Independent Variables)

x = table2array(x); % converting from table to double

% Name of the orginal features
dataname = data.Properties.VariableNames;

featurenames = dataname(:,19:118); %

%featurenames = dataname(:,19:112);
%featurenames = dataname(:,17:24);
%featurenames1 = dataname(:,27:121);
```

```

%featurenames = [featurenames featurenames1];

% font size for the graphs
fontsize = 14;

% Plot of the engine operating condition
rpm = data.Speed;
torque = data.T;
plot(rpm,torque,'o','Color','k','MarkerSize',
6,'MarkerFaceColor','k'); hold on;
plot(rpm(1),torque(1),'o','Color','r','MarkerSize',
8,'MarkerFaceColor','r');hold on;
plot(rpm(5),torque(5),'o','Color','r','MarkerSize',
8,'MarkerFaceColor','r');hold on;
plot(rpm(9),torque(9),'s','Color','r','MarkerSize',
9.5,'MarkerFaceColor','r');hold on;
plot(rpm(21),torque(21),'o','Color','r','MarkerSize',
8,'MarkerFaceColor','r');hold off;
set(gca,'FontSize',fontsize)
xlim([1000 3500])
ylim([0 120])
xlabel('Engine speed [rpm]')
ylabel('Torque [Nm]')

Feature engineering - Create new features
features = size(x,2); % n of columns of x matrix
xtot = []; % Matrix to be filled with the original
features normalized + new fetures
for feature = 1:features
    minx = min(x(:,feature));
    maxx = max(x(:,feature));
    xnew = MakeNewFeatures15(x(:,feature),minx,maxx);
    xtot = [xtot xnew];
end

% Second normalization to have every feature defined [0,1]

```

```

ns = size(xtot,2);
for i = 1:ns
    xnewnorm(:,i) = xt看(:,i) - min(xtot(:,i));
    xnewnorm(:,i) = xnewnorm(:,i)/(max(xtot(:,i)) -
    min(xtot(:,i)));
end

% Select between xt看 (one normalization) and xnewnorm
(two normalization)

%xnorm = xt看;
xnorm = xnewnorm; % This is the regression matrix

% Find nan and inf in xnorm
[rownan, colnan] = find(isnan(xnorm));
[rowinf, colinf] = find(isinf(xnorm));

% Initial checks for the regression matrix
cond_x = cond(xnorm) % higher value bad!
svd_x = svd(xnorm)
ntotfeatures = size(xnorm,2) % Total number of features

% Features mat equations. Select according to
% MakeNewFeatures function

featuresmat = {' [x]', ' [x^2]', ' [sqrt x]',
    ' [exp x]', ' [log 1+x]',...
    ' [1/(1+x)]', ' [1/(1+x^2)]', ' [1/(1+sqrt x)]',
    ' [1/(exp x)]',...
    ' [1/(1+log (1+x))]'};

Cross validation and Elastic Net
% Cross validation numbers. % I started with 4
kfolds = 5; % select the number of folds
trainsetperc = ((kfolds-1)/kfolds)*100 % percentage of

```

```

observations assigned to training data set
valsetperc = (1/kfolds)*100 % percentage of observations
assigned to validation data set
ntrain = round((trainsetperc/100)*obsers) % number of
observation assigned to training data set
nval = round(obsers - ntrain) % number of
% observation assigned
% to validation data set. This set will be
% changed kfolds times
% with the same dimension.

% Loop to change lambda. Higher value = simpler model
%(less features) and viceversa
lambda(1) = 3;
for i = 2:20
    lambda(i) = lambda(i-1)*0.75;
end

% Lasso function with alpha = 0.5 => Elastic Net
[B, FitInfo] = lasso(xnorm,y,'CV', kfolds,'Lambda', lambda,
'Alpha',0.5);
%B = coefficients of the model for each lambda value.
% FitInfo = fitting information

% ATTENTION!!! the lambda vector is automatically
% sorted in ascending order by lasso function!!
% The best lambda value is the one that gives us
% the minimum error (min MSE) for the
% validation set, meaning the model is sufficiently generalized.

% MSE vs lambda highlighting lambda value for min MSE
plot(sort(lambda), FitInfo.MSE, 'Color','k','LineStyle','--');
hold on;
% MSE is referred to the validation set
plot(FitInfo.LambdaMinMSE, min(FitInfo.MSE),'o',
'MarkerSize',

```

```

6,...
    'MarkerEdgeColor','k','MarkerFaceColor','k');
    hold off;
txt1 = {'\lambda: ' num2str(FitInfo.LambdaMinMSE),
'min MSE:
' num2str(min(FitInfo.MSE))};
t = text(0.20,0.42, txt1);
t.FontSize = fontsize;
set(gca,'FontSize',fontsize)
xlabel('\lambda')
ylabel('MSE')

% Table with the minimum MSE and the related lambda
VarNames = {'MinMSE','Lambda'};
table(min(FitInfo.MSE), FitInfo.LambdaMinMSE,
'VariableNames', VarNames)

% Matlab capabilities to plot MSE vs Lambda.
% MSE of green dot (validation set) should be lower than
%MSE blue (val + standard deviation).
lassoPlot(B,FitInfo,'PlotType','CV');
legend('show');

% Number of fetures with coefficients not zero
betanon0 = find(B(:,FitInfo.IndexMinMSE));
nbetanon0 = size(betanon0,1);

% Plot coefficient values from the model that minimize
% the MSE (coeff = 0 -> feature deleted)
nb = (1:ntotfeatures);
plot(nb,B(:,FitInfo.IndexMinMSE));
xlabel('feature number')
ylabel('coefficient value')
grid on
VarNames = {'n_coeffnotzero'};

```

```
table(nbetanon0,'VariableNames', VarNames)
Plot observations vs predictions
% I need the intercept that it is the one related to
% the minimum MSE. Same for the B matrix
% y predictions = intercept + x1*b1 + ... + xn*bn.
ypred = FitInfo.Intercept(FitInfo.IndexMinMSE) +
xnorm*B(:,FitInfo.IndexMinMSE);

% Regression statistics
[yles, rsq, rsqadj, dof] = regrparam(y,
ypred,obsers,nbetanon0);

minMSE = min(FitInfo.MSE)
minRMSE = sqrt(minMSE)

% PRESS
D = [ypred y];
xpress = press(D); % PRESS
PRESS = xpress;

% Information criterion
BIC = bicme(minMSE,ntrain,nbetanon0);

% Plot prediction performance
x1 = linspace(0,10,100);
y1 = x1;
plot(ypred,y,'o'); hold on;
plot(x1,y1,'-'); hold off;
title('Minimum MSE model');
xlabel('ypred')
ylabel('y')
xlim([3 8])
ylim([3 8])

% Table with model info and performance
VarNames1 = {'observations', 'regressors', 'BIC',
```

```

'PRESS', 'MSE','RMSE', 'Rsqadj'};
table(obsers, nbetanon0, BIC, PRESS, minMSE, minRMSE, rsqadj,
'VariableNames', VarNames1)

% Plot residuals
plot(ypred,yres,'x');
xlabel('ypred')
ylabel('Residuals')

% Plot the Normal Probability. It is useful to spot outliers.
normplot(yres)

Selected features (minimum MSE) with coefficients
% Merge original features with mat equations
featnamestot = []; %array to be filled with the original
% features name + new fetures name
for featnamecount = 1:size(featurenames,2) %counter up to
% the total n of original fetures
    for equat = 1:size(featuresmat,2)
        %counter up to the total n
        % of mat equations
        bb = (featuresmat(1,equat));
        %selecting on mat equation
        ab = strcat(featurenames(1,
        featnamecount),bb);
        %concatenate one original feture
        % with the selected mat equation
        featnamestot = [featnamestot ab];
        % append the results
    end
end

% Create a cell array with first row=feature name
% and second row=coefficient
coeffall = B(:,FitInfo.IndexMinMSE);
coeffallcol = coeffall.';

```

```

featnamesvaltot = featnamestot;
featnamesvaltot = [featnamesvaltot; num2cell(coeffallcol)];
% feature names + coeff. zeros included

betanon0coll = betanon0.'; % index of the columns not zero
featnamesvalnonzero = featnamesvaltot(:,betanon0coll);
% feature names + coeff. zeros escluded

% Delete features with lower coefficient (weight) and
% re-run elastic net (or LASSO) with the simplified regression matrix
% Set the coefficient value limit for all the features
coefflimit = 0.11;

% Find the index of abs coeff > coefflimit
indexlowcoeff =
find(abs(cell2mat(featnamesvaltot(2,:)))>coefflimit);

% Delete all the columns from xnorm (regression matrix) but
% the ones corresponding to indexlowcoeff
xnormreduc = xnorm(:,indexlowcoeff);

% ELASTIC NET with the reduced regression matrix
% Loop to change lambda.
lambda_reduc(1) = 3; % higher value = simpler model
% (less features) and viceversa
for i = 2:20
    lambda_reduc(i) = lambda_reduc(i-1)*0.75;
end

% Lasso function with alpha = 0.5 => Elastic Net
[B_reduc, FitInfo_reduc] = lasso(xnormreduc,y,'CV', ...
    kfold,'Lambda', lambda_reduc,'Alpha',0.5);

% MSE vs lambda
plot(sort(lambda_reduc), FitInfo_reduc.MSE); hold on;
% MSE is referred to the validation set

```

```

plot(FitInfo_reduc.LambdaMinMSE, ...
     min(FitInfo_reduc.MSE),'x'); hold off;
xlabel('lambda')
ylabel('MSE')

% Table with the minimum MSE and the related lambda
VarNames = {'MinMSE','Lambda'};
table(min(FitInfo_reduc.MSE), FitInfo_reduc.LambdaMinMSE, ...
      'VariableNames', VarNames)

% Matlab capabilities to plot MSE vs Lambda.
lassoPlot(B_reduc,FitInfo_reduc,'PlotType','CV');
legend('show');

% Prediction model with the reduced regression matrix
ypred_reduc =
FitInfo_reduc.Intercept(FitInfo_reduc.IndexMinMSE) + ...
    xnormreduc*B_reduc(:,FitInfo_reduc.IndexMinMSE);

% Create a cell array with first row=feature name
%and second row=coefficient
coeffall_reduc = B_reduc(:,FitInfo_reduc.IndexMinMSE);
% coeff columns that minimize MSE
betanon0reduc = find(coeffall_reduc); %find non zero values
nbetanon0reduc = size(betanon0reduc,1);
% number of non zero coefficients
coeffallcol_reduc = coeffall_reduc.';
featnamesvaltot_reduc = [featnamesvaltot(1,indexlowcoeff); ...
    num2cell(coeffallcol_reduc)];

% Regression statistics
[yres_reduc, rsq_reduc, rsqadj_reduc, dof_reduc] = regrparam(y, ...
    ypred_reduc,obsers,nbetanon0reduc);

minMSE_reduc = min(FitInfo_reduc.MSE)
minRMSE_reduc = sqrt(minMSE)

```

```

% PRESS
D1 = [ypred_reduc y];
xpress1 = press(D1); % PRESS
PRESS1 = xpress1;

% Information criterion
BICreduc = bicme(minMSE_reduc,ntrain,nbetanon0reduc);

% Relative error [%]
reverr = abs((ypred_reduc - y)./y).*100;

% Plot prediction performance
x1 = linspace(0,10,100);
y1 = x1;
y2 = y1 + x1*0.05;
y3 = y1 + x1*(-0.05);
y4 = y1 + x1*0.1;
y5 = y1 + x1*(-0.1);
loglog(ypred_reduc,y,'o','Color','k','MarkerSize',7);
hold on;
plot(x1,y1,'Color','k'); hold on;
plot(x1,y2,x1,y3,'Color','k','LineStyle','--'); hold on;
plot(x1,y4,x1,y5,'Color','k','LineStyle',':'); hold off;

set(gca,'FontSize',fontsize)
%title('Optimized model');
xlabel('log PN predicted')
ylabel('log PN experimental')
xlim([3 8])
ylim([3 8])

% Table with BIC and PRESS
table(obsers, nbetanon0reduc, BICreduc, PRESS1,
minMSE_reduc, ...
    minRMSE_reduc, rsqadj_reduc, 'VariableNames', VarNames1)

```

```
% Plot residuals
plot(ypred_reduc,yres_reduc,'x');
xlabel('ypred')
ylabel('Residuals')

% Plot the Normal Probability. It is useful to spot outliers.
normplot(yres_reduc)

Main effect plots
featgroup = xnormreduc;
feature1 = featgroup(:,1);
feature2 = featgroup(:,2);
feature3 = featgroup(:,3);
feature4 = featgroup(:,4);
feature5 = featgroup(:,5);
feature6 = featgroup(:,6);
feature7 = featgroup(:,7);

ymax = max(y)
ynorm = y./ymax

plot(feature4,ynorm,'o');
title('LS')
plot(feature5,ynorm,'o');
title('1/LF')
plot(feature6,y,'o');
title('1/M+')
plot(feature7,y,'o');
title('phi')
```

