Spray combustion in auxiliary marine boilers: an experimental and numerical study

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Publication date:
2020

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Spray combustion in auxiliary marine boilers: an experimental and numerical study

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PhD thesis
March 2020

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This dissertation is the result of three years of research, from January 2017 to December 2020, conducted at the Combustion and Harmful Emission Control (CHEC) research centre of the Department of Chemical & Biochemical Engineering (KT), Technical University of Denmark (DTU), in collaboration with Alfa Laval Aalborg. The research was performed within the framework of the Blue INNOship partnership and it was funded by Innovationsfonden, The Danish Maritime Fund and DTU. The Otto Mønsteds Fond cofunded the participation in several conferences. The PhD project was supervised by Senior Researcher Peter Arendt Jensen, Professor Peter Glarborg and Professor Kim Dam-Johansen.

I would like to express my gratitude to those that supported me in these years making this work possible.

My sincere gratitude goes to my supervisors, for believing in me from the start of this project. Peter Arendt Jensen and Peter Glarborg, thank you for helping me navigate through this work, I have learned a lot from you, both personally and professionally. Kim Dam-Johansen, thank you for your inspiring words and for giving me the chance to face this challenging work.

I would like to thank the talented KT employees for their invaluable support. A special thanks to Anders Kjersgaard and Søren Post for their help and company in taking the full-scale measurements, Peter Thomas Christensen for his excellent and quick work, Hanne Mikkelsen for her helpfulness, Ramona Valentina Mateiu for the support using the SEM and Sønnik Claussen for the support with the optical measurements and the interesting talks. The work described in the second chapter would have not been possible without the personnel from Alfa Laval, especially Lotte Sørensen, Niels B. Pedersen for operating the boiler and his interest in the project, Lars Bo Andersen and the crew of the test centre for their helpfulness.

It has been a long journey, but I was lucky enough to have plenty of company through it. I would like to thank my friends and colleagues, at CHEC, in Denmark, Italy and all over the world that cheered me and made me enjoy these years, despite my best efforts not to. I started a list, but you are too many. You know who you are anyway and I love you.

I would like to thank my family for always rooting for me and making me who I am today. A special thought goes to my granddads, who taught me the value of knowledge and the value of small things.

Finally, my deepest gratitude goes to my wife, Giulia. Without you none of this would have been possible, you are my guiding light and my strength. You make me a better person and no words are enough to thank you for it.
Emissions and pollution reduction have been topics of constant interest for any industrial processes in the past decades and the marine sector is no exception. The vast majority of the marine industry is constituted by shipping, which moves around 80% of the world trade and is therefore an essential part of the global economy and supply chain. As such, it also is responsible for a significant share of the anthropogenic emission of pollutants and greenhouse gasses (GHG). Indeed, there is an immediate necessity for solutions to improve the design of new large ships and their on-board systems. One of the systems affected by the push towards alternative fuels are the auxiliary boilers, which have also seen more and more use in recent years, due to advent of slow steaming. This study is part of the effort to cope with these new demands by achieving more efficient and flexible auxiliary boilers.

As part of this effort, a necessary step is to gain further insight into behaviour of the system at hand. While both experimental and computational methods have been applied extensively in the past to the study of liquid fuel flames and sprays, each approach has its limitations. To obtain detailed data with experimental methods is lengthy and expensive, while Computational Fluid Dynamic (CFD) simulations need to be validated before being used for practical purposes and might become cumbersome if too many phenomena are included. Therefore, a combination of the two was used in this project.

The experimental work consisted of two parts. The first was a measuring campaign on a full-scale boiler to obtain data, which could be used to validate the CFD model. The second part was a characterization study of the atomizer used in the full-scale boiler to define the fuel injection in the CFD simulations.

In addition to the collection of validation data, the measuring campaign was also a chance to fully test the boiler operating capability and to observe the effects of changing operating conditions, such as oil type, load and excess air, on flame stability and emissions.

During the project, a full-scale boiler was modified with ports and connections to insert probes into the furnace and to sample the gas at the exhaust. The experimental investigation encompassed both boiler operation change and flame mapping. For the first part, the boiler has been run at three different loads and the flow rate of combustion air was changed to obtain an oxygen concentration in the exhaust over a range between 1% and 6%. The second part of the campaign consisted of gathering data to validate future CFD simulations. The experiments were repeated for marine diesel fuel and Heavy Fuel Oil (HFO).
Both parts of the experimental campaign yielded interesting results. It was observed that using HFO compared to diesel had an almost negligible impact on heat transfer and temperatures in the boiler, but increased the emission of particulate almost tenfold, and of NO\textsubscript{x} and CO from 3 to 5 times.

It was also possible to conclude that working at higher loads had a negative effect on all specific emissions, with the sole exception of diesel particulate emissions, which were consistently lower for higher loads. The increase in CO emission with load was clear when increasing the load from 40% to 60% for both fuels. The relative changes for NO\textsubscript{x} and particulate did not show such clear trends. Moreover, an air-fuel equivalence ratio ($\lambda$) above 1.2 did not lead to a further decrease in CO emission. While particulate emissions consistently decreased with increased $\lambda$, NO\textsubscript{x} concentration showed a relatively flat behaviour.

The second experimental investigation was a spray characterization study on a spill-back atomizer, which provided the data needed as an input for the CFD calculations. The implementation of these data avoided the necessity of directly simulating the spray break-up process in the CFD simulations, thus greatly reducing their computational costs. This study also resulted in novel spray diagnostic method and further insight into the influence of key nozzle operation parameters on spray characteristics.

The atomization characteristics of the nozzle were investigated in terms of droplet size and velocity distributions. The spray seen in the full-scale boiler was replicated in a cold setup. A pulsating LED optical imaging system that employs a CCD camera was used to capture image pairs with a delay as short as 1\,µs. Positions, velocity, sizes and shapes of single droplet were obtained by analysing these images. Water-glycerol solutions with different concentrations were used as model fluids, reproducing the range of viscosities found by rheology studies for fuels used in the full-scale boiler. The nozzle was characterized by varying three parameters: liquid viscosity, supply pressure and flow rate through the nozzle. As also described in literature, the droplet size distribution shifted towards higher values with an increase in viscosity and lower values with an increase in supply pressure, while the changes in flow rate had a negligible impact on the Sauter Mean Diameter. In the same operating range, consistent trends were also quantified for other two macroscopic parameters: the spray cone angle and the mean droplet velocity. The spray cone angle increased for higher viscosities and lower flow rates, while the mean velocity increased with both flow rate and supply pressure.

Overall, in addition to the data needed for the CFD simulations, the spray characterization study provided a good understanding of the effects on atomization characteristics that results from changes in boiler load, fuel pressure and viscosity.

The data obtained from the spray characterization study was then used to model the fuel injection in CFD simulations of the full-scale boiler in the commercial software ANSYS CFX. The CFD model was validated against the data from the measuring campaign.

The comparison with the mapped flame showed that the CO\textsubscript{2} concentration profile is well predicted in the simulation, while there is a deviation in the near burner region for temperature and concentrations of CO and O\textsubscript{2}. This discrepancy was ascribed to the continuation of fuel combustion in the measuring probe. The CFD simulations reproduced quite well the trends for the exhaust conditions observed in the experiments at varying amount of excess air and load. The simulations also correctly predicted the lower limit of combustion air needed to obtain a stable operation of the boiler. For all simulations, a recirculation
zone was observed downstream of the swirling plate of the burner, which was identified as a key region for flame stability. The size and shape of its boundaries in relation to the load of the boiler were compared with the observations done during the experimental campaign and showed good qualitative agreement. The achieved CFD model provides a tool to evaluate further improvements in design and operation of the boiler and it is step stone for further practical studies of full-scale spray combustion furnaces.
Emissioner samt reduktion af forurening har været emner af stor interesse for industrielle processer i de seneste århundreder, og marine sektoren er hertil ingen undtagelse. Langt størstedelen af den maritime industri udgøres af skibsfart, der står for transport af omkring 80% af verdenshandelen og er dermed en væsentlig del af den globale økonomi og forsyningskæde. Dette gør dog også, at skibsfarten er ansvarlig for en betydelig del af den menneskeskabte emission af forurenende stoffer og drivhusgasser (GHG). Derfor er der brug for løsninger til at forbedre designet af nye store skibe og deres indbyggede systemer. Et af de systemer, der er berørt af skiftet til alternative brændstoffer, er hjælpekedlerne, der anvendes i højere grad i de senere år på grund af udnyttelsen af langsom sejlads (slow steaming). Dette Ph.d. projekt er en del af bestræbelserne på at forbedre effektivitet og fleksibilitet til forbrænding i sådanne kedler.

Tidligere er både eksperimentelle og beregningsmæssige metoder blevet anvendt i udstrakt grad til studiet af flydende sprayflammer, dog har hver af disse sine begrænsninger. At fremskaffe detaljeret data gennem eksperimenter er langvarig og dyr, mens Computational Fluid Dynamic (CFD) simuleringer skal valideres, før de kan bruges til praktiske formål og kan blive svære at udføre, hvis der er for mange fænomener, der skal inkluderes. Derfor blev en kombination af de to metoder benyttet i dette projekt.


Ud over indsamlingen af valideringsdata gav målekampagnen en mulighed for at teste kedlens fyringsegenskaber og observere virkningerne af varierende driftsbetingelser, såsom olietype, last og luftoverskud, påflammestabilitet samt emissioner.

I løbet af projektet blev en fuldskala kedel hos Alfa Laval modificeret med porte og forbindelser for at der dermed kunne indsætte prober ind i fyrrummet og der blev monteret udstyr til at måle gaskompositionen ved udgang. Den eksperimentelle undersøgelse omfattede både effekt af parametervariation på kedeldrift og flammeform og længde. For den første del blev kedlen opereret med tre forskellige lastniveauer, og mængden af forbrændingsluft blev ændret for at opnå en itkonzentration i et område mellem 1% og 5% ved udgang. Det anden del af kampagnen bestod i indsamlingen af data til validering af fremtidige CFD-simuleringer. Eksperimenterne blev gentaget for marine dieselolie og Heavy Fuel Oil (HFO).
Begge dele af målekampagnen gav interessante resultater. Det blev observeret, at brugen af HFO sammenlignet med diesel havde en næsten ubetydelig indflydelse på varmeoverførsel samt temperaturer i kedlen, men øgede emissionen af partikler med næsten en størrelsesorden, og af NOₓ og CO fra 3 til 5 gange.

Det kunne desuden konkluderes, at drift ved højere last havde en negativ effekt på alle specifikke emissioner, dog var den eneste undtagelse hertil partikelemissionen fra dieselforbrænding, som konsekvent var lavere ved højere last. Stigningen i CO-emissionen med højere last var klar, når lasten øges fra 40% til 60% for begge brændstoffer. De relative ændringer for NOₓ og partikler viste ikke så klare tendenser. Herudover medførte en stigning i luft-brændstof ækvivalentens forholdet ($\lambda$) over 1.2 ikke til et yderligere fald i CO-emission. Mens partikelemissionerne konsekvent faldt med øget $\lambda$, udviste NOₓ koncentrationen en relativt flad opførsel.

Den anden eksperimentelle undersøgelse var en spraykarakteriseringsundersøgelse på en olieforstøver, og undersøgelsen leverede de nødvendige inputdata til CFD-beregningerne. Ved at implementere disse data kunne modelleringen af sprayopbrydningsprocessen i CFD-simuleringerne undgås, hvilket reducerede beregningstiden betydeligt. Herudover resulterede denne undersøgelse i udviklingen af en ny spraykarakteriseringsmetode, samt yderligere indsigt i indflydelsen af centrale dyse driftsparametre på spraykarakteristika.


Alt i alt resulterede spraykarakteriseringsundersøgelsen i en opsamling af nødvendig data til CFD simuleringer og en udvidet forståelse af indflydelsen last, brændstofstryk og viskositet på spraykarakteristika i fuldskala kedlen.

Data opsamlet fra spraykarakteriseringsundersøgelsen blev herefter anvendt til at modellere brændstofindsprøjtning i CFD simuleringer af fuldskala kedlen i det comercielle software ANSYS CFX. CFD-modellen blev evalueret med dataene fra målekampagnen.

Sammenligning af den kortlagte flamme med CFD-resultaterne viste en god overenstemmelse med CO₂ koncentrationsprofiler, mens der var en afvigelse for CO og O₂ koncentrationsprofilerne samt

Den opnåede CFD-model bidrager med et værktøj til at evaluere yderligere forbedringer i design og drift af kedlen og er et skridt på vejen til yderligere grundlæggende forståelse spray olie flammer.
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Emissions and pollution reduction have been topics of constant interest for any industrial processes in the past decades and the marine sector is no exception.

The vast majority of the marine industry is constituted by shipping, which moves around 80% of the world trade and is therefore an essential part of the global economy and supply chain [1]. As such, it also is responsible for a significant share of the anthropogenic emission of pollutants and greenhouse gasses (GHG). The official estimate is that around 3.1% of the global CO\textsubscript{2} emission are produced by this industry and the forecast for the medium term is that they will increase from 50% to 250% by 2050 [2].

The International Maritime Organization (IMO), which is the United Nations agency for the safety and security of shipping and the prevention of marine and atmospheric pollution by ships, considers topics of paramount importance [3]:

- The reduction of the SO\textsubscript{x} emissions, to be achieved through regulations to decrease the maximum sulphur content of ships’ fuel oil from 3.5% to 0.5%, or the implementation of other measures to obtain an equivalent reduction in emissions.
- The reduction of GHG emissions, with the goal to reduce the carbon intensity of international shipping by 40% by 2030 [4], their total GHG emissions by 50% by 2050 and to completely decarbonize the sector by the end of this century.
- The reduction of marine litter, especially plastic.
- Addressing the problem of Black Carbon emissions in the Arctic, caused by the use and transport of Heavy Fuel Oil (HFO).

In particular, the GHG emissions reduction targets are mandated also by the temperature goals established by the Paris Agreement of 2016 and signed by all 195 sovereign countries [5]. Furthermore, especially related to the Danish shipping industry, more stringent regulations have been placed on NO\textsubscript{x} emissions with the designation of the North Sea and Baltic Sea as Emission Control Areas (ECAs), and thus subjected to the “Tier III” limits of the MARPOL Annex VI agreement [6].

In recent years, more and more initiatives have been devoted to meet these targets. However, there is an immediate necessity for solutions to improve the design of new large ships and their on-board systems. While improvement on the logistics and operation can be implemented on existing vessels, the design solutions for the ships that will be built in the next ten years must be adequate to comply with the
emissions limits set for 2050. This is evident when considering that the average age of the vessels composing the world fleet is around 20 years [1].

Battery-powered and hybrid ferries, ships using biofuels and hydrogen fuel cells, wind-assisted propulsion and carbon capture technologies are among several solutions that are currently being explored to decrease emissions [4]. While downstream reduction and capturing solutions are already on the market for SOx and NOx (scrubbers and SCR systems), no such methods are available for CO2 emissions. Carbon Capture and Storage (CCS) technologies are under development, but no economically viable solution has yet been found for large ships.

A possibility that has recently gained attention is the use carbon-neutral fuels, such as hydrogen produced with renewable-powered electrolysis or biofuels. However, due to logistic and technical reasons, ammonia (NH3) is currently considered one of the most promising energy carriers for the marine industry: the first ships employing NH3 engines will be deployed before 2023. While research in this sense could lead to interesting developments, the main issue with this solution is that the current world production of ammonia would cover only 20% of the marine industry needs, without considering that the entire agricultural sector depends on it as a fertilizer. Moreover, while ammonia itself does not contain carbon, currently most of the ammonia produced is derived from fossil fuels. This could be changed by producing hydrogen through electrolysis, but this is not currently viable from an economic point of view. Other carbon-neutral fuels do not lend a simple solution either: adding together the global production of biofuels, biogas, pyrolysis oil and hydrogen would cover in total less than 50% of the marine shipping industry needs, again neglecting the competition of other markets to have access to these fuels.

In the last decade, two effective ways proved to be capable of drastically reducing the CO2 emissions in the shipping industry: efficiency improvements and slow steaming. For every incremental improvement in the ship design, the fuel needed to produce the same amount of power is decreased, and thus the pollutants emitted. One of the techniques that has been developed in the recent years is to include an energy storage capacity on board of the ships, thus avoiding transient operation and partial loads of the engines at low efficiency. Other examples are the implementation of smart controlling systems, improvements on the propellers and coatings for the hull. However, the improvements in efficiency are not exclusive and their benefits can synergize with any other strategy to reduce the emissions.

Slow steaming was adopted in 2007 in the face of rapidly rising fuel oil costs and consists in decreasing the cruising speed of vessels to reduce fuel consumption. It has been calculated that, by reducing cargo ship speed from 27 to 18 knots (33 km/h), fuel consumption can be reduced by 59% [7]. Fuel saving directly affects the total amount of exhaust gases from the main engine and thus the emissions of all pollutants. This practice is nowadays common in the shipping industry and still has a large potential to further reduce emissions.

Most large ships are equipped with a waste heat recovery system (WHSR) to produce steam, which is used for electricity generation and other processes such as pumping, heating, cooling, cleaning and hot water for the accommodations. The steam production system also includes smaller auxiliary boilers mainly used to cope with the steam demand while the ship is in port. In this situation, it would be unnecessarily expensive to run the main engine to power the WHSR. The main design requirements of
the auxiliary boilers are simplicity, reliability and a small footprint. The push for emission reduction in the marine industry had an impact also on the WHSR and on the requirements for auxiliary boilers. To avoid multiple storage systems, the boilers use the same fuel as the main engine, which currently comprises a wide range of liquid fuels, but most commonly HFO and diesel fuels. With the new drive towards alternative fuels, there is a corresponding rising demand for fuel flexibility in the boilers too. Moreover, with the advent of slow steaming and the increased efficiency of the engines, the heat that can be recovered from the exhausts is not always sufficient to cope with the steam demand and these auxiliary systems have seen more and more use. This in turn has led to a more vested interest from the shipyards in more efficient and flexible boilers.

Project objectives

This project included full-scale experimental and computational studies with the aim to gain insight in the functioning of liquid fuel-fired marine boilers and to develop a predictive CFD model for their optimization, thus furthering the current capabilities of predicting practical spray flame behaviour.

More in detail, the PhD project activities and goals were:

- **Full-scale experimental campaign:** Gather detailed experimental data on a full-scale marine oil boiler, both to understand the effects of changing operating conditions on the system and to provide oil flames validation data for further modelling endeavours.
- **Atomization study:** Develop a spray diagnostic method to measure droplet size and velocity, and use it to characterize the nozzle of the full-scale boiler. Thus providing measuring data that can be used as input for CFD calculations, while gaining further insight into the influence of key nozzle operation parameters on spray characteristics.
- **Computational Fluid Dynamic (CFD) modelling:** Develop a validated predictive CFD model of the oil boiler flame, to supply a practical tool for boiler studies and gain further insight into flame dynamics and criticalities in the boiler design.

Project overview

This study was carried out on a commercial boiler produced by Alfa Laval. The boiler was rated for 2000 kg/h of steam capacity corresponding to a maximum oil input of 140 kg/h. The boiler was fitted with a horizontal swirl stabilized burner that could run on either marine diesel or Heavy Fuel Oil (HFO). The boiler consists of an air supply unit, a burner, a furnace surrounded by a water jacket and a tube heat exchanger through which the combustion gasses pass before being sent to the exhaust. When HFO (Heavy Fuel Oil) is used in the boiler an electrical fuel pre-heating system is employed to lower the viscosity. During normal operation on ships, the boiler is mostly used at minimum load (around 50 kg/h of fuel) for extended periods and rarely at higher loads.

The first step to improve a system is of course to gain insight into the way it works. Experimental and computational methods have been used in the past for simulating both liquid fuel flames and the atomization processes [8–10]. One of the most interesting of these methods is Computational Fluid Dynamics (CFD). By using the finite elements method, with CFD it is possible to obtain simulations of a
fluid domain that provide detailed information about the local temperatures, compositions and flow fields [11].

However, applying CFD on a large-scale application and at the same time simulate the droplet formation process with reasonable accuracy would require, huge computational resources. This is due to the inherent stochastic [12] nature and to the very small length- and time-scales at which the initial atomization process takes place. Moreover, CFD simulations implement a large number of models and computational methods, and therefore rely on a large number of assumptions. For this reason, they need to be validated before being used for practical purposes.

One way to limit the need for computational resources is to model the spray as an injection of particles, thus avoiding the simulation of the atomization process. In order to do so, an accurate characterization of spray droplets is needed to provide a reliable input for the simulation. In this project, a spray characterization setup has been designed, built and used to obtain the size and velocity distributions of the droplets in the spray produced by the boiler’s nozzle. The setup used an optical measuring system to measure velocity and size of single droplets. The size distributions and parameters obtained can be used to define the injection conditions in CFD simulations of the boiler and of the cold spray setup itself.

In addition, an experimental campaign on a full-scale boiler has been planned and carried out during the project, with the objective to obtain data suited to validate CFD simulations. Local temperature and gas composition have been measured in multiple positions inside the furnace chamber of the boiler and at the exhaust. Flame optical imaging and particulate emissions measurements have been carried out to supplement these data. The experimental campaign also served as a comprehensive test of boiler operation, changing the load and air to fuel ratio, thus giving further insight into the auxiliary boiler system.

To carry out this work, a collaboration has been established between the Technical University of Denmark (DTU) and Alfa Laval, which provided various resources, including access to their test centre, the full-scale test boiler and the use of their control and data-logging system. Furthermore, they provided the crew to operate the boiler during the experimental campaign and contributed with their experience in boiler operation to the planning of the experiments. Lastly, they provided access the preliminary CFD simulation of the previous boiler design done by Kim Bindesbøll Andersen (Alfa Laval) and Joakim Myung Johansen (DTU), which was the starting point for the modelling campaign presented in this work.

Structure of the thesis

This thesis is composed of five chapters, which are briefly presented below:

**Chapter 1: Project background**

The first chapter provides background information for the different parts of this work. First, an overview of atomization and spray combustion is provided, with special focus on techniques for spray characterization. Next, a summary of the techniques used in experimental studies of similar applications is presented. Lastly, an introduction to CFD and its underlying equations, with special attention to CFD for spray combustion modelling, turbulence models and the practical procedure applied in this work.
Chapter 2: Measurements on marine boiler oil flames

This chapter describes the experimental measuring campaign on a full-scale marine oil boiler, carried out at the Alfa Laval Aalborg test centre. The test boiler has been modified with ports and connections to insert probes into the furnace chamber and to sample the gas at the exhaust. The experimental investigation encompassed both boiler operation changes and flame mapping. Each of these parts has been repeated for marine diesel fuel and HFO. For the first part, the boiler has been run at three different loads and the combustion air changed to obtain an excess oxygen in the exhaust in the range between 1% and 6%. The second part of the campaign consisted of gathering data to validate the CFD simulations. The operating condition used in this case was 40% load and 4% oxygen concentration at the exhaust, for both marine diesel and HFO.

Chapter 3: Spillback nozzle spray characterization

In this chapter, the atomization characteristics of a commercial spillback hydraulic nozzle are investigated in terms of droplet size and velocity distributions. The atomizing nozzle is mounted on a cold setup that replicates the operating conditions of the test boiler. The measurements are performed using a novel pulsating LED optical imaging system, obtaining positions, velocity, sizes and shapes of single droplets for the spray currently used in a marine boiler. Mixtures of water and glycerol are used as model fluids to reproduce a range of physical properties comparable to those found with a rheology study for fuel samples from the boiler. The general performance of the nozzle is examined with a series of experiments at varying pressure drop, flow rate through the nozzle and liquid viscosity. The results of this study include droplet size and velocity distributions in different spray regions, a description of the influence of each varying parameter on global indexes such as the Sauter Mean Diameter (SMD) and a comparison with experimental correlations found in literature.

Chapter 4: CFD study of the auxiliary marine boiler

This chapter presents the CFD simulations of the marine boiler flames and the details about their validation. The results obtained though the simulations are compared with the local flame measurements presented in chapter 2. The predictive ability of the CFD simulations is also tested by comparing modelled and measured exhaust temperatures, gas compositions and soot concentrations for each operating condition. In addition, the limits of the operating range of the boiler in terms of load and excess air have been explored with further simulations. Lastly, a detailed discussion of the flame anchoring in the recirculation zone is presented and compared to the experimental observation for different boiler loads.

Chapter 5: Conclusions

The last chapter summarizes the main conclusions of this thesis and presents some suggestions for future work on the various topics tackled.
References

Atomization is the process by which a bulk liquid or slurry is transformed into droplets [1], and a spray is the resulting type of turbulent dispersed two-phase flow [2]. Spraying a liquid has three main useful effects:

- When impinging on a surface, the atomized liquid can be distributed evenly with a pattern that can be manipulated through the design of the atomizing nozzle.
- The velocity and impact force of a liquid can be easily regulated by changing the differential pressure across the nozzle orifice.
- By dividing the bulk liquid into smaller parcels, the surface of contact between liquid and gas phase can be drastically increased.

It can be easily understood that the first effect is what makes spray suitable for painting application, while the second has been exploited in more recent technologies, like pressure washers. Instead it is not so straightforward what makes sprays such an irreplaceable technology in combustion and engines.

As presented below, spray combustion was first used as a method for burning relatively involatile liquid fuels. The process involves the atomization of the liquid to produce small droplets in order to increase the contact area with the gaseous phase, which greatly enhances heat- and mass-transfer rates [3]. The time needed for a single fuel droplet to burn in an oxidizer is approximately proportional to the square of their diameter [4], so smaller droplets burn faster.

### 1.1 A historical perspective

The origin of sprays as a method to atomize a liquid is dubious. As many other technological advancements, it can be traced back to a certain period, but it is currently impossible to say where and with which application did it start. The first documented uses date back to the last decade of the 19th century for all internal combustion engines, painting and medicine delivery.

Atomization of fuel can be traced back to the first version of Brayton’s Ready Motor using liquid fuels [5], but it showed its actual advantages only with the first hot bulbs engines. Indeed, previous designs of internal combustion engines could successfully run on gaseous and light petroleum fuels, but the main obstacle to the use of heavier petroleum fuels was their difficulty in vaporizing in a carburettor. This issue was first overcome by the Akroyd-Stuart’s engines, built from the 26th June 1891 by Richard Hornsby and Sons [6]. This was the first internal combustion engine to use a pressurized fuel injection system [7].
Spraying paint with compressed air can be traced back to its use on the Southern Pacific Railway in the early 1880s and as a common practice in the locomotive and cars industry by the end of the century [8]. Some other sources claim that the first spray painting device was built in 1887 by Joseph Binks, the maintenance supervisor at Chicago's Marshall Field's Wholesale Store. He developed a hand pumped cold-water paint spraying machine to apply whitewash to the subbasement walls of the store [9]. This spray painting system was also used by the decorations director for the World's Exposition in Chicago in 1893, to apply whitewash at the Exposition, turning it into what has been called the White City [10].

In 1888 Dr. Allen DeVilbiss, a country doctor serving some rural communities in Ohio, assembled a hollow rubber ball, a metal jar, and a small tube to deliver a treatment for throat infections consisting in coating the inside of the patient's throat with petroleum jelly. The homemade device would pump out a spray of medicine when the ball was squeezed. He next added an adjustable tip to the tube that allowed him to adjust the pattern of the spray. The adjustable spray tip was unique enough that Dr. DeVilbiss applied for and received a patent for the idea. In 1905 Dr. DeVilbiss's son, joined the company and started to look for other applications for the atomizers. He found that the atomizers were also well suited to spray perfumes and, in 1907, began experimenting with industrial applications for the adjustable tip atomizer, making the first compressed air driven paint spray gun [11]. Since then, sprays have been adopted for many different purposes and are nowadays an irreplaceable technology for number of applications ranging from medicine, to coatings, to fuel combustion.

![Figure 1.1: Spray painting at the Chicago World’s Exposition of 1893](12)
1.2 Spray combustion

The combustion of sprays of liquid fuel is used in a variety of energy conversion systems from steam raising boilers and furnaces, to diesel engines and space rockets propulsion. These applications have generally been divided in two categories: engine application and stationary flames. The first are characterized by short injection times in a high-pressure environment and a sequence of ignition and extinction events, the second by a continuous operation over long periods of time and generally lower injection pressures. Both share common fundamental behavior and theories, but each also presents its own specific issues. For example, in engine application, the atomizing characteristics at nozzle opening is much more relevant than in a continuous spray.

Several fuels are commonly used in spray combustion. The most common fuels in engine applications are diesel fuels including both fractional distillate of petroleum fuel oil and non-petroleum derivate fuels like biodiesel and Gas-To-Liquid diesel fuels. Also in some gasoline engines, the fuel is sprayed directly into the combustion chamber. For aeronautical applications, unleaded kerosene or naphtha-kerosene are used as jet fuels. In boilers and furnaces, heavy fuel oil is widely used (also known as heavy oil, marine fuel or furnace oil). This is the heavier fraction obtained from petroleum distillation, aside from carbon black feedstock and bituminous residues. It is composed by long hydrocarbon chains and classified in six fuel grades: the higher grades are denser, have longer chains and a higher boiling point. While an exact official definition is not available, the working definition of Heavy Fuel Oil used by the IMO: “heavy fuel oil means fuel oils having a density at 15°C higher than 900 kg/m3 or a kinematic viscosity at 50°C higher than 180 mm²/s”[13].

The process of mixing fuel and oxidizer using an atomizer is the keystone in stabilizing the flame and strongly influences fuel conversion efficiency [14]. For example, a well-designed spray can minimize thermo-acoustic instabilities that could lead to a premature failure of the combustor. Local mixing also contributes to emission control: large amount of soot is produced in fuel rich zones, near stoichiometric mixing could lead to very high temperatures and higher NOx emissions, while mixing zones that fall outside the flammability limits can result in local quenching and CO and/or hydrocarbons emissions.

Spray combustions are highly complex systems where chemistry, fluid- and thermodynamics phenomena interact with each other. A schematic view of the main concurring interactions, both in the liquid and gas phases, is given in Figure 1.2 [15]. It should be noted that elements like droplet dispersion and turbulence are closely related to the atomizer characteristics, while in other processes an important role may be
played by the combustion chamber and burner geometry, e.g. gas mixing and turbulence. This suggests that the atomizer and the combustion chamber should be designed and analysed as an integrated unit, rather than as independent items [3].

As much as it is needed to acknowledge the complexity and relationships in spray combustion, it is also useful to simplify the issue and observe the various aspects and elements separately when possible. One such simplification consists in studying the behaviour of non-evaporating and non-combusting spray. This assumption is justified by the fact that evaporation does not dominate the behaviour of other multiphase flow phenomena in premixed spray combustion [16] and that in this case, the fuel is mixed and vaporized before combustion. Also in non-premixed systems, it has been shown that combustion and multiphase flow phenomena occur, for the most part, at considerably different levels of mixing (Figure 1.3). Therefore, it is reasonable to neglect evaporation and combustion effects as a first step toward the understanding of spray combustion in general [17].

Figure 1.3: Scalar properties for an n-pentane spray burning in air at normal temperature and pressure based on the LHF (locally homogeneous flow) approximation [15].
1.3 Spray dynamics

In a multiphase system composed of a liquid dispersed in gas, the process of liquid breakup into droplets is complex and not easily described. In general, this process can be considered as the result of disruptive forces overcoming consolidating forces at the contact surface of the two phases. The consolidating force usually being surface tension that tends to shape the liquid to achieve the minimum surface energy. In most cases, the final form of the liquid is an array of spheres, since this is the shape that minimizes the surface to volume ratio Figure 1.4. At the same time, the aerodynamic forces acting on the surface of the liquid tends to deform it, while viscosity stabilizes the process by opposing any alteration of the current geometry [18].

From a macroscopic point of view, four basic coexisting mechanism of liquid breakup can be differentiated, each characterized by a different relation between final droplet size and relative velocity between the phases ($u_r$) [19]:

- **Droplets in a steady field with high relative velocity**: This mechanism is most relevant to determine the drop size of free falling liquids and isolated droplets in a velocity field and leads to droplet size proportional to $u_r^{-2}$. The breakup of droplets impinging on a solid surface seems to follow a similar rule.

- **Droplets in a high turbulence field**: This is the dominant mechanism in distillation trays and pneumatic atomizers. The final droplet size is approximately proportional to $u_r^{-1.2}$.

- **Liquid column (or low velocity jet) breakup**: This is often an intermediate step during liquid breakup processes, it is most relevant in a few special applications (e.g. prilling towers) and the resulting droplet size is independent from the velocity (proportional to $u_r^0$).

- **Liquid sheet breakup**: this is the main breakup mechanism in hydraulic spray nozzles [2][19]. The resulting droplet size is typically proportional to $u_r^{-0.67}$ (in pressure nozzle the flow rate is proportional to the square root of the pressure drop [3]).

After the primary breakup, a secondary breakup takes place in case the resulting droplets are not stable at the given conditions. Thus, the dominant mechanism for each specific application is the one characterized by the smallest resulting droplets. An additional breakup mechanism has been studied in literature for drop breakup in viscous flow fields [18]. This is relevant for liquid injection in a liquid atmosphere and is therefore out of the scope of this report.

Lastly, a special case of droplet formation is the static drop formation. In this case, the resulting droplet size is dependent on the gravitational forces, e.g. in the detachment of droplets from a wetted horizontal surface the diameter $D$ has been found to be:

$$D = 3.3 \left( \frac{\sigma}{\rho_l g} \right)^{0.5} \tag{Eq.1}$$

Where $\sigma$ is the surface tension, $\rho_l$ is the liquid density and $g$ is the gravitational acceleration. This process is not used in practical applications due to the large resulting droplets and the necessity of higher flow rates. In addition, it has been reported that for droplet sizes below 300 µm the effect of gravitational force is negligible [18].
To give an example of atomization process, the schematic representation of a spillback nozzle is given in Figure 1.5 (left). The liquid reaches the swirling chamber (b) through tangential channels (a). The swirling liquid exits the nozzle with a strong tangential component due to the smaller radius of the orifice compared to the swirling chamber. This results in a lower pressure at the centre of the orifice that creates an air core [20] inside an expanding liquid sheer in the shape of a hollow cone. To regulate the amount of atomized liquid, part of the flow can be spilled through the return line (c). Once the liquid leaves the nozzle, the breakup mechanism described above reduce it into droplets. A possible break-up pathway for thinning liquid sheets is showed in Figure 1.5 (right) [21]. Here we can see that the shear stresses cause by the surrounding air generates wave instabilities on the thinning liquid sheet, this leads to fragmentation in long liquid ligaments, which further break into droplet to minimize the surface energy.
1.4 Spray characterization

Both the modeling and the experimental study of spray systems presents three main challenges [22]. The first one is that sprays are highly stochastic phenomena. Indeed, all formation mechanisms described above are driven by instabilities of the liquid surface. In addition to this, turbulence and cavitation play an important role in the internal flow of many atomizing nozzles. The second challenge is that, in a spray, multiple physically complex phenomena take place simultaneously and influence each other, such as primary liquid breakup, droplet collision, coalescence, and heat- and mass-transfer with the environment. The third challenge is related to the large number of droplets involved and their density. This complicates experimental measurements, which in turn result in a lack of sufficiently complete data for validation of theoretical models [23]. These obstacles are more pronounced close to the nozzle orifice. Defining exact boundaries to differentiate spray regions is not a trivial task, but a general division is usually presented as:

- The internal flow of the atomizing nozzle.
- The spray formation region near the nozzle orifice.
- A dense to moderately dense spray region, characterized by multiple scattering of the light of light when passing through it.
- The far-field region where the spray is fully developed.

In some applications, a fifth region of interest is represented by the spray-wall interaction, where droplet impinge on a solid surface.

Different measurement technologies are available to investigate each of the spray regions. An excellent topical review of the state of the art for each of these regions has been recently done by Fansler and Parrish [22], which supplement the earlier work on the same topic by Bachalo [23].

The goal of our spray characterization work is to obtain a full description of the droplet motion and size distribution of a fully developed spray. Therefore, in this work, the interest in spray diagnostic technologies is limited to the far-field region. The most common measurement technologies which can be used for dilute sprays and are summarized in Table 1.1 [22]. Several combinations of techniques are able to measure size and velocity of the droplets simultaneously, but combining different diagnostic system in a single setup increases its complexity considerably.

The techniques that can measure both droplet size and velocity are Phase Doppler Interferometry (PDI), Interferometric Particle Imaging (IPI) and high-resolution imaging.

Phase Doppler Interferometry, also called Phase Doppler Anemometry, utilizes the scattered light from two coherent laser beams and three detectors, to measure sinusoidal burst Doppler signals. For spherical droplets, Mie-scattering theory is able to relate the phase of these signals to the diameter, while the velocity can be calculated from their frequency [24].

In IPI the size of a side-illuminated droplet is calculated from the spacing of the interference fringes generated from its two glare points on a non-focal plane [22], as shown in Figure 1.5.
High-resolution imaging includes several variations, such as shadow-/back-illumination imaging [26], holography [27] and glare point imaging [28]. A detailed description of the back-illumination technique is given in chapter 3, where the complete method employed in this study for spray characterization is described.

In both high-resolution imaging and IPI, it is possible to obtain the velocity of the observed droplets by taking double exposure images, or by synchronizing the camera-illumination system to take a pair of images with a very small delay between each other, generally in the µs range. Using Particle Tracking Velocimetry (PTV), the velocity of each droplet is calculated as the ratio between the observed displacement and the time between the two observations. With the use of high-speed camera, this technique has also been employed to track the overall path of single droplets [26].
1.4 Spray characterization

Table 1.1: Measurement techniques available for spray characterization in the far-field region. Derived from Fansler and Parrish [22].

<table>
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<tbody>
<tr>
<td>Phase Doppler Interferometry</td>
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<td>x</td>
<td>x</td>
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<td></td>
<td></td>
<td></td>
<td>[24,29]</td>
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<tr>
<td>Planar Dropsizing</td>
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<td>[30]</td>
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<tr>
<td>High resolution imaging (incl. Glare point imaging and Holography)</td>
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<td>x</td>
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<tr>
<td>Forward Diffraction</td>
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<td>[23]</td>
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<tr>
<td>Interferometric Particle Imaging</td>
<td>x</td>
<td>x</td>
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<td>[29]</td>
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<tr>
<td>Femtosecond polarization ratio</td>
<td>x</td>
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<td></td>
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<td>[31]</td>
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<tr>
<td>Laser Doppler Velocimetry</td>
<td>x</td>
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<td></td>
<td>x</td>
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<td>[32]</td>
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<tr>
<td>Particle Image Velocimetry</td>
<td>x</td>
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<td></td>
<td>x</td>
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<td>[33]</td>
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<tr>
<td>Laser flow tagging</td>
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<td>x</td>
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<td>[34]</td>
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<tr>
<td>Laser-Induced Fluorescence</td>
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<td></td>
<td>x</td>
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<tr>
<td>Laser-Induced Exciplex Fluorescence</td>
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<td>x</td>
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<td>[35]</td>
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<tr>
<td>Thermographic phosphors</td>
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<td>[36]</td>
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<tr>
<td>Rainbow refractometry</td>
<td>x</td>
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<td>[29]</td>
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<tr>
<td>Raman scattering</td>
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<td>[29]</td>
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<td>Mie scattering</td>
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<td>[37]</td>
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<tr>
<td>Schlieren</td>
<td>x</td>
<td>x</td>
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<td></td>
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<td>[37]</td>
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<tr>
<td>Extinction/back-illumination</td>
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<td>[37]</td>
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</table>
1.5 Experimental studies on boiler flames

While spray combustion in internal combustion engines is extensively studied, it is difficult to find detailed experimental data in literature regarding large oil flames [38], and even more so for systems similar to a full-scale auxiliary marine boiler. Most of the comparable studies are several decades old [39–43]. The few recent studies that consider large scale combustors refer to land applications, such as power generation [44–46] and are generally focused on obtaining validation data for modeling purposes. There are however, neighboring research field that can provide insight into the boiler system and the experimental techniques that can be employed to study it.

Auxiliary boilers are fired using the same fuels as the main engines of large ships, therefore some engine studies contain useful data [47]. Studies on the fuel properties [48], combustion kinetics [49], flame and spray dynamics [50–52], and emissions [53] from marine engines are especially relevant to this project. The main limitations for this parallel is that, unlike in boiler furnaces, engine combustion happens in a discontinuous manner and at high pressure. Furthermore, the type of atomizer used for engines work at much higher injection pressure (30 to 200 MPa [54], compared to the 2 MPa of the back-spill atomizer mounted in the auxiliary boiler), in very short pulses and in a high pressure environment with a relatively small geometry (compared to the spray).

In recent studies, some attention is given to the use of bio-derived liquid fuels [55–59] including their application as fuels in industrial furnaces [60–63]. In these studies, HFO and diesel are used as reference to compare the bio-derived fuels. Data on their properties relevant to combustion and atomization is therefore reported, such as composition, viscosity, surface tension and heating values. Moreover, the investigation methods and the experimental techniques employed are often transferable to the study of marine boiler flames.

Special attention has been given to the experimental techniques used in these works, some of which have been employed in this study for the experimental campaign on a full-scale boiler, and are described in more detail in chapter 2. An overview of all the collected techniques with the corresponding reference is given in Table 1.2.
Table 1.2: List of experimental techniques used for measurements in spray combustion. Adopted techniques for this work are marked with *.

<table>
<thead>
<tr>
<th>Type of measurement</th>
<th>Technique</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>Suction pyrometer*</td>
<td>[46,49]</td>
</tr>
<tr>
<td></td>
<td>IR pyrometer</td>
<td>[44]</td>
</tr>
<tr>
<td></td>
<td>Two color optical pyrometry</td>
<td>[49]</td>
</tr>
<tr>
<td></td>
<td>Unshielded thermocouple</td>
<td>[38,40,60,64]</td>
</tr>
<tr>
<td>Gas Sampling</td>
<td>Water-cooled stainless steel sampling probe*</td>
<td>[38,39,42,46,49,60,64]</td>
</tr>
<tr>
<td></td>
<td>Water quenching probe</td>
<td>[65]</td>
</tr>
<tr>
<td>Gas Analysis</td>
<td>In line gas analyzers*</td>
<td>[38,41,42,49,60,64]</td>
</tr>
<tr>
<td></td>
<td>OH chemiluminescence</td>
<td>[63,66]</td>
</tr>
<tr>
<td>Particulate</td>
<td>Gravimetric analysis*</td>
<td>[38,60]</td>
</tr>
<tr>
<td></td>
<td>SEM analysis*</td>
<td>[38,60]</td>
</tr>
<tr>
<td>Radiation</td>
<td>Wall radiometer</td>
<td>[38,39]</td>
</tr>
<tr>
<td></td>
<td>Thermopile</td>
<td>[40]</td>
</tr>
<tr>
<td>Liquid Phase</td>
<td>Mie scattering</td>
<td>[52]</td>
</tr>
<tr>
<td></td>
<td>Deposition on magnesium coated glass with shutter</td>
<td>[42]</td>
</tr>
<tr>
<td>Flow field velocities</td>
<td>Laser Doppler Velocimetry</td>
<td>[38,41,64]</td>
</tr>
<tr>
<td>Optical</td>
<td>High speed imaging</td>
<td>[66]</td>
</tr>
<tr>
<td></td>
<td>Camera Probe*</td>
<td>[67]</td>
</tr>
</tbody>
</table>
1.6 Computational Fluid Dynamics

In the last decades, CFD modeling has become an important tool in many fields: from aerospace design and power generation, to weather simulation and biological engineering. With the recent developments in computational sciences and the improvements in numerical combustion models, the design of combustion systems has started relying on CFD simulations more and more [68]. CFD modeling has several advantages in this field when compared to traditional experimental investigation. CFD can provide a detailed description of gas composition, temperature and velocities throughout the domain, while avoiding any intrusive measurement that could potentially alter the results. Moreover, in most cases, CFD simulations are quicker and less expensive than designing and testing an experimental setup and geometry and boundary conditions are easily modified without additional costs.

1.6.1 Governing Equations

In CFD a discretization method is used to solve the governing equation of a fluid domain and calculate the fields of relevant variables (such as temperature, composition, pressure and velocity [69]). While the discretization method and additional equations used may vary, the basis of all CFD can be found in the Navier-Stokes equations (Eq.1), which describes the fluid motion as:

$$\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U \otimes U) = -\nabla p + \nabla \cdot \tau + S_M$$  \hspace{1cm} \text{Eq.1}

Where $\rho$ is the fluid density, $U$ is the flow velocity, $t$ is time, $p$ is the pressure, $S_M$ is a source term for momentum and the stress tensor is defined in relation to the dynamic viscosity, $\mu$, as:

$$\tau = \mu(\nabla U + (\nabla U)^T - \frac{2}{3} \delta \nabla \cdot U)$$  \hspace{1cm} \text{Eq.2}

These equations, together with the continuity equation (Eq.3) and a transport equation for energy, such as the total energy equation (Eq.4) are the governing equations used in CFD simulations [70].

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$  \hspace{1cm} \text{Eq.3}

$$\frac{\partial (\rho h_{tot})}{\partial t} - \frac{\partial p}{\partial t} + \nabla \cdot (\rho U h_{tot}) = \nabla \cdot (\lambda \nabla T) + \nabla \cdot (U \cdot \tau) + U \cdot S_M + S_E$$  \hspace{1cm} \text{Eq.4}

Where $h_{tot}$ is the total enthalpy, $\lambda$ is the conduction coefficient, $T$ is the temperature and $S_E$ is the source term for energy, which would include contributions such as the one from chemical reactions. The total enthalpy is defined is related to the enthalpy, $h$, by the relation:

$$h_{tot} = h + \frac{1}{2} U^2$$  \hspace{1cm} \text{Eq.5}

The CFD simulations presented in this study use Eq.1 to 5, together with additional ones for the chemical reactions, to describe the Eulerian fluid phase that constitutes the fluid domain. To do so, these equations are discretized and solved in each cell of the computational domain in an iterative manner.
1.6 Computational Fluid Dynamics

1.6.2 CFD of spray combustion

Practical simulations of fuel oil spray combustion have been carried out since the nineties [64]. A number of commercial and open-source software have been employed, but the most used are ANSYS Fluent [65,71], ANSYS CFX [72,73], OpenFOAM [63] and Star-CD [74]. While some of the issues that needs to be tackled to perform the simulation of spray combustion are common to other application of the CFD methods, their combination is quite specific.

In spray combustion simulations, homogeneous reactions are the main driver of the various phenomena, which take place in the computational domain. Various reaction models have been used in spray combustion applications, but possibly most long-lived is the Eddy Break-up Model and its modification, the Eddy Dissipation Model (EDM). While these models assume infinitely fast reaction kinetics, subsequent adaptations are able to consider slower kinetics, leading to the Eddy Dissipation Concept model or the combined EDM/Finite Rate Chemistry model. These models have been used successfully for simulations of oil fired baffle plate burners [64], large industrial boilers [72] and glass-melting furnaces [75].

Another important factor is how the liquid phase is modelled. In recent years, CFD simulation of the spray break-up process itself have been achieved using Direct Numerical Simulations (DNS) and Large Eddy Simulation (LES), but both are computationally too expensive for practical application in spray combustion [14,76]. Simpler models are used for engineering CFD simulations of sprays, but generally omit the internal nozzle flow and the near-nozzle breakup, and need experimental data to give accurate results [14,23,77]. Overall, while some studies include the modeling of the spray-break up in the CFD simulations [78–80], the majority of studies defines an injection of already-atomized fuel droplets in the computational domain [63–65,71,75]. In both cases, the Eulerian-Lagrangian approach is used to model the liquid phase.

In combustion simulations, the radiation contribution to the heat transfer in the computational domain cannot be neglected. Radiation models applicable to CFD simulations include the Discrete Ordinate (DO) model, the P1 model, the Discrete Transfer Radiation Model (DTRM) and the Monte Carlo Method [81,82]. While the latter is generally considered the most accurate, it is also the computationally most expensive. The P1 model lies at the other end of the spectrum, with its lower accuracy and computational costs. The DTRM [75] and the DO model [71] both found practical use in combustion modeling. Different sources claim the superiority of the DTRM [81], while other of the DO model [83,84].

More details about these models are given in chapter 4, together with a discussion of the used models parameter and boundary conditions. The last main issue to be considered in spray combustion modeling is turbulence, which is introduced next.

1.6.2.1 Turbulence modeling

The way turbulence is modelled in a CFD simulation is the foundation for all the other models; therefore, it is here briefly introduced.

Depending on the ratio between inertial and viscous forces, fluid flows can be divided in three categories: laminar, transitional and turbulent. The Reynolds Number (eq.6) is used to quantify the regime of fluid
flows: low $Re$ indicates a laminar flow, an intermediate range of $Re$ denotes a transitional flow and high $Re$ corresponds to a turbulent flow. The exact values for these ranges depends on the geometry that is considered.

$$Re = \frac{\rho UL}{\mu}$$  \hspace{1cm} \text{Eq. 6}$$

Turbulence representation is one of the main issues for fluid dynamics modelling and therefore of CFD. This is because the fluctuations in turbulent flows can happen on a large range of space and time scale, and produce unsteady, three-dimensional effects. This means that, while the Navier-Stokes equations can be used to describe both laminar and turbulent flows, the number of finite volumes in which a computational domain should be divided to resolve the smallest flow structures is generally impractical. However, this approach is implemented in Direct Numerical Simulations (DNS), which necessitate a number of points in the computational grid of proportional to $Re^{9/4}$, with the effect that the computational time results to be proportional to $Re^3$ [85]. Nonetheless, DNS of fluid flows has been achieved for fundamental research, and with the increase of the computational capabilities in the future, it will possibly see more application. For practical simulations, the most widespread approach is to employ a turbulence model to predict the effects of turbulence on the flow.

There are two alternatives to DNS that have been widely used in CFD in the past decades: the LES model and the RANS equations. The LES model was first proposed in 1963 by Smagorinsky et al. [86], it allows for a coarser computational grid and alleviates the computational effort required compared to DNS (as an example the number of grid elements for a LES simulation of an industrial boiler is above $23 \times 10^6$ [72]). This is achieved by solving the Navier-Stokes equations only for large-scale motion, while employing sub-grid models to consider the effects of smaller eddies. Several of these models are available including the original Smagorinsky model, the dynamic Smagorinsky-Lilly model and Wall-Adapted Local Eddy-viscosity model (WALE). While LES presents lower computational costs compared to DNS, it is still quite demanding, especially for practical application to wall-bounded flows and reacting flows with high Reynolds number [87].

Another possibility to reduce the computational costs associated with turbulence modelling is to use the Reynolds-Averaged Navier-Stokes equations. While DNS and LES directly resolve at least some part of the turbulence spectrum, the RANS equations describe a turbulent flow as a sum of an average and a time varying components. When this decomposition of the instantaneous quantities is applied to the Navier-Stokes equations, it introduces an additional unknown non-linear terms that acts like additional stresses on the fluid. For this reason, these terms are called Reynolds Stresses, $\rho u'_i u'_j$, and create a closure problem with the RANS equations. To deal with this issue a number of different RANS models have been developed. The most common of these models and their respective advantages and limitations are summarized in Table 1.3 [88]. A number of comparison between these models have been done in the past for reactive swirling flows, with a general consensus that the $k-\omega$ Shear-Stress Transport lends the best results for this application [89,90]. Regardless of the closure model used, RANS simulations are widely used for practical engineering problems since they are able to predict with good accuracy the flow phenomena and are computationally less expensive than LES or DNS [91].
### Table 1.3: Common RANS models including the number of equations they use, their advantages and limitations.[88]

<table>
<thead>
<tr>
<th>Turbulence model</th>
<th>Type</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spalart–Allmars [92]</td>
<td>One–equation</td>
<td>Suitable for wall-bounded flows with low Re number</td>
<td>Requires proper resolution near the wall (y+ &lt; 1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Not suitable for general industrial flows</td>
</tr>
<tr>
<td>k-ε [93]</td>
<td>Two–equation</td>
<td>Suitable for a wide range of turbulent flows</td>
<td>Modifications of model constants are required for specific problems</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Improved performance for modified versions</td>
<td>Weak performance for complex flows</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Boundary layer is not required to be resolved</td>
<td></td>
</tr>
<tr>
<td>k-ω, Shear Stress Transport model (SST)</td>
<td>Two–equation</td>
<td>A mixture of k-ε and k-ω models</td>
<td>Viscous sub-layer region should be resolved (y+ &lt; 5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>More accurate and reliable for a wider classes of flows compared to k-ε and</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>k-ω models</td>
<td></td>
</tr>
<tr>
<td>Reynolds Stress Model (RSM) [95]</td>
<td>7–equation</td>
<td>The most elaborate RANS turbulence model</td>
<td>Lower stability</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Rigorous and accurate for complex flows especially flows with swirl, rotation etc.</td>
<td>Requires higher computational cost than other models because of solving 7 transport equations</td>
</tr>
</tbody>
</table>

#### 1.6.2.2 Practical procedure for CFD simulation

The typical procedure for a CFD simulation starts with the definition of the computational domain with a CAD software. The geometry file is then imported to a meshing software, which is used to divide the domain into a large number of small volumes (or surface for two-dimensional models). These will be the control volumes used for the integration of the governing equations. The next step is the definition of the CFD models, boundary conditions and parameters that are used in the simulation. This information is used by the solver to calculate iteratively the solution of the simulation in the solver. For transient simulations, an inner iteration loop calculates the solution for each time-step, before moving to the next one. The results obtained from a simulation contain a huge amount of data, which needs post-processing before being analyzed. The calculated fields for some or all variables can also be used as initial conditions for further simulations. In Figure 1.6, a flow diagram shows the procedure used in this study, including the software employed for each step. Part of the process was done on a personal computer with limited computational capacity, while the CFD simulations were carried out on the central High Performance Computing cluster of DTU.
1.7 References


1.7 References


1.7 References


2

Measurements on marine boiler oil flames

2.1 Introduction

Within the framework of the INNO+ project on marine auxiliary boilers and as part of the collaboration between Alfa Laval Aalborg and the Technical University of Denmark (DTU), it was possible to carry out an experimental measuring campaign on a commercial auxiliary marine boiler. At the Alfa Laval test center, a full-scale boiler was modified with ports and connections to make it possible to insert probes into the furnace chamber and to sample the gas at the exhaust (Figure 2.3).

The main objectives of the measuring campaign were:

- To obtain point measurements of temperature and gas composition inside the furnace chamber. These data was obtained to support and validate CFD simulations of the boiler.
- To gather insight into the influence of operating changes (fuel oil type, load and amount of excess air) on the boiler emissions.

Moreover, most of the equipment used during the experiments was designed and manufactured at DTU, therefore a secondary objective of the campaign was to test it thoroughly.

In this chapter, the experimental measuring campaign of the full-scale auxiliary marine boiler is presented, starting with a brief description of the test boiler. Knowledge about how the boiler is operated has been acquired through verbal communication with Nils Brandt Pedersen, system engineering responsible for the boiler operation. In the materials and methods section, the measuring equipment is presented and discussed in detail, together with an analysis of the fuels used during the experimental campaign and the various operating conditions that have been explored. The following result section is divided into two parts: the first one presents the exhaust measurements taken for varying load and excess air, the second shows the measurements conducted inside the furnace at the reference operating condition. For confidentiality reasons, the data regarding CO, NOx and particulate emissions have been normalized to the value measured at the reference operating condition.

2.2 Materials and methods

In this section, the experimental setup and the operating conditions are presented. A summary of the measurements taken and of the boiler operating conditions during the experiments is given in Table 2.1.
Measurements on marine boiler oil flames

Table 2.1: Summary of the salient details of the material and methods used.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>Marine Diesel/Heavy Fuel Oil</td>
</tr>
<tr>
<td>Fuel flow rate</td>
<td>50/80/112 kg/h</td>
</tr>
<tr>
<td>Oxygen concentration at the exhaust</td>
<td>1/2/4/6 %</td>
</tr>
<tr>
<td>Water pressure</td>
<td>5.5 bar</td>
</tr>
<tr>
<td>Fuel heating value and composition</td>
<td>Table 2.2</td>
</tr>
<tr>
<td>Furnace chamber measurements</td>
<td>Temperature and gas composition mapping, flame imaging</td>
</tr>
<tr>
<td>Number of measuring positions</td>
<td>33</td>
</tr>
<tr>
<td>Exhaust measurements</td>
<td>Temperature, particulate, gas composition</td>
</tr>
<tr>
<td>Gas analysis</td>
<td>O₂, CO₂, CO, NO, NO₂</td>
</tr>
<tr>
<td>Flame imaging camera</td>
<td>CMOS MU9PC-MH</td>
</tr>
<tr>
<td>Flame imaging filter</td>
<td>Neutral density fused silica with metallic coating O.D.=2</td>
</tr>
<tr>
<td>Particulate analysis</td>
<td>Gravimetric and SEM</td>
</tr>
</tbody>
</table>

2.2.1 The experimental setup

The boiler object of this study was an Alfa Laval boiler, rated for 2000 kg/h of steam capacity corresponding to a maximum oil input of 140 kg/h. The boiler was fitted with a horizontal swirl stabilized burner (Figure 2.4) that could run on either marine diesel or Heavy Fuel Oil (HFO). This type of boiler is operated at a slight overpressure (ca. 3kPa), thus requiring special care and tailored connections when inserting probes in the furnace or at the exhaust, while avoiding any leak of the combustion gasses. The boiler consists of an air supply unit, a burner, a furnace surrounded by a water jacket and a tube heat exchanger through which the combustion gasses pass before being sent to the exhaust (Figure 2.2).

When HFO (Heavy Fuel Oil) is used in the boiler an electrical fuel pre-heating system is used to lower its viscosity, the exact temperature is found based on the fuel viscosity at a reference temperature using a viscosity-temperature curve given to the boiler operator. For the HFO used during the campaign the viscosity at ambient temperature was 380 cSt and to reach an acceptable level (around 8 cSt) it was heated to 140/150°C.

The exhaust gasses from the boiler can follow two different paths, depending if a scrubber is used or not. The scrubber is necessary when running on HFO, but it is bypassed when using diesel, as it requires additional crew to be operated (Figure 2.1).
During normal operation on ships, the boiler is mostly used at minimum load for extended periods and rarely at higher loads. During a test run of the boiler it was evident that already with a diesel fuel flowrate of 114 kg/h (80% of the maximum load based on the nozzle characteristics) the steam production reached 2000 kg/h, which was also the maximum capacity of the condenser connected to the system. On the other hand, based on the boiler operator experience, the minimum load used is around 47 kg/h of fuel (33% of the maximum load based on the nozzle characteristics). Hence, it was decided that these loads and an intermediate level would be used during the measuring campaign.

The load of the boiler displayed by the control system is based on the position of a valve in the fuel feeding system as a percentage (where 0% means that the valve is fully closed). Therefore, the boiler load displayed on the control system does not correspond to the amount of fuel given by the nozzle characteristics. To assess the equivalence between these two, during the test run the displayed load was incrementally changed and, once stabilized, the corresponding fuel flow was noted down (Table 2.2).

Table 2.2: Equivalence between loads and fuel flow according to the nozzle characteristic and the control system load based on the aperture of the fuel distribution valve.

<table>
<thead>
<tr>
<th>Load based on nozzle characteristics [%]</th>
<th>Calculated fuel flow [kg/h]</th>
<th>Closest control system Load [%]</th>
<th>Measured fuel flow [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>80</td>
<td>114</td>
<td>60</td>
<td>112</td>
</tr>
<tr>
<td>56</td>
<td>80</td>
<td>40</td>
<td>80</td>
</tr>
<tr>
<td>33</td>
<td>47</td>
<td>20</td>
<td>50</td>
</tr>
</tbody>
</table>

While the load is based on the fuel mass flow, the flow rate of the combustion air is regulated independently, using as a reference a portable device that measures the oxygen concentration at the exhaust of the boiler. During normal operation, the oxygen concentration at the exhaust is aimed at 5% for minimum load and it is decreased down to 3% for higher loads. The aim in this study was to collect data at 1, 2, 4 and 6 vol% O₂, but it was possible to decrease the excess oxygen to 1 vol% O₂ only at 60% load without incurring in flame stability issues.
Measurements on marine boiler oil flames

Figure 2.2: Initial design of the test boiler: lateral and front view, including probe connection position with names.

At the test centre, the boiler is connected with a closed water cycle to a condenser and a pump, here heat is removed from the saturated steam generated by the boiler that condenses and cools down before being reused in the boiler. A logging system records the boiler load, together with the steam side conditions (Figure 2.3). A sensor detects the water height in the boiler and operates the pump to keep it at a constant level. The pressure in the steam side of the boiler is kept at 5.5 bars, except when the boiler is producing an amount of steam that exceeds the capacity of the condenser, then the steam pressure increases. As mentioned above, this was the case when the boiler was operated at 60% displayed load (Figure 2.3). The change in pressure also modifies the boiling temperature of the water; however, the change is small enough that the heat exchange and surface temperatures in the boiler furnace should not be visibly affected from it (the water boiling temperature changes between 156 °C at 5.5 bar to 165 °C at 7 bar). The burner used during the experimental campaign is a swirl-stabilized burner suitable for both oil and gas firing (Figure 2.4). It uses a plate with slots to add a tangential component to part of the combustion air and to anchor a recirculation zone. A single burner lance ending in a spill-return pressure swirl atomizer is used and a spark ignition system is mounted on it. The gas injection system is embedded in a cylindrical liner around the burner lance. Despite the fact that gas supply was not used for the experiments, the gas distribution system was mounted to consider its impact on the combustion air flow field. This design resulted from the experience with two previous iterations adopted by the Alfa Laval during this project.
2.2 Materials and methods

2.2.2 Fuel analysis

During the experimental campaign, two different fuels have been used: Heavy Fuel Oil and marine Diesel. A sample of each fuel has been collected and analyzed.
Measurements on marine boiler oil flames

The Higher Heating Value (HHV) has been measured with a bomb calorimeter Parr 6300 and following the standard ASTM D240–02. The results obtained are in line with those reported in literature [1–4] and are summarized in Table 2.3.

Elemental analysis of the samples has been carried out with a FlashEA 1112 from Thermo Fisher, using a CHNS protocol with 10 repetitions for diesel and 9 for HFO. Sulphur was detected, but could not be quantified. This is because the large amount of hydrogen found in the sample produced a signal peak that overlapped with the much smaller Sulphur peak. The amount of nitrogen measured showed a clear correlation with the sample weight (see Appendix I.2.1). The reason for this was that the sample capsules were not sealed in a nitrogen free environment. In any case, these issues do not affect the hydrogen to carbon ratio, which is the most relevant parameter for mass balances in the boiler and for hydrocarbon modelling in the CFD simulations. To check the result of this analysis, the samples have also been sent to a certified external laboratory (FORCE technology) for further testing (Appendix I.2). The results in Table 2.3 confirmed that the hydrogen to carbon ratio could be calculated with reasonable accuracy regardless of the issues with the quantification of nitrogen and sulphur content. Nonetheless, given the higher accuracy, the results from the certified laboratory have been adopted for any further calculation.

While the viscosity of the HFO is given by the supplier, the Diesel sample has been studied with a Discovery HR2 hybrid rheometer lending results in agreement with those found in literature [5].

Table 2.3: Measured heating value, composition and viscosity for the fuel samples taken during the experimental campaign.

<table>
<thead>
<tr>
<th></th>
<th>Diesel</th>
<th>HFO</th>
</tr>
</thead>
<tbody>
<tr>
<td>HHV [MJ/kg]</td>
<td>45.77</td>
<td>42.76</td>
</tr>
<tr>
<td>Standard Deviation [MJ/kg]</td>
<td>0.11</td>
<td>0.16</td>
</tr>
<tr>
<td>Measured H/C ratio [mol/mol]</td>
<td>1.81</td>
<td>1.33</td>
</tr>
<tr>
<td>Standard Deviation [mol/mol]</td>
<td>0.09</td>
<td>0.10</td>
</tr>
<tr>
<td>External lab H/C ratio [mol/mol]</td>
<td>1.881</td>
<td>1.461</td>
</tr>
<tr>
<td>Standard Deviation [mol/mol]</td>
<td>0.013</td>
<td>0.007</td>
</tr>
<tr>
<td>Nitrogen [%]</td>
<td>&lt;0.1</td>
<td>0.6</td>
</tr>
<tr>
<td>Standard Deviation [%]</td>
<td>0.04</td>
<td>0.03</td>
</tr>
<tr>
<td>Oxygen [%]</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Viscosity [cP]</td>
<td>4.0</td>
<td>422*</td>
</tr>
<tr>
<td>Standard Deviation [cP]</td>
<td>0.16</td>
<td>-</td>
</tr>
</tbody>
</table>

*from the fuel supplier
2.2 Materials and methods

2.2.3 Description of the measuring equipment

The following equipment was used during the measuring campaign and it is explained in this section:

- Suction pyrometer (including logging system and ejector).
- Gas extraction probes (a long and a short water-cooled probe for sampling in the furnace chamber and a heated probe for the exhaust).
- Temperature controlled water-cooling tank to avoid condensation in the gas extraction probes.
- Gas analysis system (including CO/CO\textsubscript{2}/O\textsubscript{2} analysers, a NO\textsubscript{x} analyser, a conditioner box, calibration gasses and equipment, and heated hoses).
- Camera probe and video/picture acquisition software and hardware.
- Particulate measuring system using a direct gravimetric method (including sampling probe and filtering equipment).
- A Testo machine [6] supplied by Alfa Laval, which is a portable gas analysis system. For most part of the campaign one with CO/CO\textsubscript{2}/O\textsubscript{2} measuring capabilities was employed to regulate the boiler by reading the oxygen concentration at the exhaust. For a limited time one with also a NO\textsubscript{x} sensor has been used.

Most of the probe equipment was constructed specifically for this project.

![Schematic drawing of the suction pyrometer tip.](image)

Figure 2.5: Schematic drawing of the suction pyrometer tip.

2.2.3.1 Suction pyrometer

The suction pyrometer is a device to take temperature measurements with a thermocouple while shielding it from radiation heat exchange (see Figure 2.5). The one used in this study was built especially for the experimental campaign and according to the documentation available from the International Flame Research Foundation. With a working length of 2.2m, it was long enough to reach from the back wall to the front wall of the boiler. To generate the necessary suction a compressed air ejector is used. In the suction line, a rotameter with a temperature measurement was installed to monitor the flow through the suction pyrometer. Due to the high temperatures inside the furnace, the body of the probe is water cooled, while the tip is made of ceramic material to ensure that the temperature measured is not influenced.
During operation it was noticed that condense was forming inside the suction line and could not escape due to the vertical section needed for the rotameter. For this reason, the line was periodically drained. The temperature measurement show that the drainage was adequate, since the temperature measured did not change before and after draining. This can be observed in the example of temperature log reported in Figure 2.6: the drop in temperature recorded during the draining quickly disappears after the suction is reconnected.

2.2.3.2 Gas extraction and analysis

To obtain information about the gas composition, continuous gas analyzers had been brought from DTU and calibration gasses had been previously shipped to the Alfa Laval facility. Two gas analyzers were used, an Emerson NGA 2000 and an ECO PHYSICS nCLD 822, the first was used to measure O2, CO2 and CO, the second to measure NOx. The signal from the analyzers was logged using LabView on a dedicated computer.

![Temperature profile example during suction drain](image)

*Figure 2.6: Temperature measured by suction pyrometer the before and after draining the suction line. Measurements conducted 24/10 2018.*

![Longitudinal section schematic drawing of the gas suction probe tip](image)

*Figure 2.7: a) longitudinal section schematic drawing of the gas suction probe tip. b) Transversal section schematic drawing of the end of the gas suction probe*
Three different probes have been used for extracting gas from the system in different locations: two for in-flame measurements and one for exhaust measurements. For the in-flame measurements, one of the probes was of a similar length as the suction pyrometer and was used to sample the gas in the same positions, going across from the back wall to the front wall (Figure 2.7a). The second gas probe for in-flame measurements was designed to fit in the tight space around the boiler; this was achieved by distributing the cooling water and gas line connections on a single plane (Figure 2.7b) and integrating the gasket and probe holder inside the connection port. With these expedients, it was possible to have a working length of 0.95m with a total length below 1m. The third probe is the one used for the exhaust measurement and consist of a commercial flange probe with integrated electrical heating.

One of the main concern for gas extraction measurements is to avoid condensation in the gas lines. For this reason, the probes for in-flame measurements were cooled with water from a temperature-controlled tank that kept the water between 70°C and 80°C. The water-cooling is also instrumental in preventing reactions to continue in the gas line by decreasing the gas temperature rapidly. The short cooling time is also ensured by the small amount of gas extracted compared (1-4 l/min) to the cooling water flow (>12 l/min) and the much higher heat capacity of water compared to the gas. Lastly, a heated hose (kept at around 170°C) was used to transport the gas to a conditioner box, where condensate is removed by a cooling system and a dedicated pump (Figure 2.8C).

The gas analyzers were initially connected as shown in Figure 2.8A, this configuration ensured that each analyzer had the appropriate gas flow, and that they could work continuously and simultaneously. Unfortunately, the NOx analyzer had a slightly higher suction than the flow passing through the other analyzers and would then suck additional air from the ventilation. Switching the two analyzers was not an option as the outlet flow from the NOx analyzer includes dilution air. The solution used is show in Figure 2.8B. This configuration uses a three-way valve to direct the flow to each analyzer separately, thus
ensuring that the flow through each analyzer was correct. The drawback of this solution was that the analyzers could not work simultaneously and it was necessary to wait until steady state was reached after each switch. The logged data show that the operation of the boiler was steady enough that no inaccuracy should have been introduced by not having simultaneous measurements for the different compounds. After each change on the sampling train, the analyzers were tested with calibration gas to ensure their reliability. As no gas with a comparable amount of NOx was available, the nCLD analyser could only be tested with nitrogen. For this reason, this analyzer was tested with calibration gas at DTU before and after the experimental campaign. These tests were done using the same connections as used at the test center and showed that the analyzer worked properly and calibration is preserved regardless of the transport.

2.2.3.3 Optical imaging of the flame

A water-cooled probe was used to insert a CMOS camera in the furnace of the boiler to obtain videos of the flame. The purposes of this type of measurement are multifold. First, visualizing the flame is useful to assess macroscopic issues, such as stability and brightness of the flame, or position and shape of the recirculating zones. Moreover, the videos obtained, could be used to confirm the CFD simulations prediction regarding the position of the flame.

The camera used was a MU9PC-MH from Ximea. The camera’s maximum operating temperature is 60 °C and the maximum temperature for which its correct operations is guaranteed is 25 °C. This issue was dealt with adequately thanks to the water-cooling and a purge flow of compressed air (Figure 2.9).

Due to the high amount of radiation from the flame, to keep the sensor from saturating fused silica neutral density filters have been used. The filters used a metallic based, reflective coating and had an optical density of 2.0. Compressed air was used to generate a purge flow to ensure that no deposits would occur on the filter, while at the same time keeping the camera as cool as possible.
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The main issue with the measurements was the distortion of the images due to the rolling shutter effect deriving from the way CMOS sensors read the pixel signals. This was clearly visible when turning the probe on its axis because the flame structures movement is quite fast. The effect could be decreased by keeping the exposure of the camera above 1 ms. Regardless, this would not affect the average values through a video.

2.2.3.4 Particulate emission measurement

The method used for particulate measurement stems from an adaptation of the direct gravimetric method described in the Norwegian standard for determination of particulate emission of enclosed wood heaters (NS3058-2) with consideration for the standard ISO-29904 (Figure 2.11). Iso-kinetic calculations have not been conducted, as the particulate for this application is mainly soot and it is expected to have a small enough particle size to be fully entrained in the gas flow.

The gas sample was collected and diluted with a known volume of ambient air. A handheld thermocouple was positioned at the air suction to register its temperature for each sample and check that it would not vary during the sampling. Heating tape was used to avoid any condensation in the piping before the dilution. The dilution ratio was not directly regulated, but adjusted to avoid condensation in the sampling train and to keep the filter temperature between 25°C and 28°C. The dilution ratio is calculated to be in the range between 8 and 12 for all measurements but two (a ratio of 5 and 4 respectively was calculated for the measurements at 60% load with 1 and 2% exhaust oxygen concentration). The setup is mounted with two filter housings in parallel, so that the regulation of the dilution and stabilization of the temperatures in the system could take place while the flow was passing through a sacrificial filter. The actual sampling was started after steady state operation was achieved, by switching to the second filter line. In addition, the tubing before the two filters were slightly tilted to ensure that if any condensate was formed during the regulation, it would not interfere with the measurements.
To guarantee the reliability of the gravimetric measurement, it is important to evaluate the method used. In the case of this study, quartz fiber filters with a pore size of 2.2 μm have been employed. In Figure 2.10, a filter for each of the used operating conditions is shown. The filters have been pretreated at 550 °C for 2 hours in a muffle oven, after which they have been stored in a desiccator and weighted. To carry them to the test center, the filters have been stored in single numbered zip bags.

Table 2.4: Example calculation of the influence of humidity on the gravimetric analysis.

<table>
<thead>
<tr>
<th>Filter number</th>
<th>11</th>
<th>10</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Before the test</td>
<td>[mg]</td>
<td>696,99</td>
<td>703,46</td>
</tr>
<tr>
<td>Dried at 110 °C</td>
<td>[mg]</td>
<td>696,34</td>
<td>702,77</td>
</tr>
<tr>
<td>After storage</td>
<td>[mg]</td>
<td>696,43</td>
<td>702,81</td>
</tr>
<tr>
<td>Amount of water on total evaporated amount</td>
<td>[%]</td>
<td>4,2</td>
<td>6,1</td>
</tr>
<tr>
<td>Change in the final particulate concentration due to humidity</td>
<td>[ppm]</td>
<td>1,2</td>
<td>0,3</td>
</tr>
</tbody>
</table>

After the samples have been deposited on the filters, petri dishes were used to transport them to the laboratory and store them in a desiccator. It should be noted that the relative humidity in a desiccator is not zero, but using any thermal treatment to remove more water from the filters would cause devolatilization of other compounds too. To assess the impact that these issues have on the measurements, three filters have been weighted, and then dried in a muffle oven at 110 °C, weighted.
2.2 Materials and methods

again and then left overnight in a desiccator before weighting them one last time. The results of this experiment are summarized in Table 2.4.

From these results, it is evident that the main effect of heating the filter to 110°C is to release part of the volatiles and that the influence of the humidity in the desiccator is much smaller than the changes in particulate emissions relevant to this work.

It should be considered that the filters are stored in a desiccator also after the pretreatment even if for a shorter period. Since the particulate concentration is calculated from the difference in filter weight, if part of the humidity is present also when the filter is weighted before sampling, it will reduce the error caused by that amount. Therefore, the influence of humidity given in the last row of Table 2.4 can be considered a conservative estimate.

![Figure 2.12: SEM images of HFO (left) and Diesel (right). Quartz fibers from the filters are visible in both pictures. Large structures found in the HFO sample have been analyzed with the EDS (top left).](image)

Lastly, samples have been taken from some of the filters and observed with a Scanning Electron Microscope (Figure 2.12) Hitachi TM3000. While the resolution provided by the instrument (x500) was insufficient to observe soot particles [7–10], it showed some large structures in the sample from HFO combustion. This type of particulate, called cenospheres, has been observed in literature for HFO combustion [11] and it is easily identified by comparing the reported SEM images [12,13] with Figure 2.12 and Figure 2.15. Using the EDX (Energy-dispersive X-ray spectroscopy) attachment of the microscope, it was possible to observe that the elements present in these structures are carbon, sulphur and vanadium. The presence of these large particles could explain the fact that some of the diesel filters looked darker than the HFO filter (first filter from the top in Figure 2.10), while having less than a tenth of the particulate in weight. Compared to the clusters of soot observed in the diesel particulate, these large spherical particles contain a large amount of mass while showing a relatively small surface.
Measurements on marine boiler oil flames

Figure 2.13: SEM images of the particulate filter used during Diesel operation at 40% load and 4% exhaust oxygen. From the top: A) 1000x magnification, B) 10000x magnification and C) same image captured with the backscattered electron detector.
2.2 Materials and methods

Figure 2.14: SEM images of the particulate filter used during Diesel operation at 20% load and 2% exhaust oxygen. From the top: A) 1000x magnification, B) 10000x magnification and C) same image captured with the backscattered electron detector.
Figure 2.15: SEM images of the particulate filter used during HFO operation at 20% load and 4% exhaust oxygen. From the top: A) 1000x magnification, B) 10000x magnification and C) same image captured with the backscattered electron detector.
A Thermo Scientific™ Prisma™ E SEM has been employed to obtain further images of the samples (Figure 2.13, Figure 2.14 and Figure 2.15). While this microscope was not equipped for EDX, comparing the images obtained from back-scattered electrons (BSE) and secondary electrons (SE), gives some insight also on the materials that are being observed. This is because larger atoms are stronger scatterers of electrons, and therefore produce a higher signal for BSE. This is the case for example for the Silica present in the filter material, which remain well visible in the backscatter images (panel C for each set of images). The structures seen in Figure 2.14B seem to blend with the background in Figure 2.14C, this supports that they are mainly composed of carbon, since the background for all sample is a carbon tape. The same can be said for Figure 2.15B and Figure 2.15C, but here the effect is less clear, either because of the presence of other elements or because of the more tridimensional morphology of the HFO combustion particulate.

Overall, it is possible to conclude that the particulate for produced by the combustion of marine diesel is composed by carbonaceous material in sub-micron particles, which aggregates in clusters on the filter material when present in a large amount. For HFO combustion, the particulate is instead composed mostly of large spherical structures with diameters up to tens of microns, which contain also sulphur and vanadium. Most likely these structures are carbonaceous char material that remains after the high boiling fuel is devolatilized [14].

2.2.4 Measurements conducted

As already mentioned, the experimental investigation encompassed both boiler operation change and flame mapping. Each of these parts has been repeated for marine diesel fuel and HFO, with only minor changes due to time constrictions.

For the first part, the boiler has been run at three different loads and the combustion air changed to obtain the excess oxygen in the exhaust in the range between 1% and 6%. A complete list of the operating conditions measured is given in Table 2.5. Due to time limitations, it was not possible to have repetitions for other than those operating conditions used for the flame mapping (40% load and 4% exhaust oxygen).

In the first part of the campaign, the focus was on exhaust measurements to assess the performance of the boiler; nonetheless, the suction pyrometer has been kept at the center of the boiler from port C2 (Figure 2.2) to measure the temperature at the exit of the furnace. The camera probe was also used to record a video of the flame at each operating condition from port X2. For the exhaust measurements, the particulate rack has been used to collect a sample over a 10-minute period for each operating condition. Multiple samples were taken for diesel firing at 40% load and 4% exhaust oxygen and HFO firing at 20% load and 4% oxygen. Lastly, a sample of the exhaust gasses has been extracted in a continuous manner and sent to the gas analyzers.

The second part of the campaign concerned the mapping of the flame. As mentioned above, these data is especially useful to validate future CFD simulations. The operating condition used was 40% load and 4% oxygen concentration at the exhaust, for both marine diesel and HFO. Due to the layout of the test center in the proximity of the boiler, it was only possible to use the suction pyrometer and a long gas extraction probe only from ports C2 and C3. A compact gas extraction probe was designed and
Manufactured, so that it could be fitted into port A4. With this probe, it was possible to extract gas from the furnace up to its centerline. During the flame mapping, the long probes have been moved across the furnace (Figure 2.20) with 10 cm steps (20 cm in the port close to the exit of the furnace when the gradients were small and time was an issue) and the short gas extraction probe by 5 cm in the presence of strong gradients.

Table 2.5: Operating conditions used during the experimental measuring campaign, including time of operation and measurements performed.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Load</th>
<th>O₂</th>
<th>Day</th>
<th>Start time</th>
<th>End time</th>
<th>Particulate sampling</th>
<th>Outlet temp.</th>
<th>Flue gas comp.</th>
<th>Flame mapping</th>
<th>Optical imaging</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>20%</td>
<td>2%</td>
<td>24</td>
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<td>10:30</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>-</td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4%</td>
<td>24</td>
<td>9:09</td>
<td>9:29</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>-</td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6%</td>
<td>25</td>
<td>9:40</td>
<td>10:15</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>-</td>
<td>X</td>
</tr>
<tr>
<td>Diesel</td>
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<td>2%</td>
<td>25</td>
<td>9:05</td>
<td>9:20</td>
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<td>X</td>
<td>X</td>
<td>-</td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4%</td>
<td>24</td>
<td>11:00</td>
<td>11:20</td>
<td>X</td>
<td>X</td>
<td>-</td>
<td>-</td>
<td>X</td>
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<tr>
<td></td>
<td></td>
<td>25</td>
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<td>17:00</td>
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<td>9:50</td>
<td>9:57</td>
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<td>X</td>
<td>X</td>
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<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6%</td>
<td>25</td>
<td>8:15</td>
<td>8:50</td>
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<td>-</td>
<td>-</td>
<td>X</td>
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<td>X</td>
<td>-</td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>14:20</td>
<td>14:54</td>
<td>-</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td>X</td>
</tr>
<tr>
<td>HFO</td>
<td>20%</td>
<td>4%</td>
<td>stable</td>
<td>25</td>
<td>15:00</td>
<td>15:25</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>-</td>
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<td></td>
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<td>-</td>
<td>-</td>
<td>X</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60%</td>
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<td>X</td>
<td>X</td>
<td>X</td>
<td>-</td>
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</table>
2.3 Results

The discussion of the results of the measurement campaign is divided into two parts: results of the flame mapping with the two oil types (section 0) and results of exhaust measurements with different load and air surplus conditions (section 2.3.1). For confidentiality reasons, some values have been normalized to the values obtained for diesel firing at 40% load and 4% exhaust oxygen. These values is marked in the plots and in the tables.

2.3.1 Exhaust measurements with different lambda and load conditions

Mass balances have been carried out for the main species (carbon, nitrogen, oxygen and hydrogen) for each operating condition and using both the measurements from the Testo system and the gas analyzers. From these calculations, it was possible to obtain the amount of air injected into the boiler and the air-fuel equivalence ratio (λ).

![Graph showing temperature at furnace exit and particulate concentration against equivalence ratio.](image)

*Figure 2.16: Temperature at furnace exit (left) and normalized particulate concentration (right) against equivalence ratio for all operating conditions - based on the Testo measurements.*

In Figure 2.16 are shown the furnace outlet temperature and the particulate emission levels at different air excess levels when firing Diesel and HFO. For the same λ, when increasing the load, the furnace outlet temperature is increased as well (Figure 2.16-left). With an increased fuel input, shorter residence time and a fixed boiler heat transfer surface the exhaust temperature will increase. On the other hand, when increasing the λ and keeping the load constant, the temperature is decreased: with an increased amount of air to be heated up, but with a constant amount of fuel burned, the exhaust temperature is decreased. This effect seems negligible for the 20% load condition in the tested range of equivalence ratios.

Particulate sampling at the exhaust shows that the particulate concentration is decreased when the combustion airflow is increased (Figure 2.16 on the right). As soot is the result of incomplete combustion
of hydrocarbons and it is formed in the fuel rich zones of the flame a better soot burnout is obtained at high lambda values. The concentration found for HFO operation is 1 to 2 order of magnitude higher than that for Diesel operation at similar equivalence ratio. This can also be observed in the videos taken, as the HFO flame was much brighter than its diesel counterpart was (see Figure 2.19). Interestingly enough, the trend in soot production when increasing load is opposite for the two fuels: HFO shows a clear increase in particulate concentration at higher loads, while the highest value for diesel was found at 20% load.

In Figure 2.17 are shown CO and NOx emissions at different air excess levels when firing Diesel and HFO. CO emissions were quite low in all cases, but for the operation with 1% oxygen concentration ($\lambda=1.05$) at the exhaust. Both diesel and HFO operation consistently reported a clearly higher emission of CO for 60% load compared to 20 and 40%, and the lowest emissions for 4% excess oxygen. This could be caused by the lower residence times in the furnace chamber at high loads. NOx emissions, on the other hand, changed drastically with the fuel type used. This is probably due to the higher amount of nitrogen present in the HFO (see Table 2.3). The elemental analysis of the fuel samples supports this hypothesis since the ratio between the nitrogen content and the NOx emission is similar. In addition, as shown in the next section, the temperature profile in the boiler is almost identical for the two fuels, thus the difference observed cannot be due to changes in thermal NOx production.

Changing the excess oxygen in the range between 1% and 6% did not have a major impact on the NOx production and the only consistent trend is a feeble decrease with higher amount of oxygen, which could be ascribed to the dilution of the emission in a larger amount of gas. When the concentrations are adjusted to the same amount of excess air.

It is important to remember that for most regulations and practical purposes, the emission of a system are evaluated at a prescribed excess oxygen concentration. This is to make them comparable, and work with absolute amounts of pollutants, instead of relative concentrations. The measured gas compositions and emissions can be easily adjusted by diluting the flue gas with air (79% Nitrogen, 21% Oxygen) until
the 6% oxygen concentration is achieved. From the results presented, the only notable change is for the NOx emissions at varying lambda (Figure 2.18). It can be seen that in this case, an increase in lambda corresponds to a slight increase in NOx emissions, especially at 60% load.

Due to the transient nature of the turbulent flame, the videos taken with the camera probe are of relatively scarce usefulness, as it is quite difficult to directly compare flame shape of intensity. Therefore, they have been post-processed and various images have been created by taking statistical parameters of the intensity throughout the videos for each individual pixel. The most useful parameters proved to be minimum, average and median value. The full arrays of obtained images for all operating condition are given in the Appendix I.3. The images thus obtained can corroborate some of the results presented above, since soot is directly responsible for much of the visible radiation for this type of flame. Indeed, while soot maximum radiation intensity lies in the infrared, the human eyes spectral sensitivity makes us perceive it as a bright yellow, to dull orange, depending on the flame local temperature [15].
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This is easily seen in the increased intensity registered for the HFO flames, compared to the diesel ones (Figure 2.19). This trend is less pronounced, but still visible for varying excess oxygen, where at the same load and lower $\lambda$, a brighter flame is observed.

The complete list of results for all operating conditions is summarized in Table 2.6, including both Testo and gas analyzer measurements for completeness. The discrepancies between these are due to some technical difficulties with the $O_2$/CO/CO$_2$ analyzer, thus the Testo data has been used for further calculations regarding these quantities. For NO$_x$ on the other hand, the gas analyzer data is used, since the Testo system for NO$_x$ was not available for every operating condition, and when it was available, it was in good agreement with the NO$_x$ analyzer.

Table 2.6: Exhaust gas composition and temperature at varying operating condition of the boiler. Normalized values ($) are reported for CO, NO$_x$ and particulate, which have been obtained as the ratio with the value used for further calculation for Diesel firing at 40% load and 4% oxygen at the exhaust (shown with a *).

<table>
<thead>
<tr>
<th>Load</th>
<th>Diesel 20%</th>
<th>Diesel 40%</th>
<th>Diesel 60%</th>
<th>HFO 20%</th>
<th>HFO 40%</th>
<th>HFO 60%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2$ [%]</td>
<td>2.6</td>
<td>4.5</td>
<td>6.1</td>
<td>-</td>
<td>3.8</td>
<td>-</td>
</tr>
<tr>
<td>$O_2$ testo [%]</td>
<td>1.9</td>
<td>3.9</td>
<td>5.85</td>
<td>1.9</td>
<td>3.8</td>
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<tr>
<td>CO [ppm/ppm]</td>
<td>52</td>
<td>19.2</td>
<td>16</td>
<td>-</td>
<td>19.0</td>
<td>-</td>
</tr>
<tr>
<td>CO testo [ppm/ppm]</td>
<td>34</td>
<td>8</td>
<td>8</td>
<td>43.4</td>
<td>1.0*</td>
<td>7.0</td>
</tr>
<tr>
<td>$CO_2$ [%]</td>
<td>12.6</td>
<td>11.3</td>
<td>10</td>
<td>-</td>
<td>11.6</td>
<td>-</td>
</tr>
<tr>
<td>$CO_2$ testo [%]</td>
<td>13.9</td>
<td>12.4</td>
<td>11</td>
<td>13.8</td>
<td>12.5</td>
<td>10.9</td>
</tr>
<tr>
<td>NO$_x$ [ppm/ppm]</td>
<td>1.04</td>
<td>1.03</td>
<td>0.93</td>
<td>0.83</td>
<td>1.0*</td>
<td>0.93</td>
</tr>
<tr>
<td>NO$_x$ testo [ppm/ppm]</td>
<td>1.05</td>
<td>1.08</td>
<td>0.91</td>
<td>-</td>
<td>0.86</td>
<td>-</td>
</tr>
<tr>
<td>Particulate$_x$ [(g/m$^3$)/(g/m$^3$)]</td>
<td>2.02</td>
<td>1.33</td>
<td>0.92</td>
<td>1.31</td>
<td>1.0*</td>
<td>0.84</td>
</tr>
<tr>
<td>Tout [°C]</td>
<td>840</td>
<td>840</td>
<td>840</td>
<td>970</td>
<td>950</td>
<td>920</td>
</tr>
</tbody>
</table>

2.3.2 Flame mapping

As mentioned above mapping of a diesel and a HFO flame were done using the operation data specified in Table 2.5. Temperature and gas have been collected and analyzed by inserting probes from the back-wall of the boiler and moving them in steps across it (Figure 2.20). This process have been repeated for both diesel and HFO. In addition, the compact gas extraction probe could be inserted from the side port to obtain gas composition at burner height in a perpendicular direction. However, it was possible to complete these measurements only for HFO, while for diesel only the two positions closest to the wall were used due to a technical issue.
The measured temperature profiles obtained for both HFO and Diesel can be seen in Figure 2.21. It is apparent that the temperature profile is almost unchanged by the switch from diesel to HFO and in both cases is measured a temperature of approximately 1450°C near the burner exit. The only noticeable change is in the measurements closest to the burner, but in those measurements, the influence of the presence of the suction pyrometer has a large impact. This is because close to the burner, the velocity is highest and the probe disturbs the flow the most. Furthermore, the suction pyrometer could be kept in those positions only for a short time and, in the case of HFO, it had to be removed due to plugging by excessive deposits.

At the burner height, the temperature is relatively constant in the first half of the boiler at 1400-1500°C and then decreases to 1200-1300°C towards the back wall. At the wall, or to be more precise at the rim of the port where the probe was inserted, the temperature is drastically lower, probably due to the presence of a boundary layer on the cold wall. At the higher port, the temperature has a reverse behavior. This can be explained by considering the general flow direction as shown in Figure 2.20 and the fact that the flow heat is removed from the walls over a longer period of time for the gas that recirculates toward the bottom of the boiler. This gas is then found on the front wall section of the furnace before it reaches the outlet on the top and it has temperature between 850 and 950°C. At the back wall, a temperature in excess of 1100°C was measured. This is consistent with the mechanism presented above: these points are quite close to those measured in the same positions at burner height, the path that the gas is following is direct and therefore the residence time of the gas in this area is very short.

It should be noted that the measurement could be influenced by the presence of the probe itself (Figure 2.22). Also, due to the way the suction pyrometer works, the measured temperature should be considered as an average temperature of the volume surrounding the suction pyrometer hole, more than a point measurement. In Figure 2.23 are shown O2, CO, CO2 and NOx measurements in the diesel and HFO flames. When comparing the gas compositions measured for HFO and diesel fuel, it is possible to observe the same trends when moving across the boiler (Figure 2.23A). As one would expect, CO2 increases when
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moving away from the burner and it is constant otherwise. Oxygen has a similar but opposite trend, as it is consumed by the combustion reaction. It is also possible to notice that the minimum O₂ concentration is actually measured at 0.3-0.4 m from the burner: this is probably because part of the air is not mixed with the fuel in the main combustion zone, meaning that the spray is not able to penetrate all the way into the surrounding airflow. It should also be noted that the oxygen concentration is always lower for diesel than for HFO, even though the outlet concentration and the concentrations close to the boiler exit are the same (as seen in Figure 2.23C). This could be due to differences in mixing and consequent faster depletion of oxygen. Carbon monoxide shows a peak for both HFO and diesel at 0.2 to 0.3m from the burner and decreases while moving towards the back wall down to ppm level.

Figure 2.21: Temperature profiles across the boiler.

This is consistent with the CO₂ and O₂ measurements as CO is an intermediate product of the oxidation reactions. It is interesting to note that contrary to the exhaust value, the CO concentration for diesel fuel on the axis of the burner is higher than the one for HFO. This difference is consistently of one order of magnitude after the boiler centerline (0.6m) and disappears for the measurements from the upper port. This is most likely caused by differences in the evaporation and kinetics characteristics of the two fuels: the difference in hydrocarbons chain lengths could delay the oxidation to CO, thus decreasing its peak values.

NOₓ concentration also follows similar trends for HFO and diesel (Figure 2.23B, D and F), but with the HFO having a concentration approximately 5 times higher in all positions, both at burner height and at furnace exit. This is probably because HFO contains a higher amount of fuel bound nitrogen (Table 2.3); therefore, the same considerations about NOₓ of section 2.3.1 apply here. Also, being the temperature field almost identical for both fuels, thermal NOₓ production is unlikely to be a differentiating factor for the two fuels.

Figure 2.23F shows the gas composition measurements obtained from the side port. Here it is possible to see that the concentration of all species close to the wall resemble those at furnace exit for both HFO and diesel, further supporting the flow field shown in Figure 2.20. Moving toward the center of the boiler,
it is possible to observe a point with a maximum of oxygen concentration and a minimum of CO$_2$. This is caused by the presence of air that has not yet completely mixed into the central fuel rich region and that flows around the swirling plate (and thus the recirculation zones). In this same position, also NO$_x$ concentration is at its minimum, again due to dilution into this air stream. CO concentration presents a plateau in the center of the boiler and decreases to ppm level towards the wall. Lastly, the concentrations of all species at the point closest to the center of the boiler should resemble those obtained at 0,8 and 0,9m from the back wall with the long probe, but are instead closer to those between 0,6 and 0,7m. This could be due to the fact that the radial gradients in the flame are much higher than the longitudinal ones, or also to the disturbance in the flow introduced by the probe. A role could also be played by the fact that the long probe was oriented so that the gas did not change its direction significantly before entering it. On the other hand, when the probe was inserted from the side port, it lied orthogonal to the flow in the center of the boiler, thus interacting with the flow field in a different manner.

The measurements taken at the higher port near the furnace chamber exit show small gradients between measuring point (Figure 2.23C and D). The values obtained close to the boiler’s axis are mostly consistent with the corresponding exhaust measurement, showing that only very limited reactions take place downstream of this region. The only clear and consistent trend observed is a peak in CO concentration toward the back wall of the boiler. Even if the concentration was very low, the peak would support the general flow directions stated above and shown in Figure 2.20. Other than that, it is possible to observe that the oxygen concentration assume the same value for diesel and HFO in the measurement points closest to the outlet (near the boiler axis at 0,6m from the walls), supporting the idea that the difference observed at burner height is only a local effect. The NO$_x$ concentration decreases when moving towards the back wall, suggesting that the recirculation seen by this part of the flow could have a small NO$_x$ reduction potential, possibly due to the flow passing close to the primary combustion zone, but this could also just be an effect of further dilution with fresh combustion air.
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Figure 2.23: Gas composition across the furnace chamber from the three ports available for gas sampling. Furnace exit values for CO and NOx have been normalized to their respective measurements shown with a * in Table 2.6.
2.4 Conclusions.

The experimental campaign was successfully concluded in October, 2018. Two main activities were conducted both for diesel firing and HFO firing. The first was the investigation of changes of operating conditions of the boiler with regards to load, fuel type (HFO and diesel) and fuel to air ratio (only for diesel firing), and it included exhaust measurement of gas composition, particulate emissions, temperature and optical imaging of the flames. The second was the mapping of a diesel and a HFO flame at fixed operating conditions. This was achieved by taking temperature and gas composition measurements across the boiler at two different heights.

More specifically, it was seen that using HFO compared to diesel had an almost negligible impact on heat transfer and temperatures in the boiler, but increased the emission of particulate almost tenfold, and of NOx and CO from 3 to 5 times. Also, the morphology of the particulate emission changed drastically between the two fuels, with sub-micron particles produced by diesel combustion and particles in the range between 10-100 µm for HFO firing.

Regarding the variation of operating conditions, it was possible to conclude that working at higher loads had a negative effect on all specific emissions, with the sole exception of diesel particulate emissions, which were consistently lower for higher loads. The increase in CO emission with load was clear when increasing the load from 40% to 60% for both fuels. The relative changes for NOx and particulate did not show such clear trends. For CO emissions, a lambda value above 1.2 did not lead to a further decrease in CO emission. While particulate emissions consistently decreased with increased λ, NOx emission showed a relatively flat behaviour. When the concentrations were adjusted to the same amount of excess air, the NOx showed a slight increase with increased λ (see Figure 2.18), while all other conclusions retained their validity.

In conclusion, from the point of view of emissions and within the range explored, the boiler with the current setup was best suited to work at λ=1.2 or higher and at a low load, but the type of fuel used had a much larger impact.

The data gathered was consistent and seemed to be appropriate for CFD validation given the considerable amounts of position measured for both HFO and Diesel firing. Moreover, the availability of exhaust measurements for both modes of operation could be used as a comparison to check if the overall performance of the boiler is accurately predicted.

2.5 References


Chapter 3

Spillback nozzle spray characterization

3.1 Introduction

This chapter presents the work done on spray characterization within the project and it has been submitted with minor modifications as a scientific paper to the journal “Experimental Thermal and Fluid Science”.

As in most applications using liquid fuels, the burner mounted in auxiliary marine boilers uses an atomizer to convert the liquid stream into fine droplets and mix it with an oxidizer. This is a necessary step in order to burn any liquid fuel at an effective rate, since it drastically increases the liquid surface. Spray nozzles are used to atomize the fuel and the resulting spray properties are determining factors for flame stability and fuel conversion efficiency [1]. The atomization process relation with combustion is complex and has been the subject of numerous studies [2]. The size and velocity of each droplet influence the evaporation rate and thus the position and rate of release of the fuel to the gas phase. In turns, the concentration and mixing of fuel and oxygen in the gas phase will govern the combustion process that provides the heat for the evaporation of the fuel droplets. Understanding the atomization process and spray properties is therefore a key issue in any effort to improve auxiliary marine boilers and reduce their environmental impact. The work presented in this chapter is a study aimed at obtaining further insight into spray characteristics in this type of system.

The interactions between atomization and combustion process can be described by Computational Fluid Dynamics models. However, when applying this method to a full-scale system, the spatial discretization needed to observe the first stages of the atomization process is much smaller than the other characteristics lengths. With the recent increase in computational power and developments of DNS, it is possible to conduct such analysis, but it is still computationally very demanding [1,3–6]. As a simplification, it is possible to inject already atomized droplets in the computational domain, thus avoiding modelling directly the atomization process. To do so detailed knowledge of droplet sizes and velocities is needed as an input to the CFD simulation. Several experimental correlations to calculate these data exist for pressure swirl atomizers [7], but they are usually limited to single parameters such as the Sauter Mean Diameter (SMD), instead of describing the whole size distribution. Moreover, their accuracy is limited by the geometry and operating conditions used in the underlying experiments, and employing different correlations leads to a wide range of results. While the general effects of parameters such as surface
tension, viscosity and differential pressure on the spray are generally agreed on, their relative importance varies from source to source. As discussed in the result section, when using the correlations proposed by Lefebvre et al.[8] and Radcliffe et al. [9] on one of the spray characterized in this chapter (80 l/h of water, with a ΔP=20 bar), the results vary between 57 and 113 µm for the Sauter Mean Diameter.

Another possibility to obtain these particle size and velocity data is to characterize the spray with experimental methods, thus obtaining information pertaining to the specific nozzle geometry and operating conditions used, here for auxiliary marine boilers. This approach also has the benefit of providing a mean of assessing the predictive capabilities of the experimental correlations for the specific nozzle.

As mentioned in section 1.4, the measuring techniques currently available to measure droplet sizes and velocity are several, especially when working in the in the far-field region of a spray [10,11]. Few of these techniques also allow measuring both droplet size and velocity simultaneously, thus providing comprehensive information about droplet characteristics. Possible candidates for such measurements include: Phase Doppler Interferometry (PDI) [12,13], high-resolution imaging [14–18], Interferometric particle imaging [19,20], holography [21,22] and glare point imaging [20]. Among these, high-resolution imaging is relatively simple to implement and, with the recent development in camera sensors and LEDs, the capabilities of this technology have increased drastically [10], making it an ideal candidate for further refinement.

The aim of the work presented in this chapter is to characterize the spray structure produced by a back-spill atomizer in terms of droplet size, velocity and trajectory and to develop and evaluate a novel experimental method. The spray nozzle is investigated at various supply pressures, liquid viscosities and flow rates in order to reflect possible changes in operating conditions in a full-scale marine auxiliary boiler.

The measurements are made with a novel back-light imaging technique adapted from previous work on solid particle sizing [23]. A technique very similar to the one used has also been proposed for PIV studies under the name of Particle Shadow Velocimetry [24] and provides a solution that lends equally accurate results, with lower equipment costs and that requires significantly less power.

The optical setup used for this work differs in two ways from conventional shadowgraphy methods for droplet size and velocity measurements. The first is the use of a fast-pulsed LED as a light source, thus providing short and precise light pulses without using expensive lasers [25–29]. The second is the replacement of high speed cameras [27,30] with a standard CCV camera, decreasing substantially the costs with the only drawback of a longer sampling time.

The premise for this work is that the spray data obtained for different operating conditions represents different populations of droplets. As a preliminary step for the spray characterization work a statistical analysis has been conducted on the earlier spray data and it is reported in Appendix II.5.

3.2 Material and methods

In order to investigate the atomization process, an experimental setup was built at DTU. The setup is composed of two systems: one is the hydraulic and safety devices to reproduce at room temperature the
spray generated in the full-scale boiler (Figure 3.2), the second is a shadowgraphy system to capture the spray and measure the droplet properties (Figure 3.3).

3.2.1 The setup

The nozzle used in this study is a commercial spillback hydraulic nozzle (Figure 3.1), rated for a supply pressure of 20 bar and a maximum flow rate of 125 l/h. The nozzle has a straight orifice with a diameter of 1mm. This is the same nozzle mounted in the test boiler of chapter 2, where it is used to atomize different types of fuels including marine diesel and Heavy Fuel Oil (HFO). By regulating the fuel flow rate through the nozzle, it is possible to satisfy a variable steam demand, but for most of the lifetime of the equipment, the atomized flow rate lies in the range between 50 to 112 l/h. Therefore, the spray characterization setup was designed to supply up to 300 l/h, since it uses a single pump that also provides the liquid that is spilled for regulation and through the spillback nozzle. To explore the full range of operation of the nozzle and obtain meaningful data for the actual application, during the experiments the flow rate was kept at 50, 80 and 112 l/h. Another parameter that can be easily changed when operating the boiler is the supply pressure to the nozzle. The nozzle manufacturer gives a design value of 20 bar, but the system can support a relatively broad range of supply pressures without requiring any change. Since this parameter is of fundamental importance for atomization quality in a pressure swirl atomizer [7], the setup has been built with components able to withstand a wide range of pressures and the nozzle has been tested at supply pressures of 15, 20 and 25 bar. Also, while the manufacturer supplies the characteristic curves relating supply, spill and atomized flows to the spill pressure for 20 bar of supply pressure, experiments have been carried out to check these curves, including the effect of fouling on the filter in the supply line (Appendix II.1).

The setup is operated with the two backpressure valves, which are used to keep the respective upstream pressure constant, thus regulating supply and spill pressure for the nozzle. A volumetric pump with multiple pistons is used to deliver flow rate in excess of the required amount and part of it is spilled through the first backpressure valve. A membrane tank is used to further reduce any pulsation in the flow. Pressure gauges has been placed as close as possible in the system to the nozzle to monitor supply and spill pressure. The atomized liquid and all the liquid spills are collected into a cylindrical tank and recirculated into the system. The issue of droplets entrained in the surrounding air and recirculating to the sampling volume was taken into account and assessed through the various iteration of the setup design (Appendix II.2). In the final design, to avoid droplet recirculation in the near nozzle region, a raised lid with a hole with the diameter of the boiler burner tube is used and air is sucked by a shielded
Spillback nozzle spray characterization

ventilation connection at the bottom of the tank. The influence of these precautions on the results should be negligible, considering that the spray measurements are taken few centimetres below the nozzle orifice and that the distance to the ventilation and air escape route is approximately one meter. Moreover, it can be argued that this configuration is more similar to that of the full-scale boiler than a closed tank or a completely open environment.

Figure 3.2: Hydraulic system of the spray characterization setup.

To study the effect of changes in liquid viscosity on the spray characteristics the experiments were repeated with water and water-glycerol solutions [31,32]. This was done to reproduce the viscosities of some of the fuels used in the boiler [33], or achievable with a fuel preheating system [34]. The solutions were designed using the viscosity data found in literature [35]. Due to the higher than normal ambient temperature during the days when the measurements were taken, a slot for a hand held thermocouple has been fitted just after the backpressure valve on the spill line. This made it possible to monitor the liquid temperature throughout the experiments and calculate the actual properties of the liquid during the atomization process. A sample of the solutions has also been collected during the experiments and later analyzed with a Discovery HR2 hybrid rheometer using a Peltier plate to keep liquid at 25 °C during the measurement. Values from literature correlations for the viscosity were calculated and lie within the error range of the measurements.

The shadowgraphy setup main components are a CCD camera and an LED pulser, synchronized by a delay generator. This type of system has been described elsewhere [24] and the configuration used in this work has been thoroughly tested in a previous publication [23]. The main characteristic of this setup is that it relies on a fast-pulsed LED instead of a camera shutter to freeze the frames, thus making it possible to obtain consecutive or superimposed images with a delay as low as 1 µs to one another, while avoiding the use of expensive laser illumination systems. Moreover, since the LED can produce light pulses as short as few nanoseconds, the resulting images are “frozen”, thus showing the shape moving
3.2 Material and methods

particles with good accuracy and negligible distortion. For example, a particle moving at 50m/s would move just 1.2 µm during a pulse of 24 ns. While similar methodologies are employed in recent studies [36], the solution proposed in this work has been especially developed to replace costly high-speed cameras with a regular CCD camera by synchronizing the shutter and LED signals. The trade-off of this solution is that only pairs of images can be obtained, instead of multiple consecutive frames. While this prevents the tracking of single droplets through more than two consecutive images, it also greatly reduce the costs and droplet size, shape, speed and velocity can still be measured with the same accuracy.

Figure 3.3: Optical setup.

The CCD sensor used is composed of 1296×966 pixels for a total size of 4.86×3.62 mm, while a telecentric lens provides a magnification of 1.5×. The depth of field of this configuration is 0.86 mm, thus resulting in an observed volume of 6.72 mm³ and a pixel size of 2.5×2.5µm.

To observe different regions of the spray, the system is mounted on a railing system so that the axial and radial distances of the observed volume from the nozzle orifice can be adjusted independently. For this study, all measurements have been taken from 32 to 35 mm downstream of the nozzle orifice and the radial position has been changed in 2.5 mm steps, thus covering the whole spray cross-section. The number of droplets captured in each frame varies with the position and the spray that is being observed: on the outer fringe of the spray, most images are empty, while in the central region more than 50 droplets per image are measured. For each experiment, around 400 image pairs have been recorded at each position. In the periphery of the spray, the measurements have been stopped when less than 100 droplets were recorded in the corresponding image set. It should of course be noted that this is an arbitrary limit and that statistical significance of the findings is lower in the more dilute regions of the spray.

3.2.1.1 Droplet evaporation preliminary assessment

In the auxiliary boiler, the liquid fuel is sometimes preheated to lower its viscosity, but it is always injected several hundred Kelvins below its evaporation temperature. This implies that some after injection the droplets will need some time to heat up before evaporating. In this zone, the spray characteristics would reflect those obtained on a cold setup. The difference between the spray in the cold setup and in the boiler would be that during the heating process the liquid temperature increases and with it some of the fluid properties that influence the atomization process might change. This issue is taken into account in
chapter 4 by repeating the CFD simulations of the boiler with droplet size distributions of fluids with different viscosities in the range between injection and evaporation of the fuel.

The distance from the nozzle orifice for the measurements has been chosen after a preliminary assessment of the droplet evaporation using CFD simulation. The simulation done with ANSYS CFX commercial software employs the same models and settings presented in chapter 4, and uses a Rosin-Rammler droplet size distribution with size parameter of 25 µm and shape parameter 1.4. From the results shown in Figure 3.4, it is possible to observe that in the first 50 mm downstream of the nozzle the number of droplets and the average size is almost unchanged. Given the uncertainty on the droplet size, a conservative estimate was used and the spray measurements were taken between 32 and 35 mm from the nozzle.

![Figure 3.4: Droplet evaporation according to preliminary CFD simulations of the full-scale boiler.](Image)

3.2.2 Data treatment

To measure the droplet size and velocity accurately, a threshold based droplet recognition method was used together with filtering based on multiple criteria and a simple model to convert the planar measurements to represent the entire cross-section of the spray.

Since fixed parameters are used during these steps, the results are accurate only if the greyscale values of background and droplets are consistent within an image set. Indeed, with shadowgraphy images the background intensity varies due to the light scattering from the out of focus liquid. Thus, images taken in or through a thicker or denser region of the spray will present a lower intensity. Post processing the image sets can help in avoiding this issue. Several image post-processing algorithms have been tested with ImageJ [37], but the one that lent the most consistent results for all image sets was a simple two-step procedure. For each set of images corresponding to a measurement position and operating condition, the average intensity is calculated for each pixel and afterwards, each pixel of each image is divided by the corresponding average value.

From the images obtained, each contiguous dark region is measured if its greyscale value is below a fixed threshold and its boundary gradient above another. The thresholds have been determined based on the
3.2 Material and methods

greyscale values observed in the images after post-processing, and depend on illumination quality during the experiments. The delay between the frames is set small enough that the distance each droplet moves between frames is small compared to the distance between droplets, thus each droplet in the first frame is paired with the closest one to its position in the second frame. Since we are interested in single droplets and not gas flow velocity as in classical PIV, the velocity vector of each individual droplet is estimated by measuring the distance of the centre in two consecutive snapshots and dividing it by the delay set between the two frames. Regardless of how sparse the droplets are, it is always possible that some are very close to each other, or that a droplet leaves the sampling volume, and thus different droplets are paired together. To avoid this, it is checked that there is no significant change in droplet shape, sharpness or droplet size between the paired droplets and that the resulting droplet velocity is within reasonable limits. Also, any potential droplet that cannot be matched in the second frame or that has a diameter of less than three pixels is filtered out, since it is not possible to determine its velocity or shape respectively. This produces a floor value of 7.5 µm for the measured droplet diameters (visible in Figure 3.8b).

![Figure 3.5: Cumulative Distribution Function of the spray with and without correction for distance from the spray axis of each droplet. Experiment at 80 l/h of water at 25 bar.](image)

To characterize each of the sprays, the railing system were adjusted to move the sampling volume across the spray on a diameter of the circular cross-section of the spray cone. Assuming that the spray is axisymmetric, each sampling volume is representative of all the volume laying at the same distance from the spray axis. To take into account that these volumes are increasingly large the farther away from the spray axis, the contribution of each droplet in all calculations is proportional to its distance from the spray axis. The change that this correction causes is shown in Figure 3.5, where the cumulative distribution function of droplet size shifts because of the larger fraction of small droplets toward the center of the spray and of bigger ones on the outer region.
3.2.3 Error evaluation and discussion

The precision of the droplet diameter estimation is determined by several factors. The first is the error on the pixel size, which is calculated with an optical target, and it is subject to an error below 1%. Secondly, there was no adjustment for the depth of field calibration, and while using telecentric optics avoids any distortion of out of focus particles, the effective depth of field for different sized particles could lead to an overestimate of larger droplets. Lastly, there is an error due to the fact that pixels are not infinitesimally small, this leads to an uncertainty on the position of the boundary of each droplet. This error is reduced by processing the images in greyscale, thus also pixels partly obscured are taken into consideration. While it is difficult to give a precise error estimate for each of the contribution, the overall accuracy of the system has been tested in previous work [23] with calibration microspheres. These particles belonged to three different diameter intervals corresponding approximately to 5, 10 and 40 pixels. The measured mean diameter for each of the three groups were within the certified particles size range, which spanned respectively 6.2%, 2.8% and 1.7% of the mean diameter. Therefore, the overall relative measurement error is smaller than these percentages, with the highest uncertainty on the smaller droplets and the lowest on the larger ones.

Another concern when assessing the accuracy of particle or droplet characterization is if the sample size bears statistical significance. This kind of analysis is scarce in the spray characterization literature. A common practice to avoid this issue, is to take a very large sample, speculating that it is sufficient [26,29,38,39]. While in some works it is possible to find estimates of population size needed for spray characterization, the basis of such claims are generally not given [40,41]. A simple way to gain some insight on this issue is to calculate a relevant parameter for increasingly larger subsets of the droplet population and observe how it converges toward a constant value. While this is a useful indicator, it is very much dependant on the order in which the droplets are considered and on the specific parameter used. To surpass these shortcomings, the procedure was implemented in MatLab code (version R2016a) and repeated for different permutations of the droplet population and for both SMD and average droplet speed (Figure 3.6a). For each permutation, the number of droplets needed to obtain a relative error on the each parameter smaller than a fixed threshold was found. The number of permutation was increased until a smooth curve was obtained when sorting and plotting the results (10^4 permutations for a population of 10^5 droplets).
3.2 Material and methods

The average sample size needed to meet the error threshold was calculated (Figure 3.6b) and the process was repeated for thresholds from 1 to 10%. The results of this analysis show that the number of droplets needed to have a reasonably accurate estimate (2 to 4% relative error) of the SMD is between $10^4$ and $4 \times 10^4$, while to obtain similar uncertainties on the mean droplet velocity less than a tenth of these amounts are sufficient.

The results obtained in the sample size analysis are consistent with the main assumption needed to carry it out, which is that the sample size on which it is based is large enough to be significant. To further check on this assumption, a sensitivity analysis to assess the influence of the number of droplet measured has been conducted. This analysis showed that the average sample size needed to achieve a certain error is not influenced by the original sample size in the observed range (Figure 3.7). A more complex behaviour is observed for the SMD, but it is possible to observe that for errors above 2%, the estimate converge for a population around $8 \times 10^4$. This again confirms that the sample used is large enough to draw conclusions above this error threshold.

Figure 3.6: a) Error for the SMD and average velocity for increasingly larger sub-samples of droplets. b) Comparison of average sample size needed to meet different error thresholds for SMD and average velocity. Experiment at 80 l/h of water at 25 bar.
3.3 Results

The results obtained within this spray characterization study can be divided in two types: detailed information about the droplet size and velocity across the spray, and effects of changes in operating condition on the overall spray characteristics.

3.3.1 Single droplet measurements across the spray and trends for size fractions

While absolute values and gradients may vary, the same trends have been observed for all measurements for local size, velocity and direction of the droplets across the spray. Therefore, while local measurements have been taken for all experiments, for the sake of simplicity, the plots reported in Figure 3.8 are for operation with water at 25 bar of supply pressure and a flow rate of 80 l/h, and the average values refer to the image set taken in each position. The same plots are given in Appendix II.3 for the other tested cases. The plots report both single droplet values, and average values for each sampling position. The average values are given both for the entire population, and droplets above 40 and 80 µm (90th and 98th quantiles respectively for the measurements shown in Figure 3.8) to visualize different trends dependent on particle size. In Figure 3.8b, it is possible to see that the average droplet size increases farther away from the spray axis, as also reported in other studies [40]. While this was expected, it is interesting to observe that the average size remains constant across the spray when only the larger droplets are considered.

Figure 3.8c shows that the droplet velocities are on average lower close to the spray axis. In this region, the velocities of the droplets are relatively uniform, with very few droplets moving slower than half of the average value. On the other hand, away from the axis, both the average velocity and the spread increases. By observing the average values found for different droplet size fractions it is also clear that away from the spray axis, larger droplets move faster than smaller ones. While the average velocity increases moving outward, there is also a significant number of droplets with velocities smaller than those found in the hollow core.
3.3 Results

Figure 3.8: Angle (a), size (b) and velocity (c) across the spray, including averages for different size fractions. The red line represents the geometrical angle formed with spray origin and axis. Experiment at 80 l/h of water at 25 bar.

In addition to the magnitude of a droplet velocity, to characterize its motion, it is necessary to consider the direction of said motion. When assuming that the tangential component is negligible, it is possible to represent the direction of each droplet in the spray with the angle it forms with the spray axis. The validity of this assumption is supported by the rarity of droplets that move out of focus, compared to that of droplets moving out of the pictures in the image sets. Nonetheless, it is important to remember that in this study as well as in any form of planar measurements, tangential velocities are not measured. In Figure 3.8a, the geometrical angle has been calculated as the angle between the spray axis and the line connecting the nozzle orifice to the sampling position. This quantity is a useful reference since it would be the angle of each droplet if it moved in a straight line from the nozzle orifice to the current position. When comparing these angles to the measured ones, it is evident that they match only at the fringes of the spray and in the center. Looking at the measured angles across the spray, shows that the absolute average value is consistently smaller than the geometric angle, and it presents a complex behavior.
Spillback nozzle spray characterization

around the spray axis. When only larger droplets are taken into account, the average angle match the geometric values closely, thus showing that they follow an almost straight trajectory from the nozzle orifice to the control volume. This suggests that the deviation from the geometrical trajectory is due to the local gas flow field, since inertial and shear forces respectively affect droplets based on their volume and surfaces.

The flow field generated by the entrainment of air into the spray would be consistent with both the observation done for droplet size stratification and deviation from the geometrical trajectory. The air moving toward the hollow core of the spray deviate the droplet trajectories according to their size, thus reducing the angle they form with the spray axis, and increasing the amount of smaller droplets present toward the centre of the spray. This also means that such effects will vary when using the spray nozzle in quiescent or co-flowing air and to study them further gas flow measurements should be conducted.

3.3.2 Effects of varying operating conditions on overall spray characteristics

Three main operating conditions of auxiliary marine boilers have a direct influence on the atomization process. The flow rate of the liquid is changed when adjusting to the load of the boiler, the supply pressure to the nozzle can be adjusted with the dedicated pump and the viscosity of the liquid can be reduced with a preheating of the fuel. The experiments with the spray setup included repetitions for different values of each of these parameters to evaluate their impact on the overall spray characteristics. To summarize these results, the SMD, average droplet velocity and spray cone angle have been used.

By adjusting both the backpressure valves (Figure 3.2) in the spill and supply lines of the nozzle, it was possible to change the supply pressure maintaining the atomized flow constant. Another series of experiments instead was done by maintaining the supply pressure constant and adjusting the spill pressure to obtain three different liquid flow rates through the orifice. In this way, it was possible to observe the contribution of varying supply pressure and flow rate separately. Lastly, the viscosity of the atomized liquid was adjusted by using solutions with different concentrations of water and glycerol and adjusting the setup to obtain the same flow rate and pressures. Overall, the experiments have been carried out using pure water and water-glycerol solutions with viscosities of 1, 3 and 7 cP. The supply pressures have been adjusted to of 15, 20 and 25 bar and the flow rate from 50 to 80 and 112 l/h (Table 3.1).

The effect of changing flow rate (V), supply pressure (Δp) and viscosity (ν) on average droplet velocity (u_{avg}) and spray cone angle (β) have been investigated. The average droplet velocity shows that an increase in either of the first two parameters results in an increased droplet speed (Table 3.1). While this result was expected, it was also interesting to observe that for the same relative change, an increase in flow rate produces an effect three times bigger than a change in supply pressure. Viscosity on the other hand does not seem to affect droplet speed significantly. The spray cone angle was measured as the angle of the measurement in each set with the highest liquid fraction and it is therefore on a discrete scale. From Table 3.1, it is possible to see how the spray cone angle decreases at higher viscosities and flow rates through the nozzle, while the change in supply pressure has a negligible effect on it (as reported also by [7,28,40]).
3.3 Results

Table 3.1: SMD, average droplet velocity and cone angle for the experimental campaign.

<table>
<thead>
<tr>
<th>Δp [bar]</th>
<th>V [l/h]</th>
<th>ν [cP]</th>
<th>SMD [µm]</th>
<th>uavg [m/s]</th>
<th>β[°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>80</td>
<td>1</td>
<td>57.4</td>
<td>32.1</td>
<td>77</td>
</tr>
<tr>
<td>15</td>
<td>80</td>
<td>1</td>
<td>66.4</td>
<td>30.0</td>
<td>72</td>
</tr>
<tr>
<td>25</td>
<td>80</td>
<td>1</td>
<td>52.5</td>
<td>33.9</td>
<td>77</td>
</tr>
<tr>
<td>20</td>
<td>50</td>
<td>1</td>
<td>53.3</td>
<td>31.0</td>
<td>91</td>
</tr>
<tr>
<td>20</td>
<td>112</td>
<td>1</td>
<td>54.1</td>
<td>37.9</td>
<td>66</td>
</tr>
<tr>
<td>20</td>
<td>112</td>
<td>3</td>
<td>69.6</td>
<td>39.3</td>
<td>60</td>
</tr>
<tr>
<td>20</td>
<td>112</td>
<td>7</td>
<td>77.8</td>
<td>37.6</td>
<td>55</td>
</tr>
</tbody>
</table>

Spill-return atomizers are designed to deliver a constant atomization quality with a high turndown ratio. From the results show in Table 3.1, it is observed that large changes in the flow rate yield almost negligible changes in the SMD (D₃₂).

On the other hand, changes in supply pressure have a clear effect on the droplet size: as in other simplex atomizers [7], higher supply pressure does indeed produce finer droplets. To quantify this effect, the data obtained was compared with experimental correlations found in literature for pressure swirl nozzles, by calculating the proportionality exponent γ as:

\[ D_{32} \propto \Delta p^{\gamma_p} \]  \hspace{1cm} \text{Eq.1}

\[ \gamma_p = \log_{\Delta p_a/\Delta p_b}(D_{32_a}/D_{32_b}) \]  \hspace{1cm} \text{Eq.2}

The experiments have been carried out purposely with fixed nozzle geometry, flow rate through the orifice and liquid properties. In these circumstances, several classical experimental correlations for SMD in pressure swirl nozzles can be simplified and written in the same form as equation 1. Moreover, to use the same nomenclature found in literature, pressure difference can be used instead of the supply pressure, since they are equivalent when at constant environment pressure. A value for γ of -0.46 ±0.05 was obtained from the data, matching quite well the values reported in the cited literature, which report values in the range from -0.4 to -0.55 [8,9,42,43].

The same procedure can be applied to the SMD found by changing viscosity of the liquid using water-glycerol solutions. This is done by replacing the pressure difference in equations 1 and 2 with the dynamic viscosity of the liquid. The values obtained for γ in this case is 0.18±0.05, while values between 0.16 and 0.25 are found in literature [8,9,42,43]. While other studies could not find a clear correlation when studying the effects of viscosity [44], the large relative error on this estimate prevents us from confirming or rejecting the literature values. However, a possible explanation for this is that a tendency to entrain air bubbles in the flow was noticed during the experiments and it is suggested that a system without recirculation of the collected liquid should be used in the future.
The cited experimental correlations have also been applied to predict the SMD in each experiment and compared with the measured value. From the results of this comparison (Figure 3.9), it is quite clear that the correlation proposed by Lefebvre et al. [8] leads to the most accurate prediction. While the error found when changing flow rate or viscosity was up to 25%, the other three correlations tested instead overpredicted the SMD by a large margin. Moreover, for the range of tested differential pressures, the prediction match the measurements quite well, with an error below 3%.

### 3.4 Conclusions

The spray generated with an oil burner spill return nozzle has been studied using a LED pulsed shadowgraphy technique. A comprehensive methodology for spray characterization has been developed and presented.

The novel back-light pulsed single LED setup was able to capture pairs of frames with a delay as low as 1 µs and, pixel size of 2.5 µm with an error <1% on the measured spray parameters, proving to be a reliable and economic alternative to systems using lasers and high-speed cameras. Using the presented image post-processing algorithm and a threshold based droplet recognition method it was possible to obtain measurements with an error on the mean particle size ranging from 6.2% to 1.7% depending on the particle size. Overall, the presented configuration of the LED pulsed shadowgraphy technique was demonstrated to have the capability to measure droplet sizes down to 7.5 µm and velocities up to 50m/s.

Through the statistical analysis of the data thus acquired, it was possible to evaluate the relationship between the population size of the droplet sample and the error on the SMD and the average velocity, showing that a relative error of 2% could have been achieved with $3 \times 10^4$ droplets for the former and $10^3$ for the latter. This results both support the validity of the present study, but can also be used as a starting point to assess the sample size needed for future experimental work with similar atomizers.

Seven different operating conditions were investigated by varying the supply pressure to the nozzle (15-20-25 bar), the flow rate (50-80-112 l/h) and the liquid viscosity (1-3-7cP). It was found that a common
trend from all experiments was the radial stratification of droplets according to size and velocity, as also shown in other studies [40][45]. The larger droplets of the spray move in a straight line originating from the nozzle orifice and form a hollow cone; on the other hand, the smaller droplets are present also in the core of the cone and deviate significantly from the straight trajectory.

The relation between SMD and changes in supply pressure and viscosity was described with a proportionality exponent $\gamma$ (Eq.1) and compared to three empirical correlations found in literature [8,9,42]. The $\gamma$ obtained for supply pressure was $-0.46 \pm 0.05$, confirming the literature values. The $\gamma$ obtained for viscosity was $0.18 \pm 0.05$, and while it matches the values between 0.16 and 0.25 reported in literature, the large standard deviation suggests that other effects might be in play. The experimental correlation that best approximated our results was the one proposed by Lefebvre et al.[8] and while it could not predict the SMD for changes in flow rate or viscosity, the error for the range of tested differential pressures was less than 3%. The other correlations tested over predicted the SMD by a large margin.

Lastly, it was confirmed that changes in atomized flow have little impact on the SMD in back-spill nozzles and that the spray cone angle is increases with decreasing viscosity [25] and flow rate [7].

3.5 Bibliography


Spillback nozzle spray characterization
4

CFD study of the auxiliary marine boiler

4.1 Introduction

The following chapter will present the CFD simulations of the full-scale auxiliary marine boiler. The CFD campaign includes simulations for each of the operating conditions measured during the experimental campaign for marine diesel fuel and HFO firing.

To validate the CFD simulations, the results obtained for the reference state of 40% load and 4% exhaust oxygen (40L4O) are compared with the local flame measurements presented in chapter 2.3. The discrepancies between the experimental measurements and the values predicted by the CFD are investigated and explained.

The predictive ability of the CFD simulations is then tested by comparing for each operating condition the exhaust gas composition, temperature and soot concentration with the data obtained experimentally. The limits of the operating range of the boiler in terms of load and excess air are explored with further simulations.

Lastly, a detailed discussion of the flame anchoring in the recirculation zone is presented and compared to the experimental observation for different boiler loads. This is of practical use to understand the effect of the burner geometry and nozzle characteristics on the resulting flame.

As in any modeling endeavor, when comparing CFD results to experimental data, it is important to establish the level of accuracy achieved. This can be a precise target, but also the fact of achieving a qualitative agreement with the experimental data. Due to the spatial and temporal discretization needed, reaching a certain level of accuracy for a full-scale reacting system may not be practical, especially if the simulations should be accessible with limited computational resources. On the other hand, it is in such systems that the ability of predicting the effect of changing geometry or operating condition, without incurring in costly modification of the actual system, is most valuable.

The three-dimensional geometry of the boiler has been created using Solid Works 2016 and imported in ANSYS Design Modeler for minor adjustments. To create the computational grid, ANSYS Mesher was used and the CFD simulations have been carried out with the commercial software ANSYS CFX 17.1.
4.2 Materials and methods

In this section, the main models and parameters used in the CFD campaign are presented. The main issues that are tackled are the modeling of turbulence, multiphase interaction, radiation, chemical reactions, boundary conditions, and space and time discretization. A quick summary of the main inputs and models included in the CFD simulations is given in Table 4-1. The goal is to provide enough details for understanding and reproduction of the CFD model. Details that are not presented here can be found in the software manuals of ANSYS CFX 17.1 [1–3]. However, being ANSYS CFX a commercial code, further details on the implementation of the various models than those given in the manuals are not available.

Table 4.1: Summary of the salient models and parameters used for the CFD simulations.

<table>
<thead>
<tr>
<th>Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulence modelling</td>
<td>RANS with k-ω SST [4]</td>
</tr>
<tr>
<td>Droplet phase</td>
<td>Two-way coupled evaporating lagrangian particles [5]</td>
</tr>
<tr>
<td>Drag model</td>
<td>Schiller Naumann [6]</td>
</tr>
<tr>
<td>Particle heat transfer</td>
<td>Ranz-Marshall [5]</td>
</tr>
<tr>
<td>Latent heat</td>
<td>216 kJ/kg [8,9]</td>
</tr>
<tr>
<td>Radiation heat transfer</td>
<td>DTM with WSGG spectral model [7]</td>
</tr>
<tr>
<td>Reaction mechanism</td>
<td>Two-step global reaction [8]</td>
</tr>
<tr>
<td>Reaction rate model</td>
<td>Combined EDM/Finite Rate Chemistry Model</td>
</tr>
<tr>
<td>Reactant limiter</td>
<td>A=4 [9]</td>
</tr>
<tr>
<td>Reaction rates</td>
<td>Table 4.2</td>
</tr>
<tr>
<td>Soot formation</td>
<td>Magnussen and Hjertager model [9]</td>
</tr>
<tr>
<td>Soot diameter</td>
<td>1.785*10^-8 m [9]</td>
</tr>
<tr>
<td>Fuel carbon mass fraction</td>
<td>86%</td>
</tr>
<tr>
<td>Boiler walls temperature</td>
<td>170°C</td>
</tr>
<tr>
<td>Outlet pressure</td>
<td>2607 Pa</td>
</tr>
<tr>
<td>Reference pressure</td>
<td>101325 Pa</td>
</tr>
<tr>
<td>Inlet air temperature</td>
<td>25°C</td>
</tr>
<tr>
<td>Inlet air relative/absolute humidity</td>
<td>25%/0.48%</td>
</tr>
<tr>
<td>Mass flow of fuel and air</td>
<td>Table 4.4</td>
</tr>
<tr>
<td>Fuel injection conditions</td>
<td>Table 4.4</td>
</tr>
<tr>
<td>Number of tracked computational particles</td>
<td>10^9 1/s</td>
</tr>
<tr>
<td>Computational grid first layer thickness</td>
<td>0.1 mm</td>
</tr>
<tr>
<td>Inflation zone thickness (burner/boiler wall)</td>
<td>5/20 mm</td>
</tr>
<tr>
<td>Number of computational elements</td>
<td>7094796</td>
</tr>
<tr>
<td>Number of computational nodes</td>
<td>1811981</td>
</tr>
<tr>
<td>Time step</td>
<td>0.1 ms</td>
</tr>
</tbody>
</table>
4.2.1 Models

For turbulence modeling, Direct Numerical Simulation (DNS) of industrial size furnaces is still not attainable, while Large Eddy Simulation (LES) and Reynolds Averaged Navier Stokes (RANS) modeling have both been successfully used for this application [10]. As seen in section 1.6, both approaches present different advantages, but the lower computational cost drove the choice towards RANS simulations. While the larger computational capability needed for LES might not be an issue in other framework, for this project reducing the computational time and resources needed was one of the main concerns.

Of the various models available for RANS, for the increased stability and lower computational costs over Reynolds Stress Model and the better general performance compared to other k-ω and k-ε models [11,12], the Shear Stress Transport (SST) model based on the k-ω formulation has been adopted [4].

The oil droplets are represented in the computational domain as a lagrangian particle transport fluid. To model heat and momentum transfer between the gas phase and the droplets, there are two possibilities: one- or two-way coupling. When using one-way coupling only the effect of the continuous phase on the droplets is considered, while the continuous phase is unchanged by the presence of the droplets. Particle trajectories and evolution are calculated at the end of the simulation in a post-processing step. While one-way coupling minimizes the computational effort, it is not a feasible approach to represent spray combustion. One-way coupling is a good approximation when the dispersed phase mass is low compared to the continuous one. In a spray, there is a large variance in the local ratio between phases and in the region near the nozzle, there will always be a high amount of liquid. Also, the mass transferred from the droplets to the gas phase is the fuel for our combustion reaction: while the direct contribution to changes in the momentum of the gas phase could be negligible, the change produced by the combustion it causes, determines the flow field of the entire furnace. For these reasons, two-way coupling has been used in this study. In two-way coupling, a source term is added when solving for the local fluid properties to take into account the effect that the particles have on the gas phase. To know this source terms, the droplets position and properties have to be calculated at each time step, thus adding to the computation. To alleviate the CPU cost of particle tracking, this calculation can be solved once per time step, instead that for every iteration.

The droplets are considered spherical, isothermal and composed of an evaporating fluid. The assumption of sphericity is justified by the measurements taken on the spray characterization setup (chapter 3). Their diameter is calculated based on their mass and density, meaning that during the evaporation each droplet shrinks according to the amount of mass lost. The liquid evaporation model uses a latent heat of 216 kJ/kg [13,14] at a reference temperature of 25°C. This value is also close to those reported for HFO of 211 kJ/kg [15].

The momentum transfer between the droplets and the gas phase is calculated using the Schiller-Naumann drag model [6] as suggested by the CFX manual for spherical and small liquid particles [3]. This model uses a drag coefficient of $C_D = 24/Re_d$ for low droplet Reynolds number ($Re_d<<1$), $C_D = 0.44$ for high Reynolds number ($>10^3$) and for transition values in the interval between $0.1$ and $10^3$ uses a complex function of $Re_d$ (equation 1).
CFD study of the auxiliary marine boiler

\[
C_D = \frac{24}{Re_d} \left( 1 + 0.15Re_d^{0.687} \right) \quad \text{Eq.1}
\]

The droplet Reynolds number (eq.2) is calculated for each representative droplet as the Reynolds number of a flow around a sphere moving at the relative velocity between the droplet and the surrounding flow, \( u_r \). Thus uses as characteristic length the droplet diameter \( D \) and the density \( \rho_g \) and viscosity \( \mu_g \) of the surrounding gas [16][17]. The relative velocity can be calculated as the difference between the vectors of the droplet velocity, \( u_d \), and the local gas phase velocity, \( u_g \) (Eq.2).

\[
Re_d = \frac{\rho_g u_r D}{\mu_g} = \frac{\rho_g D}{\mu_g} \sqrt{(u_{gx} - u_{dx})^2 + (u_{gy} - u_{dy})^2 + (u_{gz} - u_{dz})^2} \quad \text{Eq.2}
\]

It should be remembered that \( Re_d \) is uses a characteristic length on the micrometers scale and velocities generally below 10 m/s, thus it is much smaller than the typical Re for flow through pipes or furnaces (Appendix III.1). The range of \( Re_d \) can be observed in Figure 4.1, where most droplets present \( Re_d \) in the transitional range between 0.1 and \( 10^3 \) and lower values are found only for droplets that lost most of their mass due to the evaporation, and thus with a very small diameter.

The droplet Reynolds number

\[C_F\] is calculated for each representative droplet as the Reynolds number of a flow around a sphere moving at the relative velocity between the droplet and the surrounding flow, \( u_r \). Thus uses as characteristic length the droplet diameter \( D \) and the density \( \rho_g \) and viscosity \( \mu_g \) of the surrounding gas [16][17]. The relative velocity can be calculated as the difference between the vectors of the droplet velocity, \( u_d \), and the local gas phase velocity, \( u_g \) (Eq.2).

\[
Re_d = \frac{\rho_g u_r D}{\mu_g} = \frac{\rho_g D}{\mu_g} \sqrt{(u_{gx} - u_{dx})^2 + (u_{gy} - u_{dy})^2 + (u_{gz} - u_{dz})^2} \quad \text{Eq.2}
\]

Figure 4.1: Spray droplets in the computational domain at the end of the CFD simulation 40L4O. Droplets are in scale 100:1 for visibility, lines show the trajectory of the droplets. Droplets completely evaporated are represented only with the trajectory.

The heat transfer between the liquid and gas phase considers thermal energy only, meaning that the contribution of kinetic energy is neglected (such as viscous heating). This approach is recommended for systems with a Mach number, \( Ma < 0.2 \) [18]. In preliminary simulations, the maximum \( Ma \) found in the computational domain was 0.115. This has also been checked in the final simulation confirming that the \( Ma \) does not approach this limit. In the this heat transfer calculation, the Ranz-Marshall correlation is used to calculate the Nusselt number [5].

The heat transfer through radiation is modeled using the Discrete Transfer Model (DTM). The other models available in CFX are the P1 and Monte Carlo models, but the DTM is computationally lighter, while offering accurate results [2,19,20]. A parameter that has been shown to affect DTM is the number of discrete rays [21], the default value used by CFX is 8 [3]. To assess the influence of this parameter a simulation with 10 tracked rays was performed and showed little difference from those with 8 (Appendix III.2), thus the default value has been adopted for the rest of the simulation campaign.
4.2 Materials and methods

In order to consider the heat exchange both between phases, and with the surrounding walls, the gas phase is included in the calculation as a participating media with a Weighted Sum of Gray Gases (WSGG) spectral model. In this approach, the gas phase absorption characteristic is described as the weighted sum of the absorption of gray media. The absorption and emission from a gas can be described as a function of the product of the partial pressure of the gas and the length of the path through the gas, and the gas temperature. In the combustion of hydrocarbons, the main species that absorb and emit radiation are carbon dioxide and water vapor, with unburned hydrocarbons, SO$_2$, NO$_x$, and CO giving a minor contribution. The coefficients used in the CFD simulation for the WSSG model are derived from the work of Beer et al. [7] as suggested in the software documentation [1] for a mixture of CO$_2$, H$_2$O and hydrocarbons. The spectral characteristics expressed by the model are related to the partial pressures of water (p$_{H_2O}$) and carbon dioxide (p$_{CO_2}$) in the gas. The coefficients could be found for p$_{H_2O}$/p$_{CO_2}$ = 1 and p$_{H_2O}$/p$_{CO_2}$ = 2, where the first case is generally suggested for liquid fuels and the second for gaseous fuels. According to the elemental analysis of the fuels used in the boiler, the composition of the exhaust gas resulting from their complete combustion would have a p$_{H_2O}$/p$_{CO_2}$ ratio between 0.72 and 1. These conditions are mostly observed toward the outlet and in low velocity regions such as the walls of the boiler. On the other hand, the region of the boiler where the radiation characteristics are fundamental for flame stability is near the burner. Here, the calculated radiation field determines the heat exchange and evaporation of the fuel droplets, and as seen in Figure 4.2, the p$_{H_2O}$/p$_{CO_2}$ ratio is well above 1, with the lowest value of 1.5 in the region where droplets are present. The simulations were run with the gray gas coefficients for p$_{H_2O}$/p$_{CO_2}$=2, since the focus of this work is on flame stability and characteristics and not on heat exchange with the walls, this ensures that the near burner region is calculated as accurately as possible.

![Figure 4.2: Ratio between partial pressure of water and CO$_2$ on the vertical cross section of the boiler in the 40L40 simulation.](image)

4.2.2 Reactions

The combustion reactions are simulated using a two-step global reaction mechanism that includes a fuel oxidation step to CO (reaction 1) and the subsequent oxidation of carbon monoxide to carbon dioxide (reaction 2) [8,22].
CFD study of the auxiliary marine boiler

\[ C_aH_b + \left( \frac{a}{2} + \frac{b}{4} \right) O_2 \rightarrow a CO + \frac{b}{2} H_2O \]  
(Reaction 1)

\[ CO + \frac{1}{2} O_2 \rightarrow CO_2 \]  
(Reaction 2)

These reactions are modeled using the combined Finite Rate Chemistry (FRC) and Eddy Dissipation Model (EDM) implemented in CFX 17.1.

The FRC is based on the definition of the Arrhenius equation for the reaction through the pre-exponential factor \( A \) and the activation energy \( E_a \). When these two parameters are substituted in equation 3 together with the local temperature \( T \), it is possible to calculate the rate constant \( k \).

\[ k = A e^{-\frac{E_a}{RT}} \]  
Eq.3

\[ \frac{d[CO_2]}{dt} = - \frac{d[CO]}{dt} = k_{CO}[CO]^{x_{CO}}[O_2]^{x_{O_2}}[H_2O]^{x_{H_2O}} \]  
Eq.4

\[ n \frac{d[CO]}{dt} = \frac{m d[H_2O]}{dt} = k_f[C_nH_m]^{x_{C_nH_m}}[O_2]^{x_{O_2}} \]  
Eq.5

The reaction rate in each computational cell is the product of the local rate constant and the local concentration of the participating species elevated to an appropriate exponent, \( x_i \) (equation 4 and 5). Values for these parameters can be calculated with experimental or numerical methods. Data from different sources was collected and evaluated.

Table 4.2: Arrhenius equation parameters for CO oxidation reaction found in literature. Units are cm, mol, kcal. The concentration exponents, \( x_i \), of the forward reaction are respectively for \([CO]\), \([O_2]\) and \([H_2O]\), and for the backward reaction, they refer to \([CO_2]\). The values used in this work are highlighted in grey.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Pre-exponential Factor, ( A )</th>
<th>Activation Energy, ( E_a )</th>
<th>Concentration Exponents, ( x_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Westbrook and Dryer [8]</td>
<td>(-10^{14.6})</td>
<td>40</td>
<td>1.0-0.25-0.5</td>
</tr>
<tr>
<td>- backward reaction</td>
<td>(&lt;-10^{8.7})</td>
<td>40</td>
<td>1.0</td>
</tr>
<tr>
<td>DuPont, Pourkashanian and Williams [23]</td>
<td>(10^{10})</td>
<td>23.88</td>
<td>1.0-1.0</td>
</tr>
<tr>
<td>Dryer and Glassman [24]</td>
<td>(-10^{14.75})</td>
<td>43</td>
<td>1.0-0.25-0.5</td>
</tr>
<tr>
<td>- when low ([C_nH_m]) is present</td>
<td>(-10^{14.6})</td>
<td>40</td>
<td>1.0-0.25-0.5</td>
</tr>
<tr>
<td>Nicol [25]</td>
<td>(-10^{14.9})</td>
<td>23.1</td>
<td>1.69-1.57</td>
</tr>
<tr>
<td>- backward reaction</td>
<td>(&lt;-10^{14.35})</td>
<td>123.8</td>
<td>1.0</td>
</tr>
<tr>
<td>Franzelli [26]</td>
<td>(10^{10.65})</td>
<td>20</td>
<td>1.0-0.5</td>
</tr>
<tr>
<td>Zheng, Miller and Cernasky [27]</td>
<td>(-10^{14})</td>
<td>40</td>
<td>1.0-0.25-0.5</td>
</tr>
<tr>
<td>- backward reaction</td>
<td>(&lt;-10^{7.08})</td>
<td>40</td>
<td>1.0</td>
</tr>
</tbody>
</table>
4.2 Materials and methods

For CO oxidation, the values found in the reference are summarized in Table 4.2. In some references a backward reaction is considered, and DuPont et al. [23] and Nicol et al. [25] report quite different parameters from the other studies, and no dependence on the water concentration. A test simulation has been run including the backward reaction proposed by Zheng et al. [27]. In this simulation the CO level at the exhaust increased by a factor of 100, leading to results very different from the experimental measurement conducted. Finally, the values chosen for the current study are those from Dryer and Glassman [24], obtained for a combustion with excess oxygen and low concentration of hydrocarbons in the carbon monoxide oxidation region (highlighted in Table 4.2). The conditions under which these data were obtained should be similar to those found in the boiler and seemed appropriate giving the relatively high water concentration (around 10% in volume at the exhaust).

Table 4.3: Arrhenius equation parameters for hydrocarbon oxidation reaction found in literature. Units are cm, mol, kcal. The concentration exponents are respectively for [CnHm] and [O2]. The values used in this work are highlighted in grey.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Pre-exponential Factor, $A$</th>
<th>Activation Energy, $E_a$</th>
<th>Concentration exponents, $x_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Westbrook and Dryer [8]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-C7H16</td>
<td>$6.3 \times 10^{11}$</td>
<td>30</td>
<td>0.25-1.5</td>
</tr>
<tr>
<td>-C8H18</td>
<td>$5.7 \times 10^{11}$</td>
<td>30</td>
<td>0.25-1.5</td>
</tr>
<tr>
<td>-C9H20</td>
<td>$5.2 \times 10^{11}$</td>
<td>30</td>
<td>0.25-1.5</td>
</tr>
<tr>
<td>-C10H22</td>
<td>$4.7 \times 10^{11}$</td>
<td>30</td>
<td>0.25-1.5</td>
</tr>
<tr>
<td>Franzelli [26]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-C10H20</td>
<td>$8 \times 10^{11}$</td>
<td>41.5</td>
<td>0.55-0.9</td>
</tr>
<tr>
<td>Gowdagiri and Oehlschlaeger [28]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-C10H22</td>
<td>$2.6 \times 10^{11}$</td>
<td>34.7</td>
<td>0.25-1.5</td>
</tr>
<tr>
<td>-C12H26</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Zheng, Miller and Cernasky [27]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-C7H16</td>
<td>$2.3 \times 10^{12}$</td>
<td>39.7</td>
<td>0.25-1.5</td>
</tr>
<tr>
<td>This work</td>
<td>$1.88 \times 10^{12}$</td>
<td>30</td>
<td>0.25-1.5</td>
</tr>
</tbody>
</table>

The hydrocarbon oxidation reaction proved to be more challenging to model, since the fuel used on the boiler, marine diesel and HFO, contain many hydrocarbon species and little data is available for global reaction rate of higher hydrocarbons. Considering the elemental analysis conducted on samples of the fuels (Chapter 2, Table 2.3) it was decided to use the reaction rates found in literature (Table 4.3) for decane [8] as a starting point. From these rates, a sensitivity analysis was conducted on the pre-exponential factor, $A$. To limit the analysis to a single parameter, the concentration exponents for the fuel and oxidizer, and the activation energy were kept constant, respectively at 0.25 [-], 1.5 [-] and 30 [kcal/mol]. This choice was based on the fact that these values are reported valid for many hydrocarbons.
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in two-step mechanisms [8], while differences of orders of magnitude can be found for the reported pre-exponential factors. The sensitivity analysis was conducted at first for the reference operating conditions of 40% load and 4% oxygen concentration at the exhaust. These simulations showed that the kinetic limitation has an effect on the shape of the flame up to a pre-exponential factor of $2.35 \times 10^{12}$ (5 times the starting value reported by Westbrook and Dryer [8]), as seen in Figure 4.3. For values of $9.4 \times 10^{11}$, the flames proved to be unstable and lifted off in a short time. The values of $1.41 \times 10^{12}$ and $1.88 \times 10^{12}$ (respectively 3 and 4 times the starting value) were further investigated by decreasing the amount of combustion air to 2% and 1% oxygen concentration at the exhaust. This is because the full-scale boiler was able to operate at 2% during the experimental campaign, but below this value it was not possible to obtain a stable operation. The flame quickly lost its anchoring in the near burner region for both simulations with $A=1.41 \times 10^{12}$, while the ones with $A=1.88 \times 10^{12}$ was stable in the 2% simulation. The value used for the pre-exponential factor in this study is $1.88 \times 10^{12}$, since it showed the best agreement with the behavior of the real boiler.

The EDM assumes that the only limitation to the reaction is the mixing rate between reactants, thus considers only the local turbulence to calculate the reaction rate, disregarding the kinetics of the process [29]. The reaction rate in EDM for turbulent flows $R_{EDM}$ is proportional of the concentration of the reactant $[I]$ that is limiting compared to the stoichiometric amount $\nu_i$ and to the ratio between the turbulent kinetic energy $k$, and the dissipation rate $\varepsilon$ (equation 6).

Figure 4.3: Instantaneous snapshots of the fuel droplets (black) and iso-surface with 2%vol concentration of CO (coloured according to the local temperature) from simulations at the 40L4O condition (Table 4.4) each with a different pre-exponential factor in the fuel oxidation reaction.
4.2 Materials and methods

\[ R_{EDM} = A \frac{\varepsilon}{k} \min \left( \frac{|v|}{v_{ij}} \right) \]  

Eq.6

Where the coefficient A, is the reactant limiter and it is obtained experimentally [9,29,30]. A sensitivity analysis for the reactant limiter has been carried out (Appendix III.3), supporting the widely used value of A=4 proposed by Magnussen [9] and also suggested in the software documentation [2].

The combined EDM and FRC model calculates the reaction rate according to the FRC and EDM, finally using in each computational cell the lower of the two. This is so that the limiting factor between mixing and kinetics is always considered. For this reason, the combined model is valid for a wide range of Damköhler number (which describes how fast is the chemistry compared to turbulent mixing rate) and it can be used also when the same reaction is limited by turbulent mixing or by kinetics in different regions of the computational domain. The drawback of using the combined model is that it has a higher computational requirement and it is less computationally robust compared to the EDM.

A last possible approach is to assume that the fuel oxidation is limited by mixing and the CO oxidation by the kinetics, thus including the FRC model only in the CO oxidation reaction [29]. This approach proved to be useful to obtain the initial values for further simulations using the combined model, since the combustion reaction can proceed at low temperature and it is more stable.

To avoid making assumption about the limiting factors in the reactions, the presented results are obtained using the combined EDM and FRC model. For simulations using the EDM it was found helpful for computational stability to introduce a maximum flame temperature. This temperature was set to 2500 K, that is above the adiabatic flame temperature of hydrocarbons from C6H14 to C12H26, which lies between 2270 to 2305 K [13].

The Magnussen and Hjertager model [9] is used for soot formation in the computational domain. This is the only possibility for soot formation available in CFX 17.1 and adds two transport equations for the specific concentration of soot nuclei and for soot mass fraction (eq.7-138 and 139 of [1]). The default values suggested in the software manual for soot material and particle diameter have been used, while the fuel carbon mass fraction has been adjusted to reflect the elemental analysis on the fuel samples reported in chapter 2.

4.2.3 Boundary conditions and particle injection

As boundaries for the CFD simulations it was chosen to use the internal surfaces of the furnace and its natural inlet and outlet, as described in chapter 2. While the flow had a sufficient space to develop before reaching the furnace, the outlet has been extended to avoid recirculation on the boundary. This helps avoiding divergence and poor mass balances in the results. Four types of boundary conditions have been defined to describe the surfaces delimiting the computational domain: inlet, outlet, adiabatic and isothermal walls (Figure 4.4).
The inlet is composed of a cylindrical surface through which the combustion air enters the domain. This is set as subsonic since the highest velocity expected in this region is below 4 m/s. The default settings for high intensity turbulence are used, since the air is fed directly from a fan system mounted on top of the burner that is not included in the simulation. Ambient air composition at 25°C and 25% relative humidity is used. The humidity was calculated using the Mollier diagram based on the ambient temperature and humidity reported for the days of the experimental campaign and adjusted to the temperature measured after the fan. The exact amount of air entering the computational domain varies according to the load and excess air of the boiler in each simulation (Table 4.4). The values used have been calculated from the mass balances for carbon, nitrogen and oxygen, based on the injected fuel and the outlet measurements presented in chapter 2.

The outlet is set as a subsonic outlet, again due to the relatively low velocities expected. This assumption has been checked during the post-processing of the results, were the maximum Mach number found at the outlet boundary was 0.02. The average pressure of 2610 Pa has been specified according to the data of the test center system based on the pressure losses of the heat exchangers downstream of the furnace.

The boiler furnace is enveloped in a water jacket, which cools some of the walls and keeps them at a relatively constant temperature. These walls, blue in Figure 4.4, have been considered isothermal with a temperature of 170°C. Due to the lack of experimental data in this regard, this value is based on the cooling water pressure kept constant by the steam drum at 5 bar, resulting in boiling temperature of 150°C and assuming a reasonable temperature difference across the wall [31–33]. A sensitivity analysis on the effect of this parameter on the flame characteristics would further validate this approach.

The other walls present in the domain have been modeled as adiabatic. For the burner outer surfaces, the bottom of the furnace, and quarl walls this condition represents quite well the reality, since these parts are made of refractory material and/or insulated. The burner inner surfaces on the other hand are
made of steel with no insulation, but are only in contact with low temperature flow (Figure 4.5), with no significant gradients that would promote heat exchange.

All walls are no-slip, smooth and opaque with an emissivity of 1. The momentum restitution coefficient for particles is set to 1, meaning that in case a droplet would collide with them, it would bounce off with the same velocity. While this is not realistic, in the presented simulations the spray droplets never impinge on the walls.

The fuel is injected in the computational domain in a particle injection region with the hollow cone option of CFX, and geometry, particle size distribution, angles and velocities as obtained from the spray measurements presented in chapter 3 and summarized for each simulation in Table 4.4. Each simulation has been repeated using the data obtained for liquid viscosities of 1 and 3 cP. The measured viscosity of the diesel fuel is 4cP at 25°C, but after injection, its temperature increases, decreasing its viscosity while the atomization process is taking place (Figure 4.6) [34]. Therefore carrying out the simulation at 1 and 3 cP should encompass the possible range of viscosities for the fuel. Comparing the results of these simulations with the experimental measurements will also contribute in assessing which viscosity better represents the atomization process in the boiler. For the simulation using HFO, H40L-40, some parameters have been changed from those reported in in Table 4.1. For these simulations, the spray data from the experiments with 7 cP viscosity are used, due to the higher viscosity of HFO. Also, as mentioned in chapter 2, to achieve this viscosity the fuel is pre-heated to 140°C, thus the temperature of the particles injected into the computational domain had to be adjusted. The carbon mass fraction of the fuel has been adjusted to match the results of elemental analysis of the HFO sample (89%), and the latent heat of evaporation to the value reported in literature (211 kJ/kg) [15].
The particles number of position, that represent the number of representative computational particles actually tracked during the simulation, is set to $10^5$ particles per second. This value was chosen as a compromise between particle track file size and computational stability, after a series of preliminary simulations. It was noted that the increase in computational time needed for particle tracking when increasing this parameter is small compared to the overall time needed for the simulations, but it might be an important contribution in other applications. The list of conducted simulations shown in Table 4.4 covers variations in the input parameters of fuel and air mass flows and fuel injection parameters.

Table 4.4: Summary of the operating conditions simulated in the CFD campaign.

<table>
<thead>
<tr>
<th>Name</th>
<th>Load</th>
<th>Fuel in</th>
<th>$\text{O}_2$ out</th>
<th>Air in</th>
<th>Vel oil</th>
<th>Angle</th>
<th>SMD</th>
<th>Fuel</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>[%]</td>
<td>[kg/s]</td>
<td>[vol%]</td>
<td>[kg/s]</td>
<td>[m/s]</td>
<td>[°]</td>
<td>[µm]</td>
<td></td>
</tr>
<tr>
<td>20L-10</td>
<td>20</td>
<td>0.0156</td>
<td>1</td>
<td>0.233</td>
<td>32.7</td>
<td>83</td>
<td>54.1</td>
<td>Diesel</td>
</tr>
<tr>
<td>20L-20</td>
<td>20</td>
<td>0.0156</td>
<td>2</td>
<td>0.248</td>
<td>32.7</td>
<td>83</td>
<td>54.1</td>
<td>Diesel</td>
</tr>
<tr>
<td>20L-40</td>
<td>20</td>
<td>0.0156</td>
<td>4</td>
<td>0.276</td>
<td>32.7</td>
<td>83</td>
<td>54.1</td>
<td>Diesel</td>
</tr>
<tr>
<td>20L-60</td>
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<td>6</td>
<td>0.310</td>
<td>32.7</td>
<td>83</td>
<td>54.1</td>
<td>Diesel</td>
</tr>
<tr>
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<td>Diesel</td>
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<td>2</td>
<td>0.368</td>
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<td>70</td>
<td>54.1</td>
<td>Diesel</td>
</tr>
<tr>
<td>40L-40*</td>
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<td>0.406</td>
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<td>Diesel</td>
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<tr>
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<td>70</td>
<td>54.1</td>
<td>Diesel</td>
</tr>
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<td>0.490</td>
<td>40</td>
<td>60</td>
<td>54.1</td>
<td>Diesel</td>
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4.2 Materials and methods

<table>
<thead>
<tr>
<th>Volume</th>
<th>Diameter</th>
<th>Thickness</th>
<th>Initial Diameter</th>
<th>Final Diameter</th>
<th>Temperature</th>
<th>Combustion Product</th>
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<td>83</td>
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<tr>
<td>20L-20-3cP</td>
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<td>2</td>
<td>0.248</td>
<td>32.7</td>
<td>83</td>
</tr>
<tr>
<td>20L-40-3cP</td>
<td>20</td>
<td>0.0156</td>
<td>4</td>
<td>0.276</td>
<td>32.7</td>
<td>83</td>
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<tr>
<td>20L-60-3cP</td>
<td>20</td>
<td>0.0156</td>
<td>6</td>
<td>0.310</td>
<td>32.7</td>
<td>83</td>
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<tr>
<td>40L-10-3cP</td>
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<td>0.0231</td>
<td>1</td>
<td>0.345</td>
<td>33.9</td>
<td>70</td>
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<tr>
<td>40L-20-3cP</td>
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<td>0.0231</td>
<td>2</td>
<td>0.368</td>
<td>33.9</td>
<td>70</td>
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<tr>
<td>40L-40-3cP</td>
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<td>0.0231</td>
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<td>70</td>
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<tr>
<td>40L-60-3cP</td>
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<td>6</td>
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<tr>
<td>60L-10-3cP</td>
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<tr>
<td>60L-60-3cP</td>
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<td>0.635</td>
<td>40</td>
<td>60</td>
</tr>
<tr>
<td>H40L-40</td>
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<td>4</td>
<td>0.391</td>
<td>33.9</td>
<td>64</td>
</tr>
</tbody>
</table>

*Reference flame simulation

4.2.4 Grid and time step sensitivity analysis

The computational grid used for the final simulations is an unstructured grid with three refinement zones (Figure 4.7A) and inflation layers on the wall boundaries (Figure 4.7B). The first refinement zone is in the burner body, since there are several small features in the geometry that might influence the flow field in the quarl. The second encompasses the region downstream of the swirling plate, since here the gradients for species concentration, temperature and velocity will be the highest. The last refinement zone is around the central region of the boiler in order to have a good resolution of the fields in the flame area. The starting size of the inflation is chosen so that \( y^+ < 5 \) (Eq.7), thus ensuring a proper resolution of the viscous sub-layer region.

\[
y^+ = \frac{y_1 u_T}{v}
\]

Eq.7

Where \( y_1 \) is the distance of the first grid point from the wall, \( u_T \) is and the wall friction velocity and \( v \) is the kinematic viscosity. This resulted in a first layer thickness of 0.1 mm, with an inflation zone of 12 layers for a total thickness of 5 mm in the burner and 20 mm on the boiler walls.
A grid independency study has been carried out employing four different computational meshes (2.4, 4.7, 7.1 and 10.6 millions of elements), to ensure that the solutions are not influenced by the spatial discretization of the computational domain (Figure 4.8). While complete grid independency could not be achieved, as there are still some differences between the results obtained with the composed of 10.6x10^6 elements and the one with 7.1x10^6, nonetheless, the latter was chosen for further simulations. This is because the amount of computational overhead that the finer mesh required was substantial and the change incurred were too small to justify it. More details on the grid independency study are presented in Appendix III.4.
4.2 Materials and methods

time discretization of the computational problem. The main parameter in this discretization is the time step. The time step choice can be based on the Courant number (eq.8), which in a one-dimensional flow represent the amount of cells that the fluid traverses in a single time step. The Courant number calculated in CFX is a multidimensional generalization of this formula based on the mass flow into the control volume and its size, but can be interpreted in the same way. While CFX is an implicit code, and thus does not require \( Co \) to be close to unity, it can still be used as a target parameter for adaptive time stepping, or to give an idea of the time discretization.

\[
Co = \frac{u \Delta t}{\Delta x}
\]

Eq.8

The time step chosen for further simulation was of \( 10^{-4} \) second as a compromise between computational time and error compared to the time step independent solution. This time step is small enough to capture all the vortex shedding observed in the fluid domain (frequency of 200 to 400Hz).

![Figure 4.9: Instantaneous and time-averaged CO at the boiler outlet normalized on the final value for 40% load and 4% oxygen at the exhaust.](image)

On the other end of the simulated timescales, in transient simulation it is important that the simulated time is long enough to include the slower oscillations of all variables. The drawback of increasing the simulated time is that it is computationally demanding, since the computational time and the simulated time are proportional to each other, when the time to write backups and intermediate solution files is not taken into account. Aside from checking the behavior of individual parameters and how their average evolve during a simulation, the average residence time was used as a starting point to consider a suitable simulated time. The average residence time can be calculated in a complex fluid domain as:

\[
t = \frac{V}{\dot{V}} = \frac{V}{m/\bar{\rho}} = 0.65 \, s
\]

Eq.9

While the volume \( V \) and mass flow rate \( \dot{m} \) are fixed for the flow through the domain, the density is function of the local temperature and pressure, thus the average quantity \( \bar{\rho} \) has been used. The resulting average residence time shows that significant average results could be obtained with a simulated time \( >1s \). Such
timescale proved to be reasonable also when looking at the results of the simulations. As an example, the time-average CO at the exhaust of the boiler has been plotted in Figure 4.9. Here it is possible to see that already after 0.1 s the average value is within 3% of the final value.

![Figure 4.10: Instantaneous and time-averaged CO at the boiler outlet normalized on the final value for 40% load and 4% oxygen at the exhaust, after changing particle size distribution.](image)

While these results are representative for oscillations during steady operation, to reduce the total computational time, some of the simulations used as initial values the results obtained for different operating conditions. When inputs such as particle size distribution or flow rate of fuel and air are changed, more time was necessary to reach a steady operating condition. During each of these transition simulations, monitor quantities such as temperature, CO emission and pressure during the simulation were tracked to evaluate if a steady operation had been achieved. After the transition simulation is completed, its final instantaneous results are used as initial conditions in a new simulation to obtain the time averaged results. An example of this is given in Figure 4.10, where the fluctuation in the CO concentration at the outlet is observed after the particle size distribution was modified.
4.3 Results

The results of CFD simulations can include the values of dozens of variables for each of the millions of cells that form the computational domain. Moreover, in transient simulations these data can be given for each of the thousands of time steps that compose the simulation, summing up to tens, if not hundreds of billions of values. Therefore, it is necessary to select representative and meaningful parameters or samples of data that can be recorded and communicated. During this study, it was found that sections of the fields for some variables were especially useful to understand the system behavior:

- The velocity field shows the fluid dynamics in the furnace, such as recirculation zones, general direction of the flow, vortex shedding, stagnant flow regions and viscous boundary layer thickness. This information is relevant for combustion studies, since it determines the mixing conditions, transport and diffusion processes, and residence time for the various species.
- The temperature field is important to understand the heat exchange in the boiler. It also provides insight on the flame behavior, especially for hot spots where the flame is stabilized. The evaporation of the fuel droplet is also primarily determined by the temperature field.
- The concentration of key species for the combustion process gives information about the mixing, but more importantly about the reactions in which they participate. In this study, the local concentration of carbon monoxide is especially interesting to observe, since CO is the only intermediate product of the two-step global reaction mechanism used. Thus, the presence of CO shows that the hydrocarbon oxidation reaction is taking place, while its decrease is generally due to the second step of the reaction (or to mixing/diffusion with a flow with lower CO, but this can be ascertained from comparative observation of the flow field).

In addition to these three fields, in section 4.3.1, the fuel droplet positions and trajectory are important to know where the fuel is released in the gas phase. Lastly, an iso-surface showing the location where the CO concentration is 2% in volume was used to help visualize the flame behavior in a way that can be related to what is the normal “human” way of experiencing it. In section 4.3.2, to assess the accuracy and validate the CFD model, local gas compositions and temperatures are compared with the equivalent furnace measurements taken in the experimental campaign (chapter 2). The time-average values for outlet gas composition and temperature for all simulations are discussed and compared to the experimental measurements in section 4.3.3. Lastly, a closer look of the near burner area and its role in stabilizing the flame is presented in section 4.3.4.

In the graphs showing the detailed CFD simulation results, it should be noted that CO and hydrocarbon concentrations are shown on a logarithmic scale, given the importance of their concentrations with values of the order of $10^{-1}$ in the flame region, and of values in the ppm and ppb range at the furnace exhaust.

4.3.1 Reference simulation results

The simulation 40L-4O (Table 4.4) has been chosen as the reference condition for the CFD campaign. This is because it reproduces the operating conditions of the boiler during the flame mapping in the experimental measurement campaign (chapter 2) and therefore its local temperature and gas
composition data is available. In this section, these data are compared with the results of the CFD model in order to validate it.

The two most noticeable features in the temperature field (Figure 4.11a) are the injection in the furnace of the cold air from the inlet and the heat release in the center of the boiler due to the combustion of the fuel, with peak temperatures of around 2000K. The heat exchange with the boiler walls is much less pronounced, but results in a final temperature below 1100K. Also, less apparent but equally important is the high temperature spots seen in front of the swirling plate. As discussed more in detail in section 4.3.4, the recirculation of the flow in this region is essential to anchor the flame, since without it the temperature would be the same as that of the surrounding cold jet. Temperature and velocity fields also show quite distinctly the recirculation zone on the swirling plate, which was also observed during the full-scale measurement with the same annular shape (Figure 2.19).

As one would expect, the velocity field (Figure 4.11b) shows that the flow velocity increases in the flame region in front of the burner, and when the flow is forced through the smaller area around the swirling plate. The corners of the boiler present a relatively stagnant flow, which also explain the lower
temperatures caused by the longer residence time in proximity of the cold boiler walls. In front of the swirling plate, it is possible to observe a recirculation zone as mentioned above. It is also apparent that a large part of the flow moves toward the bottom of the boiler after impinging on the back-wall, then recirculate towards the front-wall before moving toward the outlet on top of the computational domain. Lastly, it is possible to observe vortex shedding in the quarl area, on the side of the main flow entering the furnace. This in turns corrugates the boundaries of the flow and improves the mixing and heat exchange with the surrounding flow.

Figure 4.12: Vertical sections of the instantaneous concentrations fields of CO$_2$ (a), oxygen (b), fuel in the gas phase (c) and water (d) in the boiler during the simulation 40L-40.

From the fuel droplets positions (Figure 4.11d), the general behavior of the liquid fuel can be observed. Most droplets move downstream in the flame region before evaporating, but some droplets evaporate when passing in the wake of the recirculation zone, thus sustaining it and helping to anchor the flame. Few of the large droplets are able to penetrate the recirculation zones and the cold airflow, thus releasing fuel in the gas phase on the side of the main gas flow.
The reaction progression can be observed from the evolution of the concentrations of the reacting species and products (Figure 4.11c and Figure 4.12). It is quite apparent that in the bottom and top part of the boiler different processes are happening.

The bottom part of the boiler has high concentrations of CO, CO₂, water and uncombusted hydrocarbons still in the ppm range, while the oxygen level is close to zero. The higher oxygen concentration in the upper part of the boiler is due to the fact that part of the combustion air moves directly to this region without taking part in the oxidation reaction. Water is produced only in the fuel oxidation reaction (reaction 1), while CO₂ is the product of the CO oxidation (reaction 2), thus it is possible to see the regions where each reaction happens and with which intensity by observing the differences between Figure 4.12a and Figure 4.12d.

As one would expect, the increase in H₂O precedes the one of CO₂ and both concentrations decrease when moving to the upper part of the boiler, confirming that the exhaust gas are diluted with part of the
air that did not participate in the combustion process. In the recirculation zone there is a relatively high concentration of all species aside from oxygen, this is expected given the high temperature and residence times in this region, any oxygen that enters it, is immediately consumed.

In Figure 4.12c, the fuel concentration in the gas phase shows that the release of the fuel to the gas phase due to droplet evaporation happens close to the burner, but part of the fuel is then transported downstream in pockets without enough oxygen to combust. The fuel is present in the bottom part of the boiler in the ppm range, and reacts when enough oxygen is present, resulting in concentrations of few ppb in the upper part of the boiler.

While the concentration of each species gives specific information on the furnace, the CO concentration field shows the progress of the reaction itself, since it is the only intermediate product of the global reaction mechanism.

While the instantaneous results are easier to interpret, the process happening in the furnace has very pronounced transient characteristics. For this reason the time-average value of each variable in each cell of the domain has been calculated (Figure 4.13). Comparing this with the instantaneous results, almost all of the observations made are still valid, but it can now be seen that all gradients are smoother and the shape of the various profiles is more regular. Of course, part of the information on the transient behaviour of the system is lost, such as the corrugation of the flame front or of the cold air jet when entering the furnace. On the other hand, some other patterns are now clearly visible, while in the instantaneous results they could only be guessed. The connection between the recirculation zone and the main body of the flame is clear, both in the CO concentration and in the temperature fields. Moreover, it is clear that regardless of the oscillations of the flame, there is a well-defined hot region in the centre of the boiler that is relatively stable. The slight increase in the time averaged CO concentration field just on outside the cold air jet confirms that some droplets complete their evaporation here, releasing fuel in the gas phase that quickly react producing carbon monoxide.

The results of simulation H40L-4O, using HFO, did not show any significant deviation from those presented in this section for diesel firing. This is partly explained by the observing that also in the experimental measurement presented in chapter 2, the main difference between diesel and HFO firing lied in NOx production, which is not included in the simulations. The lack of difference in the CO concentration field between H40L-4O and 40L4O, implies that this change is not caused by parameters that have been adjusted to simulate HFO. The factors that has not been changed for HFO, which could have a bearing on this matter, are the fuel oxidation kinetic parameters. Another possibility is that, due to the complex nature of HFO, to obtain a more accurate model it is necessary to use a multi-component fuel model to reproduce its evaporation and reaction characteristics [35,36]. For completeness, the results for the simulation H40L-4O are given in appendix III.8.

4.3.2 Validation against the experimental data

It is possible to extract from the CFD data the temperature and species concentration profiles along a specific path. Since in the experimental campaign measurements have been taken inside the furnace on the burner axis, the corresponding variables have been sampled from the time-averaged computational results and plotted against the experimental ones (Figure 4.14 and Figure 4.15).
While this comparison has been done for the simulation 40L40 using both the 1 and 3cP spray data, the 1cP simulation showed a much better agreement with the experimental data, and it is presented in this section. This agreement suggests that the viscosity of the fuel at a temperature of around 100°C is more representative than that at injection temperature (Figure 4.6) to obtain the droplet size distribution for the CFD simulations. The results for the simulation 40L40-3cP are reported in appendix III.6.

When doing such comparison it is important to remember the techniques used to obtain the experimental measurements mentioned in chapter 3 and their limitations. In particular, both gas concentration and temperature have been obtained inserting water-cooled probes into the furnace, thus modifying the flow field and possibly the heat exchange. In the presence of sharp gradients and high velocities, e.g. near the burner, these effect would be even more marked.

Moreover, while we consider point measurements, the sampled gas would originate from a volume around each point, due to the alteration to the local flow field caused by the suction. Regarding the gas sampling to measure the concentration, it should be remembered that the gas in quenched from the water-cooled walls of the probe, but this process is not instantaneous and might affect the measurements, especially in high temperature regions.

Lastly, the thermocouple used in the suction pyrometer is shielded with ceramic material to avoid heat exchange by radiation with the surrounding, for obvious reasons this part of the probe cannot be water-cooled. This means that from the sampling to the temperature measurement, the gas flows on very high temperature ceramic surfaces, which could be promoting further reactions in the gas.

Regarding the CO₂ concentration (Figure 4.14a), as one would expect the steady increase shows the progression of the fuel and CO oxidation reaction. The simulation shows good agreement with the experimental measurements both predicting the gradient and the absolute values across the boiler. Since
4.3 Results

CO$_2$ is the final product of the two-step global reaction mechanism, this validation supports that the flame dynamics can be captured by the CFD model.

The oxygen concentration (Figure 4.14b) on the other hand shows a good agreement in terms of trends, but the curve from the CFD results is consistently shifted away from the front wall. This could be due to several reasons. For example, a too fast CO oxidation combined with a too slow fuel reaction could justify the accuracy of the CO$_2$ prediction, but the higher amount of oxygen. Another possibility is that the gas is not quenched quickly enough by the sampling probe and the fast reaction of fuel oxidation continues in it, leading to a smaller amount of measured oxygen than what is actually present in the measuring position. This hypothesis is supported by the comparison between measured and predicted CO concentration (Figure 4.15a). These results are qualitatively similar in terms of trends, but in the first half of the boiler, the amount of CO measured is higher of several percentage points than the one shown by the CFD. Again, this would be consistent with both proposed causes of the discrepancy for the oxygen profile. In the first case, the faster reaction rate of the CO would decrease its local concentration. In the second case, the fuel oxidation reaction would continue in the probe, using the oxygen and producing CO. Since the CO oxidation is much slower than the hydrocarbon oxidation (Table 4.2), the flow is quenched before the CO can react, thus resulting in the correct amount of CO$_2$, lower O$_2$ and higher CO than what is actually present in the measuring position. It should be noted however that the CO concentration farther away from the front wall is predicted quite closely by the CFD.

The last comparison we can do with the experimental results regards the temperature (Figure 4.15b). Here we can see that the temperature close to the back wall are predicted quite well, moving toward the center of the boiler the measured temperature is higher than the calculated one, and near the front wall the measured temperature presents a plateau, while the CFD results show a sharp decrease. This might
be caused by the flame stabilizing on the ceramics of the suction pyrometer, thus increasing the temperature measured near the burner.

Since most of the discrepancies between the CFD prediction and the experimental results could be caused by the fuel oxidation reaction taking place in the measuring system, to check if this could be the case, the diesel oil concentration in the gas phase has been plotted for the same axis as the previous graphs (Figure 4.16). Indeed, while it is not a definitive proof, the large amount of uncombusted hydrocarbon in the near burner zone is supports the veracity of our supposition.

It should also be noted that near the burner the gas condition make the measurements less reliable and given the very sharp gradients in temperature and concentrations, a small disturbance in the flow field can lead to drastically different results. Indeed, looking at the temperature fields from the CFD simulations (Figure 4.13A), a small change in the position will induce a large change in temperature. This issue is more pronounced for the temperature measurement, since the gas sampling uses a relatively low suction flow rate (0.06 to 0.24 Nm$^3$/h), while the typical flow rate of the suction pyrometer is 10 Nm$^3$/h. As an example, the average values in a sphere around the measuring point is shown in Figure 4.15B, where the temperature peak value of the volume average reflects quite well the experimental one.

4.3.3 Results for varying operating condition

In this section, the results from the outlet measurements for different operating conditions presented in chapter 2 are compared with the equivalent values calculated from the CFD simulations. As in chapter 2, some of the results are normalized to the correspondent value from the reference simulation case (40L4O) for confidentiality reasons.

As mentioned above, all simulations have been repeated using both the droplet size distribution for liquid with viscosity of both 1cP and 3cP (Table 4.4). While the comparison with local gas concentration and temperature showed that the 1cP simulation reproduces the experimental data much better (Appendix
4.3 Results

III.6), it was also noted that the outlet conditions are generally in agreement between the two sets of simulations, as shown in later in this section (see Figure 4.18, Figure 4.19 and Figure 4.21). However, simulations using the 1cP particle size distribution showed a tendency to destabilize the flame when lowering the amount of combustion air and when increasing the load to 60%. In these cases, the flame lifted off after a short, unstable transient lasting up to 0.05 s. In the actual boiler, a spark system is used to ignite the flame that could help achieve a stable condition and a flame detection system that shuts off the boiler in case the flame lifts off. During the experimental campaign, this happened multiple times when lowering the inlet air to achieve and excess oxygen of less than 2% at 40 and 20% load. These conditions must be close to the lower limit of the operating range of the boiler for $\lambda$. This shows a good agreement between the CFD simulation and the experience gained by operating the boiler. In fact, even if the oxygen level at which the flame is unstable is slightly higher than in the experiments, the fact that the flame does not lift off for the simulation using the 3cP data for droplet distributions shows that also in the CFD model the limit of the operating range is close to the 2% excess oxygen value. For these reasons in this section the results of both 1cp and 3cp simulations are included.

![Figure 4.17: Exit flue gas moisture content at each operating condition - CFD results. The dotted lines show the estimate range based on the experimental data, with the lower limit obtained assuming dry air and the upper limit considering a moisture content of the inlet of 0.5% in mass.](image)

When the flame loses its anchoring to the recirculation zone, it moves downstream in the boiler and tends to stabilize on the back wall (shown in Appendix III.9). Nonetheless, this operating mode would quickly lead to a deterioration of the back wall, thus it is not considered in this chapter. For the operating condition at which it was possible to obtain a stable flame, the results of the outlet temperature, gas and soot concentrations matched closely those of the simulations at 3cP.

It should also be noted, that while the results from the CFD results are taken at the outlet of the furnace, before the tube heat exchanger situated above it, the experimental measuring points for gas composition and particulate sampling are further downstream due to layout limitations of the boiler. Assuming that the gas is quenched quickly enough, this should have only a negligible effect on the gas composition, but
it cannot be excluded that some reaction might still be happening in the first section of the heat exchanger.

In the experimental campaign, the gas sampled from the boiler exhaust passes through a conditioner box where the moisture is removed to avoid damage to the gas analyzer. The data presented has been adjusted to represent dry concentrations of the gas species and it is therefore comparable to the values presented in chapter 2. For this same reason, the experimental results do not include moisture content of the exhaust gas, while this information is provided from the CFD (Figure 4.17). An estimate of the water content of the exhaust gas can be obtained from the mass balances based on the experimental data and assuming the humidity of the inlet air. Generally, we can see that the moisture content in the exhaust decreases with an increase of combustion air.

![Figure 4.18: Comparison between exhaust CO concentrations from the CFD simulations (using 1 and 3 cP viscosity) and experimental data for marine diesel. Values are normalized on the results of 40L40.](image)

This can be explained by simply observing that water produced in the combustion is proportional to the amount of fuel injected, thus increasing the amount of combustion air dilutes it. The CFD results lie in the range estimated from the experimental data and follow the same trend when the excess oxygen at the exhaust is changed.

As mentioned previously, being CO an intermediate product in the global reaction mechanism, its exhaust concentration is a good indicator of the completeness of the combustion in the furnace. The CFD simulations are able to capture the trends for changing air to fuel ratio and, given the low range of CO at the exhaust, show a good accuracy for the simulations at 40 and 60% load (Figure 4.18). A possible explanation for the quantitative discrepancy in the 20L2O simulation is that due to its high concentration, the CO oxidation continues in the first section of the heat exchanger after the furnace before reaching the sampling probe. Unfortunately, not enough data about this part of the system is available to check this hypothesis.

While oxygen and carbon dioxide are not of interest for regulations on emissions and they are mostly determined by the mass balances, the comparison between measured and simulation data lends more
insight into the predictive capabilities and limitations of the CFD model. In Figure 4.19, it is possible to see that since CO$_2$ is produced by consuming the oxygen, in the cases where there is an overestimation of one, the other is under predicted. The values obtained from the simulations are close to the experimental one, with a larger deviation in the simulations using spray data for 3 cP viscosity. In these simulations, the discrepancy increases at low air-fuel ratios, thus pointing at a possible issue with incomplete combustion. In this scenario, part of the fuel injected would not react with oxygen and thus producing a lower amount of CO$_2$.

![Comparison between CFD simulations (using 1 and 3 cP viscosity) and experimental data for exhaust oxygen (above) and CO$_2$ concentrations (below).](image)

To check this hypothesis the amount of unburned hydrocarbons in the gas phase at the exit of the furnace has been calculated from the CFD simulations (Figure 4.20). In all simulations where a significant amount of unburned hydrocarbons is found, there is also a deviation from the experimental data for the CO$_2$ and O$_2$ concentration. It can also be observed that the simulations using the spray data for 1cP viscosity matched quite well the outlet concentrations of CO$_2$ and O$_2$ and have less than 6ppm of unburned fuel at the exhaust. On the other hand, the simulations with the 3cP data 20L-2O, 40L-2O, 40L4O, 40L6O and 60L10, which showed a larger discrepancy with the experimental measurements, have between 20 and 270ppm of unburned fuel at the exhaust. Even considering that each mole of fuel would react with approximately 19 moles of oxygen, in these concentration it cannot account for the discrepancies.
observed for $O_2$ and $CO_2$. Nonetheless, this points to a decrease in the accuracy of the CFD model in relation to cases where the combustion is not complete and fuel is released in the gas phase throughout the computational domain. Another possible cause for these deviations might lie in the uncertainties in the inlet conditions.

![Figure 4.20: Diesel oil concentration in the gas phase at the furnace exhaust in the CFD simulations.](image)

The reported exhaust temperatures for the simulation campaign show the same trend when changing the amount of combustion air observed in chapter 2 for the experimental measurements: the larger amount of air and lower residence time for higher $\lambda$ lead to a decrease in temperature. This trend is more accentuated in the simulations and, contrary to the experimental data, persists when at 20% load (Figure 4.21). This might be caused by the constant wall temperature for all simulations. While the trends are well captured, from a quantitative point of view, the simulations seem to underestimate the outlet temperature. This was expected since in the simulation the outlet temperature can be obtained as the mass flow average of the temperature on the furnace outlet section, while in the experimental campaign the temperatures were obtained by placing the suction pyrometer in the center of the boiler 137mm below this section.

![Figure 4.21: Comparison between exhaust temperatures from the CFD simulations (using 1 and 3 cP viscosity) and experimental data for marine diesel.](image)
As shown in Figure 4.22, the position where the suction pyrometer is placed is at a higher temperature than the average of the exhaust section. Moreover, the suction pyrometer position is in a region with large gradients of the temperature field, making it challenging to guess the effects on it of the presence of the probe. Considering these factors, the agreement between experimental and simulation temperature is satisfactory.

The last quantity taken into consideration for comparison of the different operating conditions and the respective experimental measurements is soot. While the sampling method as presented in chapter 2 is meant for qualitative analysis, the information gained by such comparison is relevant to establish the limitation of the CFD model of the boiler. The results of the simulation capture some of the trends observed in the experimental data and lends results in the same range of the measurements (0-10 mg/Nm³). To improve such comparison a more detailed study of the morphology of the soot particles should be carried out and the input parameter for the Magnussen and Hjertager model should be adjusted to reflect the measured soot particle size.
4.3.4 Recirculation zones

As pointed out in paragraph 4.3.1, the recirculation zone that forms downstream of the swirling plate is of primary importance for stabilizing the flame. While it is quite difficult to gain insight into this region experimentally, with CFD it is possible to have a closer look at how it works, thus gaining further insight into the flame.

As the name says, the recirculation zone is characterized by an inversion of the flow thus forming a region with a high residence time, where hot flue gas recirculates and mixes with fresh air and fuel. In Figure 4.24 a black line encompasses the areas where the axial velocity is negative both on the vertical and horizontal planes. In the same region, we find high temperature (shown by the color map) that is sustained by the quick oxidation of any fuel entering it. This is shown by the overlap of the recirculation zone and the pink CO iso-surface in Figure 4.24. Part of the fuel evaporated (seen in Figure 4.12c) and of the hot gas is carried downstream generating a diffusion flame with the surrounding jet of cold air.

**Figure 4.24**: Close up of the burner/quarl area in the 40L4O simulation. The vertical and horizontal sections of the temperature field is shown (the colour map), with the reverse flow boundary (black slid lines) and the 2% CO iso-surface (pink).

As the name says, the recirculation zone is characterized by an inversion of the flow thus forming a region with a high residence time, where hot flue gas recirculates and mixes with fresh air and fuel. In Figure 4.24 a black line encompasses the areas where the axial velocity is negative both on the vertical and horizontal planes. In the same region, we find high temperature (shown by the color map) that is sustained by the quick oxidation of any fuel entering it. This is shown by the overlap of the recirculation zone and the pink CO iso-surface in Figure 4.24. Part of the fuel evaporated (seen in Figure 4.12c) and of the hot gas is carried downstream generating a diffusion flame with the surrounding jet of cold air.

**Figure 4.25**: Sections of the Temperature (a), CO (b) and Velocity (c) fields, parallel to the swirling plate in the 40L4O simulation. Sections a and b are 9cm downstream of the swirling plate, while c is at 6 cm.
One notable point regarding this early stage of the combustion process for the simulation 40L40-1cP, is that there is an asymmetry on the horizontal plane. On the right, the recirculation zone is smaller and downstream of it there is a “hole” in the CO surface, showing that locally the fuel is not combusting. The most probable cause for this is the asymmetry in the flow field caused by the spark system mounted on the burner lance. This is confirmed by the fact that the asymmetry in the flow field can be observed upstream of those in the temperature and CO concentration fields (Figure 4.25). While this is not interfering with the stability of the flame for the simulated operating conditions, removing this issue might help increase the operating range of the boiler. This could be done easily by reducing the size of the spark system.

Observing the recirculation zone in simulations at different loads, it can be noticed that it changes shape and size according to the load of the boiler (Figure 4.26): both the high temperature and the reverse flow zones become bigger and more elongated with increased load. This is explained by the different amount of air passing through the burner and the difference in spray angle for each fuel flow rate (wider for lower loads, Table 4.4). It is also evident that the area close to the swirling plate is unaffected by the load, and reflect closely the geometry of the swirling plate. Resorting to nozzles with a different relation between flow rate and spray angle and modifying the swirling plate geometry would therefore help tailor the shape and size of the recirculation zone to stabilize the flame when changing operating range or using different fuels.

Lastly, the shape of the recirculation zone found for different loads can be compared with the respective optical measurements on the full-scale boiler (Figure 4.27). While a quantitative comparison is not feasible, the same effects of changing load is observed, with a progressively smaller bright region when the load is decreased, further supporting the validity of the CFD simulations.

In conclusion, flame anchoring with this burner is achieved thanks to recirculation induced by the presence of the swirling plate. From the results of the CFD simulations, it was possible to observe in detail how the flame stability is dependent from the burner design.
4.4 Conclusions

In this chapter, the CFD simulations of the full-scale boiler have been carried out using ANSYS CFX 17.1. The simulation campaign includes all the operating conditions tested during the experimental campaign (presented in chapter 2): 2, 4 and 6% excess oxygen for 20 and 40% loads, and 1, 2, 4 and 6% excess oxygen for 60% load. The data obtained from the spray characterization work described in chapter 3 was used to model the fuel injection in the computational domain.

For the reference operating conditions (40L4O), the results of the CFD simulation have been compared to the local temperature and gas concentration measurements along the burner axis. While the CO₂ concentration profile is well predicted in the simulation, the temperature and concentrations of CO and O₂ show a deviation from the experimental ones in the first half of the boiler. This discrepancy was ascribed to the continuation of the combustion of the fuel in the measuring probe. The unburned hydrocarbon concentration shown by the CFD in the same zone supported this hypothesis.

To assess the predictive capability of the CFD simulations at varying operating conditions, the exhaust gas composition, temperature and soot have been calculated for all simulations and compared to the experimental data. As in the experimental campaign, the CFD simulations showed a lower limit of the operating range at 2% oxygen concentration in the exhaust at 20 and 40% load and 1% at 60% load. Overall, the CFD simulations reproduce quite well the trends for all quantities when varying the amount of excess air or load. A discussion regarding the quantitative discrepancies is given for each parameter.

A recirculation zone was observed in all simulations just downstream of the swirling plate of the burner and recognized as the anchoring point of the flame. This phenomenon has been described in detail and it was observed a change in size and shape of its boundaries in relation with the load of the boiler. These changes were also compared to those observed in the experimental data, showing good qualitative agreement.
In conclusion, the CFD simulations were validated against the experimental data. Most of the discrepancies between the results can be attributed to limitation of the measuring techniques such as precision of the sampling location and continuation of the oxidation reaction in the tip of the measuring probes. Moreover, the simulations were able to capture the overall trends in exhaust gas composition, temperature and soot emission when varying the operating conditions of the boiler and to provide relevant insight into the phenomena occurring in the near-burner region.
4.5 References


4.5 References


CFD study of the auxiliary marine boiler

The main objective of this work was to investigate spray combustion in auxiliary marine boilers, by achieving reliable CFD simulations of these systems. During the project, two critical issues needed further study in order to complement the CFD modelling: full-scale measurements on a marine oil boiler and characterization of the fuel atomizer it employs. The full-scale measurements were needed to obtain data on the specific boiler, which could be used to validate the CFD model. The characterization of the atomizer was necessary to define the fuel injection in the CFD simulations at different operating conditions.

An experimental measuring campaign on a full-scale boiler was planned and undertaken during the project in order to provide suitable data for validation of the CFD simulations of the same system. This was also a chance to fully test the boiler operating capability and to gain data on the effects of changing operating conditions on flame stability and emissions.

The experiments included several changes of operating conditions of the boiler in terms of excess air, and boiler load, for both diesel and HFO firing. For three different loads, the excess air was adjusted to obtain 1, 2, 4 and 6% oxygen volume concentration at the exhaust. After a steady state operation was achieved, measurements of the exhaust gas composition, temperature and particulate emission were taken. To supplement these data, a water-cooled camera probe was used to obtain videos of the flame at each operating condition.

Switching from HFO to diesel firing had a large impact on the emissions with a reduction of NOx and CO at the exhaust between 75 and 85% and up to 97% for particulate. With a SEM, it was possible to observe that also the morphology of the sampled particulate changes drastically between the two fuels, with sub-micron particles produced by diesel combustion and cenospheres of 10 to 100 µm for HFO firing.

Stable operation could not be obtained for the lower loads of the boiler below 2% oxygen at the exhaust. The specific NOx and CO emissions decreased consistently when lowering the boiler load. Particulate emission increased at higher loads for diesel firing, and decreased for HFO firing. Increasing the amount of excess air led to a decrease in particulate emission and a substantial reduction of CO emissions. This effect became negligible above 4% oxygen concentration at the exhaust. NOx emission did not show any significant trend with changes in excess air.

A second part of the experimental campaign was dedicated to obtain a mapping of the furnace chamber for CO/CO2/O2/NOx concentrations and temperature. This was done at a set operating condition for both diesel and HFO firing. The data shows that switching between these two fuels had a negligible impact on
the temperature field in the boiler. On the other hand, the NO\textsubscript{x} production showed a local increase consistent with the outlet values, while the peak values of CO for diesel firing was noticeably higher.

The data gathered is consistent and appropriate for CFD validation given the availability of both local and exhaust measurements of gas composition and temperature for both HFO and Diesel firing. Moreover, the availability of exhaust measurements for both modes of operation could be used as a comparison to check if the overall performance of the boiler is accurately predicted.

The development and design of the equipment used for the full-scale measurement was also a challenging activity that contributed to the knowledge gained from the project, and that will surely be of use to all parts involved.

A spray characterization study was carried out on the spill-back atomizer that is used in a full-scale boiler and resulted in a novel spray diagnostic method which provided data needed as an input for the CFD calculations. At the same time, further insight was gained into the influence of key nozzle operation parameters on spray characteristics.

The oil burner spill return nozzle was characterized using a novel shadowgraphy technique. Which, with its back-light pulsed single LED setup, proved to be a reliable and economic alternative to systems using lasers and high-speed cameras. A wide range of operating conditions were investigated by varying the supply pressure to the nozzle. To reproduce the spray of the full-scale boiler, three different flow rates were employed (50-80-112 l/h). The liquid viscosity was adjusted by using different concentrations of water-glycerol solutions, thus reproducing the properties of different fuels. Lastly, three supply pressures were tested (15-20-25 bar). The proportionality exponent γ was used to describe the relations between Sauter Mean Diameter (SMD), supply pressure and viscosity. The values of γ\textsubscript{p} obtained from the experiments at varying supply pressures was -0.46 ±0.05, while the γ\textsubscript{v} obtained for viscosity was 0.18±0.05. Both results are in line with those found in literature. Furthermore, the data confirmed that changing the flow rate at constant supply pressure has little impact on the SMD in back-spill nozzles and that the spray cone angle increases with decreasing viscosity and flow rate.

Through the statistical analysis of the data acquired, it was possible to evaluate the relationship between the population size of the droplet sample and the error on the SMD and the average velocity. It was shown that to obtain an accurate estimate of the SMD, a much larger sample is needed than for the average velocity. With a sample of 3x10^4 droplets, it was possible to achieve a relative error below 2%.

Overall, in addition to the design and manufacturing of the setup itself, the spray characterization study achieved a detailed nozzle characterization including the influence of pressure, flow rate and viscosity.

Using the data obtained from the spray characterization study to model the fuel injection, CFD simulations of the full-scale boiler have been carried out for all the operating conditions investigated during the experimental campaign.

The CFD model was validated by comparing its results with the local temperature and gas concentration measured along the burner axis. While the CO\textsubscript{2} concentration profile is well predicted in the simulation, the temperature and concentrations of CO and O\textsubscript{2} show a deviation from the experimental ones in the first half of the boiler. This discrepancy was ascribed to the continuation of the combustion of the fuel in
the measuring probe. The unburned hydrocarbon concentration shown by the CFD in the same zone supported this hypothesis.

When compared with the experiments at varying amount of excess air and load, the CFD simulations reproduced quite well the trends for the exhaust values of all measured quantities. Moreover, as observed in the experimental campaign, also in the CFD simulation flame lift-off and unstable operation were observed when decreasing the excess air below 2% oxygen at the exhaust at low load.

In all the CFD simulations, a recirculation zone was observed just downstream of the swirling plate of the burner. The size and shape of its boundaries in relation to the load of the boiler were compared with the observations done with the camera probe, showing good qualitative agreement.

In conclusion, the project has been successful in achieving a complete study of the auxiliary boiler with CFD simulations based on the measured spray characteristics, which were validated against the experimental data and proved their predictive ability for changes in operating conditions, both in terms of outlet conditions and of internal flow. The CFD model provides a tool to evaluate further improvements in design and operation of the boiler and step stone for further practical studies of full-scale spray combustion furnaces.

**Future work**

While the PhD project achieved its goals, it also highlighted several issues and challenges that still need to be tackled.

A stepwise increment of the spray characterization setup capabilities could bring several interesting results both in the field of spray diagnostic and to collect more accurate data for further modelling:

- Experiments using surfactants in the water-glycerol solutions to extend the spray characterization study. This step would be instrumental in the evaluation of alternative fuels for spray combustion applications.
- A modular design of the spray characterization setup would enable the study of a wider range of spray nozzles, starting with air-blast atomizers, which are used for viscous fuels and slurries without preheating.
- A modification of the spray setup to work safely with real fuels would eliminate the necessity of model fluids altogether.

Regarding the experimental work on full-scale systems, the investigation of other commercial auxiliary marine boiler or general utility boilers could prove valuable in an effort to improve such systems. Also, in-line spray diagnostic, an Infra-Red camera probe, an integrated portable solution for the gas analysers, and velocity measurement techniques (such as Laser Doppler Velocimetry) would be valuable additions the current measuring capabilities. Moreover, switching to non-intrusive measurement techniques would add to the accuracy of the results by removing artifacts caused by the measuring probes.

The CFD model that was developed and tested in this work could be expanded and used to assess possible improvements on the boiler design and operation:
- NO\textsubscript{x} formation should be included in the model and compared with the measured data from the experimental campaign, with focus on the results for different fuels. This should be possible also by adding a post-processing step on the existing simulations.
- LES simulation could be carried out to evaluate the potential for improvement of the computationally lighter RANS model.
- Implementation in the CFD simulation of the gas combustion and combined oil and gas combustion.
- The CFD model should be used to evaluate alternative geometries of the burner and different fuels. Items that should be the focus of the work on the burner are the geometry and position of the gas distribution system, the shape and size of the swirling plate, possible solutions to introduce air staging or to automatically adjust the geometry of the burner based on the operating conditions of the boiler.
Appendix I.

I.1 Furnace probes and interfaces design

As mentioned in chapter 2, one of the technical challenges to carry out intrusive furnace measurement in auxiliary marine boilers, is the necessity of sealed connections for the probes, due to the overpressure in the furnace. After the test boiler was modified, the components necessary to insert the probes were designed and fabricated. The main concern was to ensure the safety of people involved in the measurements, by avoiding any leak of combustion gasses in the test center. The second concern was to ensure a steady support of the probe, thus ensuring the accuracy of the position of the measurement. A gate valve was provided on each of the ports to insert the probes (Figure I.1A). The connection for each of the probes included two well aligned supports and a heat resistant gasket (Figure I.1B and C). To avoid gas leaks, the interfaces were first mounted on the boiler ports, then the probe was inserted in the connection and only after the gasket had been tightened the gate valve was opened and the probe slid into the furnace chamber.

![Figure I.1: A) Suction pyrometer inserted in the boiler through its port connection. B) Schematic drawing of the connection for the camera and gas suction probe for the back wall. C) Compact connection designed for the side ports of the boiler and the short gas suction probe.](image)

I.2 Further details about elemental analysis of the fuel samples

Below are reported the complete results of the elemental analysis on the fuel samples sent to the external laboratory. The samples have been collected during the experimental campaign directly from the feeding line leading to the boiler.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Method</th>
<th>Unit</th>
<th>Results as received</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulphur (S)</td>
<td>ASTM D 3177 (2007), mod.</td>
<td>%</td>
<td>0,03</td>
</tr>
<tr>
<td>Carbon (C)</td>
<td>ASTM D 5291 (2016)</td>
<td>%</td>
<td>86,5</td>
</tr>
<tr>
<td>Hydrogen (H)</td>
<td>ASTM D 5291 (2016)</td>
<td>%</td>
<td>13,6</td>
</tr>
<tr>
<td>Nitrogen (N)</td>
<td>ASTM D 5291 (2016)</td>
<td>%</td>
<td>&lt; 0,1</td>
</tr>
<tr>
<td>Oxygen (O)</td>
<td>Calculated (100 - C, H, N, S)</td>
<td>%</td>
<td>-</td>
</tr>
</tbody>
</table>

Table I.1: Marine Diesel composition from a certified laboratory at FORCE technology.
Appendix I

Table I.2: HFO composition from a certified laboratory at FORCE technology.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Method</th>
<th>Unit</th>
<th>Results as received</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulphur (S)</td>
<td>ASTM D 1552 (2008)</td>
<td>%</td>
<td>2,3</td>
</tr>
<tr>
<td>Carbon (C)</td>
<td>ASTM D 5291 (2016)</td>
<td>%</td>
<td>87,2</td>
</tr>
<tr>
<td>Hydrogen (H)</td>
<td>ASTM D 5291 (2016)</td>
<td>%</td>
<td>10,7</td>
</tr>
<tr>
<td>Nitrogen (N)</td>
<td>ASTM D 5291 (2016)</td>
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</tr>
<tr>
<td>Oxygen (O)</td>
<td>Calculated (100 - C, H, N, S)</td>
<td>%</td>
<td>-</td>
</tr>
</tbody>
</table>

I.2.1 Influence of sample weight on in-house elemental analysis

Below the results of the elemental analysis carried out at DTU and plots showing the influence of sample weight on the results Table I.3. It is clear from the large standard deviation compared to the absolute value that nitrogen from these analyses cannot be trusted, while carbon and hydrogen are consistent.

Table I.3: results of the elemental analysis carried out at DTU.

<table>
<thead>
<tr>
<th></th>
<th>N [%]</th>
<th>C [%]</th>
<th>H [%]</th>
<th>molH/molC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diesel</td>
<td>Mean</td>
<td>2.36</td>
<td>84.8</td>
<td>12.8</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>1.24</td>
<td>0.68</td>
<td>0.68</td>
</tr>
<tr>
<td>HFO</td>
<td>Mean</td>
<td>3.24</td>
<td>87.1</td>
<td>9.7</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>1.60</td>
<td>1.30</td>
<td>0.75</td>
</tr>
</tbody>
</table>

The in-house elemental analysis showed a dependency of the sample weight and the nitrogen content, regardless of the fuel used (Figure I.2). This effect was ascribed to the air trapped in the sample capsule upon sealing it. Normally the sample is deposited into a smooth wall silver capsule, which is then sealed using a sealing device that creates and hermetic seal, thus preventing liquid spills or that the evaporating the sample mass would change. This procedure has been followed for both HFO and diesel.
Further details about elemental analysis of the fuel samples

To check if the sample preparation was responsible for the nitrogen content results, alternative methods have been used for both Diesel and Heavy Fuel Oil (HFO) sample. Two diesel samples (Diesel3cs in Figure I.2) have been used in a standard pressed tin capsule together with a Chromosorb® W (SiO₂), which soaks up the liquid preventing spills when the capsule is closed. In addition, a HFO sample (HFO3 tin) has been packed in a standard pressed tin capsule, in a similar manner as a solid sample.

The results of this test show that preparation of the sample using the smooth wall capsule should be done under a purge flow of inert gas, and, if the sample are processed just after packing, standard pressed tin capsule with an inert adsorbent are a valid alternative for marine Diesel or HFO.

A video demonstration of all the used methods can be found at the Elemental Microanalysis Ltd. Youtube channel.
I.3 Flame images arrays

Below images for mean and minimum pixel intensity are reported for all tested operating conditions.

Figure I.3: Average pixel intensity at various operating conditions.
Figure I.4: Minimum pixel intensity for various operating conditions.
### I.4 Flame mapping data

The numerical values for the flame mapping obtained at 40% load and 4% oxygen concentration at the exhaust are given in the tables below. Concentrations reported are dry concentrations. Furnace exit values are not given for confidentiality reasons.

*Table I.4: Results of the furnace measurements at burner height.*

<table>
<thead>
<tr>
<th>Position [m]</th>
<th>T [°C]</th>
<th>O₂ [%]</th>
<th>CO₂ [%]</th>
<th>CO [%]</th>
<th>NOx [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Diesel</td>
<td>HFO</td>
<td>Diesel</td>
<td>HFO</td>
<td>Diesel</td>
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Appendix II.

II.1 Back spill nozzle characteristic curves and fouling effect

The characteristic curves of the atomizing nozzle supplied by the manufacturer for operation at a supply pressure of 20 bar is compared with the ones measured on the spray characterization setup. This is because the pressures cannot be measured in the atomizer itself, and in the case of the spray setup, the closest measuring positions are at the inlet and spill outlet of the nozzle holder. Therefore, the characteristic curve depends on the pressure losses (and therefore geometry) in the flow up to these measuring points, which are not necessarily identical at the manufacturer’s facilities and on the spray characterization setup (Figure II.1). The spill flow rates are nearly identical, probably because the spill line up to the measuring point is a smooth metal tube with very little viscous losses. On the other hand, the supply flow rate, and consequently the output, are slightly lower than in the manufacturer data. This could be caused by the turns and the small passages and in the nozzle holder (a perforated ring was used as a spacer to keep the spill line pipe centered at the center of the holder).

![Figure II.1: Characteristic curves supplied from the nozzle manufactured and measured on the spray characterization setup.](image)

On the supply line of the nozzle, there is a mesh filter, on which fouling material may accumulate. The characteristic curves of the system have been measured also in conditions of heavy fouling of this filter and are shown in Figure II.2. This test was done to gain insight into possible effects of fouling and more importantly to observe fouling symptoms to recognize them during operation of the setup.
Appendix II

Fig. II.2: Measured characteristic curves of the spray characterization setup with clean and fouled filter.

Lastly, since the setup needed to be operated at various supply pressure and the manufacturer’s characteristic curve are only for the design pressure of 20 bar, the curves have been measured also at 15 and 25 bar of supply pressure (Fig. II.3). The results of these tests did not give any particular insight, but were especially useful during the operation of the setup, to know the pressures needed on the back-pressure valves to obtain a certain flow rate, instead of regulating them only by trial and error. Also, such test was necessary to test the setup for safe operation at higher pressures, before equipping it with the delicate optical components.

Fig. II.3: Measured characteristic curves for output at various supply pressures.

A last characteristic curve experiment has been carried out to assess if the type of gasket used on the nozzle holder had any influence on the operation of the setup (Fig. II.4). This is because the first design of the setup used a Teflon gasket, while the final design used a copper gasket instead.
Back spill nozzle characteristic curves and fouling effect

Figure II.4: Measured characteristic curves for output, spill and supply flow using two different nozzle gaskets.
II.2 Spray setup design

II.2.1 First setup design

In Figure II.5 is represented the design of a spray setup built at Risø campus from Sønnik Clausen and Morten Søe Jepsen, which was the starting point for the design of the setup used in this work. The water tank had a water inlet line (not shown) to fill it with tap water. Once the tank is filled, the line is closed and it is not used during operation of the setup. The tank is then pressurized by compressed air coming from a splitter in the compressed air line. The tank has a membrane to keep water and air separated, while keeping the pressure constant during operation. The nozzle holder is made by two concentric tubes. Pressurized water flow through the inner one and air through the outer one.

![Diagram of the previous design of the spray setup.](image)

Figure II.5: Previous design of spray setup.

II.2.2 Adapting the setup for the spillback nozzle used in auxiliary boilers

Two were the main issues in using the back spill nozzle from Alfa Laval in this setup. The first was that the compressed air is not needed for atomization, but instead a return line for the water should be present. This line should have a system to regulate either flow or pressure and possibly monitor both of them. Also, the nozzle holder for the back spill nozzle should be made according to the new nozzle dimensions.

The second is that the current setup is meant to work with water pressures below 10 bar, while the nozzle manufacturer information sheet specifies an operating pressure of the back spill nozzle of 20 bar.

A less important, third issue is that the distances at which the spray measurements are taken in the current setup (0.5-2m) are much farther from the nozzle than what would be relevant for our project (<0.3m).
In conclusion, only the image capture system and the connections of the current setup can be used in this project. Equivalent of some of the components could be found for higher pressures, but it is not possible to use compressed air from the workshop line to pressurize a tank to 20 bar, since it is only at around 7 bar. An alternative solution could be to have a pump delivering the water or filling a membrane tank able to withstand the pressure (Figure II.6).

Also, it is important to take into account the fuel flow rates both going to the nozzle and in the return line. While this is probably dependent on the characteristic curve of the fuel pump used at Alfa Laval, a first idea can be taken from the data collected during the cold test.

II.2.3 Spray setup design using a gas cylinder

The second draft of the spray setup is shown in Figure II.7 and included a gas cylinder to pressurize the water tank. In this configuration it was estimated that the gas bottle should be replaced every 94 minutes of operation, considering a gas bottle volume of 50 l, at 200 bar, a spraying pressure of 20 bar and maximum flow of 5 l/min.

The advantage of this design was that the supply pressure to the nozzle could be increased easily, even to values used in internal combustion engine fuel injection. On the other hand, the replacement of the gas bottle and components to withstand such pressure would be expensive.

The final design of the spray characterization setup is described extensively in chapter 3.
II.2.4 Supporting CFD simulations

CFD has been used to during the design of the spray setup and compared to the results obtained from it. These simulation were done using the same modelling approach used in chapter 4, but without the heat transfer and chemical models. The velocities measured from the setup showed good agreement with transient simulations carried out in this way (Figure II.8).
One of the issues with the first prototype of the spray setup was the recirculation of droplets entrained in the airflow to the near nozzle region, where the measurements are taken (Figure II.9). Simulation have been run to assess the impact of this issue on the measurements and showed that even setting the water surface to capture all impinging droplets, a substantial amount of smaller droplet remains entrained in the airflow, and recirculate to the near-nozzle region (Figure II.10).

**II.2.5 Uncertainty sources in the hydraulic system**

The sources of errors in the hydraulics of the setup are relative to the accuracy of the measuring devices present. The flow meters used have a sensitivity of 1.5 l/h and the pressure gauges of 0.5 bar. However, it should be noted that these errors are similar if not smaller to those in the equipment of the full-scale boiler, thus while reducing them could be useful from theoretical understanding of the spray, it would bear no real effect on the application of the results. Another source of error is that the temperature of the system is not controlled and, while the temperature of the liquid has been monitored and considered for all calculations, this account for the average temperature and not for smaller fluctuations.
II.3 Single droplets plots for all operating conditions

Below are reported the plots for single droplet measurements equivalent to those shown in Figure 3.8, for all tested nozzle operating conditions. Supply pressure was changed between 15, 20 and 25 bar, viscosity between 1, 3 and 7 cP, and atomized flow rate between 50, 80 and 112 l/h. Overall, the same trends described in chapter can be observed in all experiments. As mentioned in the conclusions of chapter 3, the water-glycerol solutions showed a tendency to entrain bubbles in the liquid, which could have caused some artifacts in the measurements. In this experiment also a tendency to form a mist of suspended droplet in the surrounding air was observed, thus the experiments were concluded at the spray axis, instead of continuing across the whole spray. Another effect of this phenomenon, is that the quality of the image taken was inferior, in terms of contrast. Since the post processing has been kept unchanged, this might be reflected in poorer accuracy of the data. Lastly, the suspension of small droplets in the surrounding air for these measurements is likely the cause of the deviation of the average velocity on the outer fringe of the spray seen in Figure II.21 and Figure II.22.

Figure II.11: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm). Experiment at 50 l/h of water at 20 bar of supply pressure.
Figure II.12: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 80 l/h of water at 20 bar of supply pressure.

Figure II.13: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 112 l/h of water at 20 bar of supply pressure.
Figure II.14: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 112 l/h of water-glycerol solution with a viscosity of 3 cP at 20 bar of supply pressure.

Figure II.15: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 112 l/h of water-glycerol solution with a viscosity of 7 cP at 20 bar of supply pressure.
Single droplets plots for all operating conditions

Figure II.16: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 80 l/h of water at 15 bar of supply pressure.

Figure II.17: Single droplet velocities across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 80 l/h of water at 25 bar of supply pressure.
Figure II.18: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 50 l/h of water at 20 bar of supply pressure.

Figure II.19: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 80 l/h of water at 20 bar of supply pressure.
Figure II.20: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 112 l/h of water at 20 bar of supply pressure.

Figure II.21: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 112 l/h of water-glycerol solution with a viscosity of 3 cP at 20 bar of supply pressure.
Figure II.22: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 112 l/h of water-glycerol solution with a viscosity of 7 cP at 20 bar of supply pressure.

Figure II.23: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 80 l/h of water at 15 bar of supply pressure.
Figure II.24: Single droplet trajectory angles across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). The red line represents the geometrical angle formed with spray origin and axis. Experiment at 80 l/h of water at 25 bar of supply pressure.

Figure II.25: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 50 l/h of water at 20 bar of supply pressure.
Appendix II

Figure II.26: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 80 l/h of water at 20 bar of supply pressure.

Figure II.27: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 112 l/h of water at 20 bar of supply pressure.
Figure II.28: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 112 l/h of water-glycerol solution with a viscosity of 3 cP at 20 bar of supply pressure.

Figure II.29: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 112 l/h of water-glycerol solution with a viscosity of 7 cP at 20 bar of supply pressure.
Figure II.30: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 80 l/h of water at 15 bar of supply pressure.

Figure II.31: Droplet diameters across the spray (blue dots), including averages for different size fractions (solid line considers all droplets, dashed line only larger than 40 µm, dotted line larger than 80 µm). Experiment at 80 l/h of water at 25 bar of supply pressure.
II.4 Near nozzle images of droplet breakups

During the testing phase of the experimental setup a number of images was taken to check the positions of the various spray regions and make sure that the measurements were taken after the secondary atomization. Some of the obtained images show details of various breakup mechanisms, such as bag- and ligament-breakup, and are reported here.

Figure II.32: Image obtained with the spray setup at DTU, showing evolving non-spherical droplet.
Figure II.33: Images obtained with the spray setup at DTU, showing liquid break-up before the final droplet size is achieved.
Near nozzle images of droplet breakups

Figure II.34: Images obtained with the spray setup at DTU, showing liquid break-up before the final droplet size is achieved.
II.5 Report on statistical analysis of the early spray data

The work presented in this report was carried out within the PhD course “Introduction to statistics and R” under the supervision of Assistant Professor Andreas Baum of the Department of Applied Mathematics and Computer Science of DTU.

II.5.1 Section summary

The data from a spray characterization setup has been analysed using several statistical methods and tools. The scientific question to be addressed was if the data from experiments at different operating conditions could be considered as having the same mean or as part of a common population. The statistical tools used to answer this question are one-way ANOVA, Kruskal-Wallis and Kolmogorov-Smirnov two-sample tests. During the study it was found that the data sample do not follow a normal distribution. To overcome this issue a series of transformations including log-transformation and Box-Cox transformation were used. All tests that have employed are unanimous in reaching the conclusion that the three groups of samples cannot be considered to belong to the same population or to have the same mean.

II.5.2 Introduction

This work is part of a PhD project to obtain predictive simulations of a full-scale auxiliary marine boiler. One of the main issues in this process is that including the detailed modelling of the atomization requires considerable computational resources. In a mechanistic approach, the spray could instead be modelled as an injection of particles. To use this approach, the size distributions have been obtained for a spillback nozzle mounted on a cold spray setup at three different operating conditions. To use this data in the CFD simulations it is important to have a good understanding of it and of possible simplification when dealing with varying operating conditions.

In this context, the aim of this study is to use statistical tools to assess if the data from experiments at different operating conditions could be considered as having the same mean or as part of a common population.

II.5.3 Data description

The data are collected from images of droplets taken with a spray characterization setup. The setup reproduces a spray used in auxiliary marine boiler to atomize liquid fuel. For the purposes of this study, the spray itself may be imagined as an axisymmetric cone of droplets originating from a single point. An optical system is used to capture images of the moving droplets. This system captures only droplets present in a control volume of 2.41 x 3.24 x 0.86 mm. All measurements have been taken on a plane perpendicular to the spray axis at increasing distances from the center of the spray (5 mm intervals). The distances from the axis are then scaled to accommodate for the change in spray angle at each specific operating condition. As the scaling factor varies for each set of measurements, the scaled measured
position are not aligned. To use comparable data, three points where the scaled positions are within a 5% range had been selected for the statistical analysis (Figure II.35). To summarize, the data considered in this report consist of nine groups of observations: one for each of the three operating conditions, for each of the three chosen measurement positions.

Table II.1: Head of the raw data for one of the samples.

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The data are organized in a data frame (Table II.1) containing droplet diameter (Diam), position in the image’s x- and y-axes (X and Y), velocity magnitude (Vel) and direction (Angle). A further variable called “Load” has been added to data-frame that tells to which of which the three data sets belongs the observation.

As the research questions only concerns the droplet size relationship with varying operating conditions, the other variables can be removed from the data-frame. It should also be noted that while the diameters are positive continuous data, Load is a nominal variable that only represents the group to which the observation belongs, without a particular order.

Figure II.36: Plot of the raw data, colored according to the operating conditions.
Also, in this report the 75% measurement position is used as an example for all plots and results, if not otherwise specified. This is because most of the characteristics, observations and results are valid for all three measurement positions.

II.5.4 Statistical Analyses

In this section, the statistical analyses that have been carried out on the data will be presented. For each type of analysis, the necessary assumption will be declared and discussed, and the eventual results will be reported individually. A more general summary is given in the next section.

II.5.4.1 One-way Analysis of Variance (ANOVA)

It is clear from the research question that the statistical tools to be used should aim at comparing the data from the different groups. One such tool is the one-way analysis of variance or ANOVA. The ANOVA is used to compare means in more than two groups and gives a joint test for any difference between the groups. This is done by comparing the variance between groups to the variance within the groups [1].

Assumptions

The assumptions of the ANOVA test are that:

- The observation are independent from each other
- The data is normally distributed within each group
- The variance is homogeneous for all groups
The first assumption is valid in our case, as all measurement has been taken so that each single droplet was measured only once and all precautions were taken so that the measurements are separate and independent.

To check for data normality Q-Q plots of the data have been observed (Figure II.38). It is clear that the untreated data does not follow a normal distribution. Using a logarithmic transformation lead to a distribution much closer to the normal. Still the normality assumption is not completely fulfilled, due to the differences in the distribution’s tails.

Lastly, the assumption of variance homogeneity has been tested. Using only graphical means (Figure II.39) the assumption could have been considered valid, the results from the Levene’s test report for all measured positions a p-value $< 10^{-3}$, thus rejecting the null-hypothesis of homoscedasticity.

Results and discussion

Even if log-transforming the data led to a distribution more close to the normal, since both the assumption of normally distributed data and that of variance homogeneity do not apply to our data, the ANOVA cannot be used.
II.5.4.2 Box-cox transformation

The Box-Cox transformation is a tool used to obtain distributions closer to normality in non-normal dependent variables and, as seen in the previous paragraph, the normality of the distribution is a prerequisite to analyze data with ANOVA. The Box-Cox transformation has been developed especially to be able to run a broader range of tests on statistical data.

The transformed data is found applying the following formula:

\[
Diam_{boxi} = f(Diam_i) = \frac{Diam_i^\lambda - 1}{\lambda} \quad [\text{Eq. 1}]
\]

The transformation is based on the correct estimation of the parameter (\(\lambda\)) so that the new distribution of the dependent variable (Diam in our case) is as close as possible to normal. For further details about the parameter estimation, the reader is referred to the original publication [2].

Table II.2: Skewness and Kurtosis comparison.

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</table>

Normality tests

After using the transformation, the data has been stored as a new variable (\(Diam_{box}\)) and tested for normality. From Table II.2 is evident that the calculated skewness and kurtosis are much closer to those of a normal distribution and within the limits used in [3].

Figure II.40: Q-Q plot and comparison with normal distribution for Box-Cox transformed data.

To observe the normality graphically a histogram of the transformed data was compared with the normal distribution and also a Q-Q plot was considered (Figure II.40). Aside from some small trends in the tails of the distribution, both plot seem to match the normal distribution quite well.
As a last test for normality, it has also been used the Shapiro-Wilk test. This showed that while the null hypothesis of the test was rejected in all cases, it was observed that the test result is highly dependent on sample size. To have a better understanding of this the test was run for 100 subset each taken without replacement from the data, for 100 sample sizes equally spaced from 50 to 5000. The resulting p-values have been plotted as a series of box plots for each sample size (Figure II.41). In all cases, it was evident that the Box-Cox transformed data performed better than the log-transformed and of the raw data. Also for all three positions, the null-hypothesis cannot be rejected for sample sizes < 1000.

ANOVA on Box-Cox transformed data

The same considerations and assumptions stated for ANOVA in the previous section apply also here. To check for variance homogeneity, a Levene’s test has been used, obtaining a p-value of 10^{-4}, and even if this value is well below 5%, it was deemed appropriate to use ANOVA, while still keeping some reservation on its results. This is because ANOVA is considered a robust test [4], and the normality assumption has been partially justified in the previous paragraph for the Box-Cox transformed data.

Results and discussion

The ANOVA run on a linear model for the transformed data found an F >30 for all three positions. The F value is a representation of the ratio between the variance between the groups to the one within each group. In all cases the test probability represented by the p-value is found to be <<10^{-10}. Therefore, the null hypothesis of equal means for all three groups is rejected. Lastly, a pairwise comparison has been carried out between the three groups. This showed that the null hypothesis of equal means is rejected in all cases (pairwise p-value <0.05), but one. That is when considering solely group 1 and 2, for the measurement taken at a scaled distance of 75% from the spray axis. The comparison was done both with and without the Bonferroni correction obtaining the same results for all cases. This result is confirmed by observing that the 95% confidence intervals for the mean obtained with the linear model are overlapping in the specific case of group 1 and 2 at 75% position.
II.5.4.3 Kruskal-Wallis non-parametric Test

The Kruskal-Wallis test is a non-parametric test to assess if the mean ranks of different groups of data are the same. While the information gained from such test is much less than what a one-way ANOVA, if the null-hypothesis of equality of mean rank is rejected, it would also mean that the different groups cannot be considered as belonging to the same population. It is quite common to use the Kruskal-Wallis test when dealing with a categorical variable and a numerical variable, but the latter does not meet the assumption necessary for the ANOVA [4].

Assumptions

Non-parametric tests are tests that do not assume that data samples can be described solely based on parameters, such as standard deviation and median or mean, and therefore do not require the data to approximate any specific distribution. The assumptions of the test are that:

- The sample are mutually independent.
- The measurement scale is at least ordinal.
- If the test is used as a test of dominance, it has no distributional assumptions. If it used to compare medians, the distributions must be similar apart from their locations.
- The test is generally considered to be robust to ties. However, if ties are present they should not be concentrated together in one part of the distribution (they should have either a normal or uniform distribution).

The first, second and fourth assumption are justified by the nature of the data itself. Regarding the third, it is possible to refer to literature on spray and atomization [5] for general considerations on the nature of size distributions. Nevertheless, it is important to acknowledge that such assumption should be validated for the specific dataset at hand and therefore the results obtained with the Kruskal-Wallis test could be not completely accurate.

Results and discussion

The null hypothesis is rejected for all three positions with p-values <<10^{-10}. When instead the test is applied excluding in turns one of the groups, thus checking that the mean ranking is the same between groups 1+2, 2+3 and 1+3, it is observed that the null hypothesis is not always rejected for groups 1+2. In fact, the corresponding p-values at positions 0%, 75% and 125% are respectively 0.026, 0.044 and 0.0013. The p-values for groups 2+3 and 1+3 are again <<10^{-10}. This shows that the change in operating conditions from group 1 to 2 have a possibly negligible influence on droplet size distribution, while the change to group 3 has a greater effect on it. Also, as the Box-Cox transformation does not alter the order of the observations, the results from a Kruskal-Wallis test are the same for raw and transformed data.

II.5.4.4 Kolmogorov-Smirnov two-sample Non-parametric test

The Kolmogorov-Smirnov test is another non-parametric test and it can be used to compare a data sample with a reference distribution (one-sample K-S test) or with another data sample (two-sample K-S test). It is reported as one of the most useful and general non-parametric tests. This is because it is sensible to both location and shape of the sample distribution [6]. The null hypothesis of the two-sample test is that the sample are drawn from the same (or identical) populations.
Assumptions

The consideration on non-parametric tests done for the Kruskal-Wallis test are of course valid also in the case of the Kolmogorov test. The assumptions for the two tests are also the same, aside for the third one that is not necessary. Therefore, all the assumptions for the Kolmogorov test are met.

Results and discussion

As the test can only compare two samples, it has been used separately on groups 1+2, 2+3 and 1+3 for each of the measurement positions. The null hypothesis is rejected in all cases. Notably, the p-values for groups 1+2, while being <<5%, are several orders of magnitude higher than the ones obtained for the other groups. This is true for the tests in all measurement positions.

II.5.5 Conclusions

The data from a spray characterization setup has been analyzed using several statistical methods and tools. The scientific question to be addressed was if the data from experiments at different operating conditions could be considered has having the same mean or as part of a common population.

One of the main challenges of this analysis has been that the data is inherently non-normally distributed and that the sample variance is not homogeneous. This was proved using the Levene’s test and Q-Q plots of the raw and log-transformed data. Also, it meant that the one way ANOVA could not be applied.

To overcome this issue the Box-Cox transformation has been employed and the data thus obtained was tested for normality. The outcome of this test has not been univocal. In fact, while the transformed data presented the appropriate values for skewness and kurtosis, and passed a graphical observation both using histograms and Q-Q plots, it could not pass the Shapiro-Wilk test. Regardless some uncertainty on its assumptions ANOVA has been applied to the transformed data. To check the results thus obtained, also two non-parametric tests have been employed: the Kruskal-Wallis test and the Kolmogorov-Smirnov two-sample test.

The result of all the tests are summarized in Table II.3. All tests agree that the three groups cannot be considered to belong to the same population (in the table shown as an X). It is also notable that in all tests when considering only groups one and two the p-values were several order of magnitude higher (blue X) and in a few cases also significant (green V). This means that the effect on droplet size distribution of changing operating condition from group 1 to group 2 are not as pronounced as the change to group 3.

Table II.3: Summary of the statistical analyses. X=null hypothesis rejected, V=null hypothesis could not be rejected.

<table>
<thead>
<tr>
<th>Position</th>
<th>0%</th>
<th>75%</th>
<th>125%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Groups</td>
<td>1+2+3</td>
<td>1+2</td>
<td>2+3</td>
</tr>
<tr>
<td>ANOVA</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>Box-Cox ANOVA</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Kruskal-Wallis</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Kolmogorov-Smirnov</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>
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II.5.6 References

[1] Lecture slides, One and Two-way Analysis of Variance, Elisabeth Wreford Andersen.


II.5.7 R Code used

The R code used in the project is given below. The data files necessary to reproduce the analyses can be obtained by contacting the author:

```r
setwd("C:/Users/gioc/Desktop/roba part analysis/matlabmio/excel-files")
# uncomment acquisition lines depending on necessity
radialdist<="75perc"
table33<-read.table(sprintf("33-36a-%s-data.dat",radialdist), sep="", dec=".")
table66<-read.table(sprintf("66-36a-%s-data.dat",radialdist), sep="", dec=".")
table100<-read.table(sprintf("100-36a-%s-data.dat",radialdist), sep="", dec=".")
#table33<-read.table("33-36a-0r-data.dat", sep="", dec=".")
#table66<-read.table("66-36a-0r-data.dat", sep="", dec=".")
#table100<-read.table("100-36a-0r-data.dat", sep="", dec=".")
#table33<-read.table("33-36a-0r-a-data.dat", sep="", dec=".")
#table66<-read.table("66-36a-0r-a-data.dat", sep="", dec=".")
#table100<-read.table("100-36a-0r-a-data.dat", sep="", dec=".")
Header <- c("X","Y","Diam", "Vel", "Angle")
names(table33)<- Header
names(table66)<- Header
names(table100)<- Header

table33$Load <- "1"
table66$Load <- "2"
table100$Load <- "3"
# uncomment to use only part of the data
#table33<-table33[sample(1:nrow(table33), 1000, replace=FALSE),]
#table66<-table66[sample(1:nrow(table66), 1000, replace=FALSE),]
#table33<-table100[sample(1:nrow(table100), 1000, replace=FALSE),]
#table66<-table100[sample(1:nrow(table100), 1000, replace=FALSE),]
#table100<-table100[sample(1:nrow(table100), 1000, replace=FALSE),]
```

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#table33$vol<-(4*pi/3)*(table33$Diam/2)^3
#table66$vol<-(4*pi/3)*(table66$Diam/2)^3
#table100$vol<-(4*pi/3)*(table100$Diam/2)^3
#table33$Diam<-(4*pi/3)*(table33$Diam/2)^3 #to use volumes instead
#table66$Diam<-(4*pi/3)*(table66$Diam/2)^3
#table100$Diam<-(4*pi/3)*(table100$Diam/2)^3
tableOr<- rbind(table33, table66, table100)
#first plots to look at the data and summary
plot(tableOr, col=tableOr$Load)
#plot(tableOr, col=as.factor(1+is.integer(tableOr$Load))) #how to use different colors?
tableOr$X < - NULL #dropping unused variables
tableOr$Y < - NULL
tableOr$Vel < - NULL
tableOr$Angle < - NULL
#tableOr$Diam<-(tableOr$Diam_box) #to do analysis with box-cox transformed data
#tableOr$Diam<-(4*pi/3)*(tableOr$Diam/2)^3 #to use volumes instead
#names(tableOr)<- Header #redundant
par(mfrow = c(2,2), mgp = c(2,0.7,0), mar = c(3,3,2,2)) #residual plots
boxplot(Diam ~ Load, data = tableOr, xlab = 'Load', ylab = 'Diameter', las = 1, col = 1+1:3)
stripchart(Diam ~ Load, data = tableOr, vertical = TRUE, xlab = "Load", ylab = "Diameter", method = "jitter", las = 1, col = 1+1:3)
boxplot(log10(Diam) ~ Load, data = tableOr, xlab = 'Load', ylab = 'log10(Diameter)', las = 1, col = 1+1:3)
stripchart(log10(Diam) ~ Load, data = tableOr, vertical = TRUE, xlab = "Load", ylab = "log10(Diameter)", method = "jitter", las = 1, col = 1+1:3)
par(mfrow=c(1,1))
summary(tableOr)
by(tableOr$Diam, tableOr$Load, summary) #first look at the data divided by load
#checking if data is normally distributed (sums of normal distributions is a normal distribution)
par(mfrow = c(2,2), mgp = c(2,0.7,0), mar = c(4,4,2,2)) #residual plots
qqnorm(tableOr$Diam, main= "Normal Q-Q Plot")
qqline(tableOr$Diam, lty=2, col="red")
qqnorm(log10(tableOr$Diam), main = "Normal Q-Q Plot for log10(Diameters)")
qqline(log10(tableOr$Diam), lty=2, col="red")
qqnorm(sqrt(tableOr$Diam), main = "Normal Q-Q Plot for sqrt(Diameters)")
qqline(sqrt(tableOr$Diam), lty=2, col="red")
par(mfrow=c(1,1))
par(mfrow = c(2,2)) # residual plots
qqnorm(table33$Diam, main = 'Normal Q-Q Plot for Load 1', ylim=c(0,120))
qqline(table33$Diam, lty=2, col="red")
qqnorm(table66$Diam, main = 'Normal Q-Q Plot for Load 2', ylim=c(0,120))
qqline(table66$Diam, lty=2, col="red")
qqnorm(table100$Diam, main = 'Normal Q-Q Plot for Load 3', ylim=c(0,120))

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qqline(table100$Diam,lty=2,col="red")
qqnorm(table0r$Diam , main= "Normal Q-Q Plot", ylim=c(0,120))
qqline(table0r$Diam,lty=2,col="red")
par(mfrow=c(1,1))
table0r$LogD<log10(table0r$Diam)
model1<lm(LogD ~ Load, data = table0r)
anova(model1)
summary (model1)
confint(model1)
qqnorm(residuals(model1),
   ylab="Sample Quantiles for residuals") #qq plot of residuals (to check normal distribution of residuals)
qqline(residuals(model1),
   col="red")
library(car)
leveneTest(model1) #testing variance omogeneity
par(mfrow = c(2,2)) #, mgp = c(2,0.7,0), mar = c(3,3,5,10)) #residual plots
plot(model1, which=1:4)
par(mfrow=c(1,1))
library(MESS)
qqwrap <- function(x, y, ...) {qqnorm(y,main="",...); abline(a=0,b = 1)}
wallyplot(model1, FUN=qqwrap) #not so difficult to guess...
#further look at the data
orderedDiam<sort(table0r$Diam, decreasing = FALSE)
#plot(orderedDiam)

h<-hist(orderedDiam, breaks=100, col="skyblue", xlab="Diamater",
   main="Histogram with Normal Curve", border = F , xlim = c(0,60))
xfit<seq(min(orderedDiam),max(orderedDiam),length=400)
yfit<-dnorm(xfit,mean=mean(orderedDiam),sd=sd(orderedDiam))
yfit <- yfit *diff(h$mids[1:2]) * length(orderedDiam)
lines(xfit, yfit, col="blue", lwd=2)
#truncating the upper part of the data
orderedDiam2<orderedDiam[orderedDiam<=45] #change accordingly to previous plot
qqnorm((orderedDiam2) , main= "Normal Q-Q Plot for the Diameters")
qqline((orderedDiam2),lty=2,col="red")

h<-hist(orderedDiam2, breaks=20,col="skyblue", xlab="Diamater",
   main="Histogram with Normal Curve of truncated data", border = F, ylim = c(0,1200))
xfit<seq(min(orderedDiam2),max(orderedDiam2),length=400)
yfit<-dnorm(xfit,mean=mean(orderedDiam2),sd=sd(orderedDiam2))
yfit <- yfit *diff(h$mids[1:2]) * length(orderedDiam2)
lines(xfit, yfit, col="blue", lwd=2)
#Box-Cox transformation

#1: Transforming the data
library(MASS)
Box = boxcox(Diam ~ Load, data = table0r, lambda = seq(-6,6,0.1))
Report on statistical analysis of the early spray data

```r
Cox = data.frame(Box$x, Box$y)
Cox2 = Cox(with(Cox, order(-Cox$Box.y)),)
Cox2[1,]
lambda = Cox2[1, "Box.x"]
table0r$Diam_box = (table0r$Diam ^ lambda - 1)/lambda
boxplot(Diam_box ~ Load, data = table0r, xlab = 'Load', ylab = 'Box-Cox transformed diameter', col =c(topo.colors(6)))
#2-performing AnOVA and checking residuals
model2 = lm(Diam_box ~ Load, data = table0r)
library(car)
qqnorm(table0r$Diam_box , main= "Normal Q-Q Plot")
qqline(table0r$Diam_box,ty=2,col="red")
leveneTest(model2) #testing variance omogeneity
par(mfrow = c(2,2)) #, mgp = c(2,0.7,0), mar = c(3,3,5,10)) #residual plots
plot(model2, which=1:4)
par(mfrow=c(1,1))
library(MESS)
qqwrap <- function(x, y, ...) {qqnorm(y,main=",,...); abline(a=0,b = 1)}
wallyplot(model2, FUN=qqwrap) #not so difficult to guess...
Anova(model2, type="II")
pairwise.t.test(table0r$Diam_box, table0r$Load, p.adj = "none")
pairwise.t.test(table0r$Diam_box, table0r$Load, p.adj = "bonferroni")
summary (model2)
confint(model2)
x = residuals(model2)
library(companion)
plotNormalHistogram(x) #normal histogram of residuals
plotNormalHistogram(table0r$Diam_box) #normal histogram of residuals
qqnorm(residuals(model2), ylab="Sample Quantiles for residuals") #qq plot of residuals (to check normal distribution of residuals)
qqline(residuals(model2), col="red")
h<-hist(table0r$Diam_box, breaks=20, col="red", xlab="Diamater", #checking out box-cox transformed data
main="Histogram with Normal Curve")
xfit<-seq(min(table0r$Diam_box),max(table0r$Diam_box),length=400)
yfit<-dnorm(xfit,mean=mean(table0r$Diam_box),sd=sd(table0r$Diam_box))
yfit <- yfit*difft(h$mids[1:2])*length(table0r$Diam_box)
lines(xfit, yfit, col="blue", lwd=2)
library(moments)
skewness(table0r$Diam_box) #drastic improvement
kurtosis(table0r$Diam_box)
skewness(table0r$Diam)
kurtosis(table0r$Diam)
#shapiro-wilkins and dependance from sample size
map<-matrix(data=NA, nrow = 100,ncol = 100)
```

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```r
for(i in 1:100) {
  for(k in 1:100) {
    shap<-shapiro.test((table0r[sample(1:nrow(table0r), i*50, replace=FALSE),]$Diam)) #or Diam_box for trasformed
    map[k,i]<-shap$p.value
  }
}

boxplot(log10(map),col=(c(rainbow(200))),xlab="Sample size used/50", ylab="Log10 of Shapiro-Wilkins p-value",ylim=c(-30,0))
lines(c(0,100),c(log10(0.05),log10(0.05)), col="red", lty = 5, lwd=2)
map<-matrix(data=NA, nrow = 100,ncol = 100)
for(i in 1:100) {
  for(k in 1:100) {
    shap<-shapiro.test(table0r[sample(1:nrow(table0r), i*50, replace=FALSE),]$Diam_box) #or Diam_box for trasformed
    map[k,i]<-shap$p.value
  }
}

boxplot(log10(map),col=(c(rainbow(200))),xlab="Sample size used/50", ylab="Log10 of Shapiro-Wilkins p-value",ylim=c(-15,0))
lines(c(0,100),c(log10(0.05),log10(0.05)), col="red", lty = 5, lwd=2)
library(vioplot)

#Kruskal-Wallis Test (non-parametric test)
kruskal.test(Diam ~ as.factor(Load), data = table0r) #as expected result with and without box-cox are the same
kruskal.test(Diam_box ~ as.factor(Load), data = table0r) #this is because the trasformation does not change order of the elements
kruskal.test(Diam ~ as.factor(Load), data = subset(table0r,Load<"3"))
kruskal.test(Diam ~ as.factor(Load), data = subset(table0r,Load>"1"))
kruskal.test(Diam ~ as.factor(Load), data = subset(table0r,Load=="1"|Load=="3"))
library(ggplot2)
ggplot(table0r, aes(Diam, fill = Load)) + geom_histogram(alpha = 0.5, aes(y = ..density..),
  color = "white", position = 'identity', binwidth = 1 )
ggplot(table0r, aes(Diam, fill = Load)) + geom_histogram(alpha = 0.5, aes(y = ..density..),
  color = "white", position = 'identity', binwidth = 1 ) + xlim(0,100)
library(scales)
hist(subset(table0r,Load=="2")$Diam,xlim=c(0,100),col="yellow",breaks = 50,border=F)
hist(subset(table0r,Load=="3")$Diam,add=T,col=scales::alpha('skyblue',5),breaks = 50,border=F)
hist(subset(table0r,Load=="1")$Diam,add=T,col=scales::alpha('red',2),breaks = 50,border=F)
#kolmogorov-smirnov 2 sample test - test to see if samples come from the same population
ks.test(subset(table0r,Load=="2")$Diam,subset(table0r,Load=="1")$Diam)
ks.test(subset(table0r,Load=="2")$Diam,subset(table0r,Load=="3")$Diam)
ks.test(subset(table0r,Load=="1")$Diam,subset(table0r,Load=="3")$Diam)
```
Appendix III.

III.1 Reynolds number in the furnace chamber

To gain an overview on the turbulence inside the boiler, the Reynolds number was calculated from the simulation 40L4O for the computational domain using the local velocity, density and the distance to the closest surface as a characteristic length in the following equation.

\[ \text{Re}_g = \frac{\rho g u D}{\mu_g} \]  

Eq. III.1

In Figure III.1, it is possible to see how the region with the highest Reynolds number corresponds to the flame region, reaching its peak values where the combustion air that passed around the swirling plate is mixed with the central fuel-rich stream. It is also evident that the high Reynolds number in this area is mainly caused by the high velocity of the gas.

---

Figure III.1: Reynolds number on the vertical cross-section of the boiler furnace for the 40L4O simulation.
Appendix III

III.2 Effect of the number of tracked rays in the DTM

During the initial CFD campaign on the first burner design, two simulation has been carried with the same setting and initial conditions, but using a different number of tracked rays for the Discrete Transfer Model, 8 in one and 10 in the other. The results of the two simulations showed no noticeable discrepancy in the fields of velocity, temperature or composition, any difference between the two was smaller than the transient fluctuation on the same values. However, when it was observed that the temperature on the wall in the quarl area (which is an adiabatic wall) presented a pattern showing 8 and 10 stripes with higher temperature, suggesting that this was an artefact caused by the radiation model (Figure III.2). The temperature difference between these bands is most likely small enough compared to the temperature gradients in the boundary layer, that it did not affect the heat exchanged by radiation significantly.

Figure III.2: Temperature on the adiabatic wall in the quarl area for 8 (right) and 10 (left) tracked rays in the radiation model.
III.3 Sensitivity analysis on the reactant limiter of the EDM

A sensitivity analysis has been carried out on the reactant limiter \( A \) of the Eddy Dissipation Model, introduced in equation 6 of chapter 4.2. The same simulation has been run varying \( A \) between 1, 4 and 10. The results of the three simulations are shown respectively in Figure III.3, Figure III.4 and Figure III.5. Here we can see that there is a drastic change in the flame shape and thus in the CO concentration field, with a much shorter flame for \( A=1 \) and a strangely long one for \( A=10 \). The results obtained for \( A=4 \) best reproduced the experimental observations of the flame. For this reason and because it is widely used and recommended in literature, this value was used for further simulations.

Figure III.3: Vertical sections of the instantaneous temperature (top-left), velocity (top-right) and CO concentration (bottom-left) fields in the boiler for a simulation using \( A=1 \). In (bottom-right) the 2\% CO iso-surface is shown to represent the flame shape with fuel droplets in black.
Appendix III

Figure III.4: Vertical sections of the instantaneous temperature (top-left), velocity (top-right) and CO concentration (bottom-left) fields in the boiler for a simulation using $A=4$. In (bottom-right) the 2% CO iso-surface is shown to represent the flame shape with fuel droplets in black.
Sensitivity analysis on the reactant limiter of the EDM

Figure III.5: Vertical sections of the instantaneous temperature (top-left), velocity (top-right) and CO concentration (bottom-left) fields in the boiler for a simulation using A=1.0. In (bottom-right) the 2% CO iso-surface is shown to represent the flame shape with fuel droplets in black.
Appendix III

III.4 Grid independency results

The grid independency study mentioned in Chapter 4 was carried out by observing both local and exhaust gas parameters. All quantities showed a converging behavior with an increase in number of grid elements, showing that a grid with 7 million elements provides a reasonable tradeoff between accuracy and computational overhead.

Figure III.6: Additional outlet conditions plots from the simulations of the grid independency study. Similar trend was observed for CO, which cannot be reported for confidentiality reasons.
Figure III.7: Additional plots for gas temperature and compositions on the burner axis from the simulations of the grid independency study.
III.5 Monitors of simulations with different time step

On top of the analysis presented in chapter 4, an indication of the influence of the time step on the results was gained by repeating the same simulation with increasingly smaller time step. Quantities of interest have been used as monitors during these simulations and showed the same transient behavior when decreasing the time step below 0.5ms.

*Figure III.8: 0.1 ms timestep temperatures monitors.*
Monitors of simulations with different time step

**Figure III.9:** 0.5 ms timestep temperatures monitors.
III.6 Comparison of simulations with different fuel viscosities

The same comparison between CFD simulations and experimental data presented in chapter 4 has been carried out also using a liquid viscosity of 3 cP (Figure III.10). The simulations with the lower viscosity match much better the experimental data.

*Figure III.10: Comparison between experimental data (black dots) and CFD results with a viscosity of 1cP (blue line) and 3cP.*
III.7 Sensitivity analysis on plate slots

During the development of the new burner design, CFD simulations have been run for different swirling plate geometries and the changes they produced in the flame. The change was in the shape of the slots in the plate, which are crucial to impart a tangential component to the combustion air velocity. The simulation showed that both modification achieved the same result on the flow. The tangible effects on the simulation of the use of the modified swirling plate was an increase in the velocities in the recirculation zone and a reduction in the flame length.

![Diagram showing the standard plate, 2x taller slots, and 2x wider slots](image)

*Figure III.11: Tested modification of the swirling plate and effect on the amount of flow through the slots.*
III.8  HFO simulation results

As discussed in chapter 4, the results of the simulation H40-40 (Figure III.12) are almost identical to those of 40L-40 using diesel (Figure 4.13).

*Figure III.12: Vertical sections of the average temperature (top-left), velocity (top-right) and CO concentration (bottom-left) fields in the boiler during the simulation H40L-40. In (bottom-right) the 2% average CO iso-surface is shown to represent the flame shape.*
III.9 Flame lift-off in CFD simulations

Figure III.12 and Figure III.13 show an example of lift off event observed in the CFD simulations: the flame detaches from the recirculation zone and it is carried towards the back wall, where it stabilizes again. In this case, the combustion reactions continue in the recirculation zone.

*Figure III.13: Snapshots of the 2% CO concentration iso-surface from a lift off event.*
Appendix III

Figure III.14: Snapshots of the 2% CO concentration iso-surface from a lift off event.
Several contributions from this work have been presented to the scientific community at international conferences, thus giving the project visibility and providing useful insight to other experts in the field of atomization and combustion:

- Oral presentation at the Nordic Flame Days 2017 conference – Stockholm, Sweden
- Oral presentation at the International Flame Research Foundation 2018 – Sheffield, UK
- Poster presentation at the International Symposia on Combustion 2018 – Dublin, Ireland
- Oral presentation at the conference of the Institute for Liquid Atomization and Spray Systems 2019, Paris – France
- Oral presentation at the Nordic Flame Days 2019 conference – Turku, Finland

The merits of this research were also recognized by the Otto Mønsted Fond that sponsored the participation for three of these conferences.

The work has also been presented in several occasions internally at DTU including at the annual day of the Combustion and Harmful Emission Control, on three editions of the PhD yearbook of the Chemical Engineering Department and during six internal seminars organized from the department. A video introduction to the project has also been chosen to advertise the department to prospecting student through their official social media platform.

The paper “Spillback nozzle characterization using pulsating LED shadowgraphy” resulting from this work has been submitted for publication to the journal Experimental Thermal and Fluid Science. A further publication on the CFD work presented in chapter 4 will also be submitted for publication during the next months.