On the atomization and combustion of liquid biofuels in gas turbines

Towards the application of biomass-derived pyrolysis oil

J.L.H.P. Sallevelt

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Summary

The combustion of liquid biofuels in gas turbines is an efficient way of generating heat and power from biomass. Gas turbines play a major role in the global energy supply and are suitable for a wide range of applications. However, biofuels generally have different properties compared to the conventional fossil fuels. This can lead to various problems when biofuels are directly used in existing installations.

This thesis aims to provide better insights into the combustion of biomass-derived pyrolysis oil in gas turbines. Pyrolysis oil can be produced from non-edible biomass via the fast pyrolysis process. In this process, the organic matter is thermally decomposed under mild conditions ($\sim 500\text{ }^{\circ}\text{C}$, 1 atm) through rapid heating in an oxygen-free environment. The vapors formed in the reactor are subsequently condensed to obtain a combustible liquid as the main product. In comparison to the most common biofuels of the first generation, i.e. bioethanol and biodiesel, pyrolysis oil has advantages regarding cost and environmental benefits. From a technical point of view, however, it is a less favorable fuel due to properties such as a low heating value, high water content, high acidity, high viscosity, increased surface tension and poor stability. Gas turbines therefore need to be modified before they can successfully operate on pyrolysis oil in pure form. One of the essential tasks is to develop a suitable burner for liquid fuels of such low quality. In this thesis, two research objectives have been formulated to support the development of pyrolysis oil combustion technology.

The first objective is to describe the evaporation and flame characteristics of pyrolysis oil. This objective has been addressed by developing a CFD model based on the Euler-Lagrange method in ANSYS Fluent. The modeling approach was first applied to simulate the combustion of ethanol in a modified, downscaled diesel burner of the OPRA OP16 gas turbine rated at 1.9 MW_e . This part of the numerical work can be regarded as a first step to validate the model against experiments and literature. Ethanol is a suitable replacement of pyrolysis oil for this purpose, since it is a single-component, nonviscous, volatile and clean burning biofuel that has been studied more extensively in the past. In the next step, the model was further developed to simulate the full-scale combustion of pyrolysis oil in a burner that was recently designed by OPRA for biofuel applications. The complex composition of pyrolysis oil has been approximated by means of a surrogate fuel containing seven components: methanol, water, acetic acid, acetol, phenol, eugenol and levoglucosan. Each com-

ponent is known to be present in pyrolysis oil and is used to represent a group of constituents with similar properties. The initial mass fractions of the seven components are chosen such that the surrogate fuel matches the volatility, water content, elemental composition and heating value of a typical pyrolysis oil.

The CFD model shows that the peak temperature reached in the combustor is about 200 K lower for pyrolysis oil than for ethanol. This result cannot be fully explained by the lower adiabatic flame temperature of pyrolysis oil, and therefore also relates to the multicomponent evaporation and mixing process in the combustor. Furthermore, it is observed that the pyrolysis oil spray causes a stronger decrease in temperature in the region close to the injection location. More than twice the amount of evaporation heat is required for this fuel, whereas the vapors released during the first half of the droplet lifetime have only a low heating value. Combustion reactions in this region are thus expected to proceed at a low rate. This effect has been observed as a decreased flame stability during experiments with pyrolysis oil in the full-scale burner. The model predicts that the evaporation time of a pyrolysis oil droplet is roughly 60% longer compared to an ethanol droplet of the same size, which is mainly due to the higher density and the high water content (25 wt.%). The impingement of fuel droplets on the liner is therefore a major point of concern, even in such a wide combustion chamber. This is confirmed by burning tests with pyrolysis oil, after which some droplet tracks on the liner indicated an area where fuel could impact on the wall. Insufficient atomization also led to minor coke deposits on the relatively cold parts of the liner surface. The high heating rate predicted for typical drop sizes in a well-atomized spray indicated a low tendency to form secondary char. Experiments showed that char particles indeed hardly appear in the flue gas in case the fuel is injected using an airblast atomizer. The present model appears to describe the main burning characteristics with reasonable accuracy, although further experimental work is required to validate the results in the combustion zone itself.

The second objective is to determine the effect of fuel viscosity on the atomization and combustion in a gas turbine. Given that pyrolysis oil is an unstable fuel, preheating for reducing the viscosity is only possible up to a limited temperature. Pyrolysis oil is therefore more viscous than standard gas turbine fuels, which can deteriorate the performance of the atomizer. This issue has been studied by conducting measurements in sprays and relating these to burning tests in a micro gas turbine.

A test rig is built to visualize the sprays in the near field of the atomizer using high-resolution shadow imaging. The optical system is chosen such that droplets as small as 15 μm can be recognized with sufficient accuracy. The image data is analyzed to determine the spray quality at varying liquid temperatures and pressures on basis of droplets as well as ligaments. Measurements with biodiesel and straight vegetable oil have been performed to examine the spray characteristics for a range of viscosities. In addition, the combined effect of high density and surface tension on the atomization has been evaluated by testing with glycerin. The pressure-swirl atomizer that generated the sprays originates from the micro gas turbine setup that

is used for the combustion tests. The results show that viscous damping strongly affects the primary breakup length. Increasing the viscosity deteriorates the breakup process, so that the liquid film and the ligaments travel further downstream before disintegrating into droplets. However, the influence of viscosity on the mean droplet size in terms of the Sauter mean diameter (SMD) is observed to be insignificant. Regarding the SMD of the spray, a more important role is attributed to the surface tension: the SMDs of the glycerin sprays were 10–30 μm larger compared to sprays of the other liquids at the same pressure. For all tested liquids, the SMDs are found to be sensitive to the injection pressure in the investigated range (10–30 bar).

In order to relate the measured spray characteristics to combustion efficiencies, the same atomizer is used for combustion experiments with a micro gas turbine. Standard diesel, biodiesel and straight vegetable oil are chosen as the test fuels because of their similar chemical properties. This enables to study the effect of viscosity by changing the fuel temperature, with minimum interference of other fuel properties that influence the combustion. The built-in fuel supply system has been replaced by an external system to control the fuel temperature, to easily switch between fuels during operation, and to achieve a constant rotational speed of the turbine at all test conditions. The CO emissions in the exhaust gas were similar for the three fuels when injected at the viscosity of standard diesel at room temperature. In the experiments with biodiesel as well as vegetable oil, the CO emissions increased proportionally with viscosity. Above a viscosity of 9 cP, however, a visible increase in opacity of the exhaust gas indicated that the atomization quality was clearly unacceptable. Since the mean droplet size was found to be rather constant in this viscosity range, it is concluded that the combustion is sensitive to an increase in breakup length. Pyrolysis oil will generally exceed the viscosity limit identified for this configuration, even when preheated. This implies that the application of pyrolysis oil in the unmodified micro gas turbine will fail, regardless of several other properties impeding the combustion process.

The results obtained in this research can be used to formulate a number of guidelines for the combustion of pyrolysis oil in gas turbines. Both the simulations and the experiments point out that the flame tube of a pyrolysis oil combustor must be at least 70% wider than that of a typical diesel combustor to accommodate the increased spray length. The total volume of the primary zone should also be increased because of the lower flame temperature, which results in slower combustion kinetics. The pyrolysis oil flame is characterized by a lower stability due to the limited heat release close to the atomizer. Therefore, the addition of a miscible, volatile fuel such as ethanol or the use of a pilot flame can be necessary to stabilize the combustion, especially at part load. Good atomization, i.e. an SMD of about 30 μm , is essential to limit the spray length and minimize char formation inside the droplets. The use of pressure-swirl atomizers is not advised due to the strong influence of fuel viscosity on the breakup length and the relatively large droplets produced at reasonable injection pressures. Twin-fluid atomizers should be able to provide superior spray quality, in particular for viscous fuels. Still, to prevent the buildup of sediments in

case a minor part of the pyrolysis oil spray impacts on the liner, it is important to maximize the inner surface temperature of the flame tube.

The present study provides insights that may speed up the application of pyrolysis oil or other biofuels in gas turbines. The combustion of pyrolysis oil in gas turbines is technically possible, but requires specially designed combustion chambers and highly effective atomization methods for viscous fuels. Further research is recommended to validate the proposed models in more detail and to improve the understanding of the spray combustion process.

Samenvatting

De verbranding van vloeibare biobrandstoffen in gasturbines is een efficiënte manier om elektriciteit en warmte te genereren uit biomassa. Gasturbines spelen een belangrijke rol in de wereldwijde energievoorziening en zijn geschikt voor een breed scala aan toepassingen. Biobrandstoffen hebben doorgaans echter afwijkende eigenschappen ten opzichte van de conventionele fossiele brandstoffen. Dit kan tot diverse problemen leiden wanneer biobrandstoffen direct worden gebruikt in bestaande installaties.

Het algemene doel van dit proefschrift is om beter inzicht te geven in de verbranding van pyrolyseolie uit biomassa in gasturbines. Pyrolyseolie kan worden geproduceerd van niet-eetbare biomassa via het snelle pyrolyseproces. In dit proces wordt het organische materiaal onder milde condities ($\sim 500^\circ\text{C}$, 1 atm) thermisch ontleed door snelle verhitting in een zuurstofarme omgeving. De dampen die vrijkomen in de reactor worden vervolgens gecondenseerd tot een brandbare vloeistof als hoofdproduct. In vergelijking met de meest gangbare biobrandstoffen van de eerste generatie, d.w.z. bioethanol en biodiesel, heeft pyrolyseolie voordelen als het gaat om kosten en milieu. Vanuit technisch oogpunt is het echter een minder gunstige brandstof vanwege eigenschappen zoals een lage verbrandingswaarde, hoog watergehalte, hoge zuurgraad, hoge viscositeit, verhoogde oppervlaktespanning en matige stabiliteit. Gasturbines zullen daarom moeten worden aangepast om een succesvolle werking op pyrolyseolie mogelijk te maken. Eén van de belangrijkste opgaven is het ontwikkelen van een geschikte brander voor vloeibare brandstoffen van dergelijk lage kwaliteit. In dit proefschrift zijn twee onderzoeksdoelstellingen geformuleerd om de ontwikkeling van verbrandingstechnologie voor pyrolyseolie te ondersteunen.

Het eerste doel is om de verdamping en de vlamkarakteristieken van pyrolyseolie te beschrijven. Voor deze doelstelling is een CFD model ontwikkeld dat is gebaseerd op de Euler-Lagrangemethode in ANSYS Fluent. De modelaanpak is allereerst toegepast om de verbranding van ethanol te simuleren in een aangepaste, teruggeschaalde verbrandingskamer uit de OPRA OP16 gasturbine met een nominaal vermogen van 1.9 MW_e . Dit deel van het numerieke werk kan worden beschouwd als een eerste stap, met als doel het model te valideren op basis van experimenten en literatuur. Ethanol is hiertoe een geschikte vervanger voor pyrolyseolie, aange-

zien het een pure, niet-visceuze en vluchtige brandstof is met een schone vlam, die bovendien tot nu toe veelvuldiger is onderzocht. In de volgende stap is het model verder ontwikkeld om de verbranding van pyrolyseolie te simuleren op ware grootte, in een recentelijk door OPRA ontworpen brander voor de toepassing van biobrandstoffen. De complexe samenstelling van pyrolyseolie is hierbij benaderd door middel van een brandstofmodel bestaande uit zeven componenten: methanol, water, azijnzuur, acetol, fenol, eugenol en levoglucosaan. Elk component is een bekend bestanddeel van pyrolyseolie en wordt hier gebruikt om een hele groep bestanddelen met vergelijkbare eigenschappen te vertegenwoordigen. De initiële massafracties van de zeven componenten zijn zodanig gekozen, dat de gemodelleerde brandstof sterk overeenkomt met een typische pyrolyseolie wat betreft vluchtigheid, watergehalte, elementaire samenstelling en verbrandingswaarde.

Het CFD model toont aan dat de maximale temperatuur die wordt bereikt in de verbrandingskamer ongeveer 200 K lager is voor pyrolyseolie dan voor ethanol. Dit resultaat kan niet volledig worden verklaard door de lagere adiabatische vlamtemperatuur van pyrolyseolie, en is daarom ook gerelateerd aan de niet-gelijktijdige verdamping van de brandstofcomponenten. Het model laat tevens zien dat de pyrolyseoliespray een sterkere afkoeling veroorzaakt in de buurt van de brandstofinspuiting. Om deze brandstof te verdampen is namelijk meer dan twee keer zo veel energie nodig, terwijl de dampen die tijdens de eerste helft van dit proces vrijkomen uit de druppel nauwelijks verbrandingswaarde hebben. De verbrandingsreacties in deze zone zullen naar verwachting dus langzamer verlopen. Het effect hiervan werd tijdens experimenten met pyrolyseolie in deze verbrandingskamer waargenomen als een verminderde vlamstabiliteit. Verder voorspelt het model dat de verdampingstijd van een druppel pyrolyseolie grofweg 60% langer is vergeleken met een druppel ethanol van dezelfde grootte. Dit wordt voornamelijk veroorzaakt door de hogere dichtheid en het hoge watergehalte (25 wt.%). De inslag van druppels op de wanden van de vlamhuis (voering) is daarom een punt van zorg, zelfs in een relatief brede verbrandingskamer. Dit werd bevestigd door de verbrandingsexperimenten met pyrolyseolie, waarna druppelsporen en enige aanslag op de voering een gebied markeerden waar de spray de wanden kon bereiken. Onvoldoende verneveling van de brandstof leidde daarnaast ook tot lichte afzetting van koolstofrijk materiaal op de relatief koude delen van het voeringoppervlak. Het model voorspelt hoge verhitingsnelheden voor typische druppelgroottes in een goed vernevelde spray. Dit wijst op een geringe vorming van secundaire kool in de druppel tijdens de verdamping. De experimenten hebben aangetoond dat zulke kooldeeltjes inderdaad nauwelijks worden aangetroffen in de productgassen in het geval van luchtgeblazen verneveling. Het huidige model lijkt de belangrijkste verbrandingskarakteristieken met redelijke nauwkeurigheid te beschrijven, maar verder onderzoek is nodig om de resultaten te valideren in de verbrandingszone zelf.

De tweede doelstelling is om het effect te bepalen van de brandstofviscositeit op de verneveling en verbranding in een gasturbine. Gezien de thermische instabiliteit van pyrolyseolie is voorverwarming om de viscositeit te verlagen slechts mo-

gelijk tot een beperkte temperatuur. Pyrolyseolie is om deze reden viskeuzer dan de standaard brandstoffen voor gasturbines, wat als gevolg heeft dat de verneveling verslechtert. Deze kwestie is onderzocht door de spraykarakteristieken te meten bij verschillende viscositeiten, en de resultaten hiervan te relateren aan de verbrandingskwaliteit in een microgasturbine.

Een experimentele opstelling is gebouwd om sprays te visualiseren in het nabij veld met behulp van schaduwfotografie. De optiek is zodanig geselecteerd dat druppels met een minimale diameter van 15 μm kunnen worden herkend met voldoende nauwkeurigheid. Het beeldmateriaal is geanalyseerd om de spraykwaliteit op basis van zowel druppels als 'ligamenten' (langwerpige structuren) te bepalen bij verschillende vloeistoftemperaturen en inspuitdrukken. De invloed van viscositeit op de spraykarakteristieken is onderzocht door te testen met biodiesel en plantaardige olie. Daarnaast is het gecombineerde effect van een hoge dichtheid en hoge oppervlaktespanning op de verneveling bepaald door te testen met glycerine. De pressure-swirl verstuiver waarmee de sprays zijn geproduceerd komt uit de microgasturbine die gebruikt is voor het beoordelen van de bijbehorende verbrandingskwaliteit. De resultaten van het sprayonderzoek laten zien dat viskeuze demping voornamelijk effect heeft op de lengte die nodig is voor primaire opbreking van de vloeistof. Dit proces wordt vertraagd bij verhoogde viscositeit, waardoor de vloeistoffilm en ligamenten verder stroomafwaarts kunnen reizen alvorens uiteen te vallen in druppels. De invloed van viscositeit op de gemiddelde druppelgrootte, uitgedrukt in de Sauter mean diameter (SMD), is echter niet significant. Wat de SMD van de spray betreft kan een grotere rol worden toegeschreven aan de oppervlaktespanning: de SMDs van de glycerinesprays waren 10–30 μm groter vergeleken met sprays van de andere vloeistoffen bij gelijke druk. Voor alle vloeistoffen geldt dat de SMDs sterk afhankelijk zijn van de inspuitdruk in het onderzochte bereik (10–30 bar).

Om de gemeten spraykarakteristieken te kunnen relateren aan het verbrandingsproces is dezelfde verstuiver gebruikt voor experimenten met een microgasturbine. Standaard diesel, biodiesel en plantaardige olie zijn gekozen als de testbrandstoffen vanwege de gelijkenis in chemische eigenschappen. Op deze manier kan het effect van viscositeit worden onderzocht door de brandstoftemperatuur aan de passen, terwijl de invloed van andere brandstofeigenschappen op de verbranding tot een minimum worden beperkt. De ingebouwde brandstofregeling is vervangen door een extern systeem om de brandstoftemperatuur en het toerental te kunnen regelen onder alle test condities, en om eenvoudig te kunnen schakelen tussen brandstoffen tijdens bedrijf. Bij een viscositeit gelijk aan die van diesel op kamertemperatuur zijn de gemeten CO emissies voor alle drie de brandstoffen ongeveer hetzelfde. Verhoging van de viscositeit leidt tot een lineaire toename in CO emissies in zowel de experimenten met biodiesel als met plantaardige olie. Boven een viscositeit van 9 cP duidt een zichtbare hoeveelheid rook in de uitlaatgassen op een onacceptabele vernevelingskwaliteit. Aangezien de gemiddelde druppelgrootte in de spray bij deze viscositeiten nagenoeg constant is, kan worden geconcludeerd dat de verbranding vooral gevoelig blijkt voor de opbrekengte van de spray. Pyrolyseolie zal de ge-

vonden viscositeitslimiet in het algemeen overschrijden, zelfs wanneer deze wordt voorverwarmd. Dit betekent dat de toepassing van pyrolyseolie in de microgas-turbine niet mogelijk is zonder verdere aanpassingen. Hierbij zijn een aantal andere eigenschappen die het verbrandingsproces belemmeren nog buiten beschouwing gelaten.

De resultaten die in dit onderzoek zijn verkregen kunnen worden gebruikt om een aantal richtlijnen te formuleren rondom de verbranding van pyrolyseolie in gasturbines. Zowel de simulaties als de experimenten wijzen erop dat de vlambuis in een verbrandingskamer voor pyrolyseolie minstens 70% breder moet zijn ten opzichte van die in een typische verbrandingskamer voor diesel. Hiermee wordt ruimte geboden aan de grotere spraylengte. Het totale volume van de primaire verbrandingszone dient bovendien te worden vergroot om meer verblijftijd te creëren, aangezien de lagere verbrandingstemperatuur resulteert in trage reactiekinetiek. The pyrolyseolievlam wordt gekenmerkt door een lagere stabiliteit vanwege de beperkte warmteproductie dicht bij de verstuiver. Toevoeging van mengbare, vluchtige brandstof zoals ethanol of het gebruik van een waakvlam kan daarom noodzakelijk zijn om de verbranding te stabiliseren, vooral bij lagere bedrijfslasten. Een goede verneveling, d.w.z. een SMD van rond de 30 μm , is essentieel om de spraylengte te beperken en om de vorming van vaste kooldeeltjes te minimaliseren. Het gebruik van pressure-swirl verneveling wordt afgeraden, gezien het sterke effect van viscositeit op de opbreek lengte en de relatief grote druppels die worden gevormd bij gematigde inspuitdrukken. Tweefasenverneveling zou een superieure spraykwaliteit kunnen leveren, vooral in het geval van viskeuze brandstoffen. Niettemin is het belangrijk om de binnenwanden van de vlambuis zo hoog mogelijk te houden ter voorkoming van brandstofafzettingen op het oppervlak.

Deze studie geeft inzichten die de toepassing van pyrolyseolie of andere bio-brandstoffen in gasturbines kunnen versnellen. De verbranding van pyrolyseolie in gasturbines is technisch mogelijk, maar vereist speciaal ontworpen verbrandingskamers en zeer effectieve vernevelingstechnieken voor viskeuze brandstoffen. Nader onderzoek is aanbevolen om de voorgestelde modellen in meer detail te valideren en om de verbranding van sprays verder te doorgronden.

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Chapter 1

Introduction

1.1 The renewed interest in biomass as a fuel

The large-scale exploitation of fuels from fossil carbon reserves starting around 1850 gave rise to a drastic change in the worldwide energy supply. Biomass resources were rapidly replaced by fossil fuels such as coal and crude oil, which contained more energy and allowed for more efficient heat and power generation. The availability of large amounts of cheap energy boosted the industrialization process ongoing in many countries and provided the conditions for reaching the high standard of living in today's modern societies.

At present, however, most of the developed countries strive to reduce the consumption of fossil fuels for several reasons. Firstly, it is evident that fossil energy sources are finite and increasingly scarce ('economics'). Although the total proven reserves of oil, gas and coal are sufficient for many years, it is nevertheless expected that fossil energy becomes expensive in the near future due to depletion of reserves that are easily accessible. The second reason is the increasing dependency of a nation's energy supply on foreign reserves ('security of supply'). These resources are geographically concentrated in regions that are generally not controlled by the countries with the highest energy demand. A third issue is the large contribution of fossil fuel combustion to the global climate change ('environment').

Due to these concerns related to fossil energy, there is a strong interest in diversification of the energy mix by developing sustainable alternatives. Biomass is one of the suitable alternatives that can play a significant role in this shift. Raw biomass can be converted into biofuels that allow for efficient heat and power generation in the current or in future energy systems. Since the feedstock material of biofuel production is renewable and can be supplied from a variety of local sources, these fuels are attractive for improving the national energy security. Biofuels are furthermore effective in reducing CO₂ emissions as they are essentially carbon neutral. Depending on the conversion method and the type of feedstock, biofuels can be obtained in solid,

liquid or gaseous form. Among these, liquid biofuels are of special interest because they are easily transportable and are characterized by a high energy density.

1.2 A general introduction to pyrolysis oil

The vast majority of the liquid biofuels currently used worldwide are categorized as biofuels of the first generation, which are typically derived from the edible parts of food crops. The sugars, starch or vegetable oils contained in these crops are converted into fuels via conventional, relatively simple technologies. First generation biofuels are nowadays applied as transportation fuels on a large scale in the form of bioethanol or biodiesel. These fuels are mostly mixed with a large excess of conventional fuel to prevent technical failures in unmodified vehicles.

It is important to note that first generation biofuels have been criticized because of their potential effect on food prices, the intensive use of agricultural resources for growing the crops and several related issues [30, 35, 43, 63, 70, 108]. The sustainability and environmental performance of these fuels are therefore considered to be questionable. In the past few decades, however, several technologies have been developed to produce fuels from inedible types of biomass. Such biofuels of the second generation are largely derived from lignocellulosic materials, which are most abundantly available, relatively cheap and not related to the food chain. The source materials are moreover used efficiently by converting all main components of the feedstock into useful products. Possible feedstocks are agricultural and forestry residues and industrial waste streams, but may also include dedicated non-food crops if the cultivation is regulated and monitored according to strict sustainability criteria [35, 43].

Second generation biofuels are thus preferred above those of the first generation regarding cost and environmental benefits. However, the production of liquid fuels from non-food materials is technically much more challenging and requires more advanced thermochemical conversion methods. One of the most recent and viable technologies for converting lignocellulosic biomass into a liquid fuel is the fast pyrolysis process [7, 22, 79, 104]. Fast pyrolysis refers to the thermochemical decomposition of biomass through rapid heating in an inert atmosphere under mild conditions ($\sim 500\text{ }^{\circ}\text{C}$, 1 atm). When subjected to high heating rates for a short period of time, the macromolecules that make up the organic material (cellulose, hemicellulose and lignin) are cracked to form a wide range of smaller fragments. This process converts the biomass largely into vapors, of which the majority can be condensed to obtain a liquid product referred to as pyrolysis oil (Fig. 1.1). With a yield of typically 50–75 wt.% of the original feedstock, pyrolysis oil is the main product. The remaining mass is recovered as charcoal and non-condensable gases, which can be burned to provide the heat required for the endothermic decomposition reactions or converted into usable products [22].

To date, however, the application of biomass-derived pyrolysis oil as a second

Property	PO	Diesel
Density (kg/L)	1.1–1.3	0.83
Viscosity (cP, 40 °C)	15–300	2–4
LHV (MJ/kg)	13–19	43
pH	2–3	–
Water content (wt.%)	15–30	< 0.02
Solids content (wt.%)	< 0.5	0.01
Elemental analysis		
C (wt.%)	37–55	86
H (wt.%)	6–8	14
O (wt.%)	39–55	< 0.5

Figure 1.1 & Table 1.1: Typical appearance of wood-derived pyrolysis oil [47] and some of its properties compared to diesel (EN 590) [17, 22, 74, 110].

generation biofuel has been very challenging. The difficulties arise from the fact that, in contrast to what the term ‘oil’ might suggest, the composition of pyrolysis oil is not similar to that of conventional fuel oils [22, 90, 91, 96, 110]. Whereas conventional fuels are specific fractional distillates of petroleum and contain only hydrocarbons, the fast pyrolysis of biomass results in a complex mixture of mostly oxygenated compounds. In addition to 15–30 wt.% of water, which is the most abundant constituent, pyrolysis oil contains hundreds of compounds which can roughly be divided into ketones, aldehydes, alcohols, phenols, organic (carboxylic) acids, furans, sugars and pyrolytic lignin. Given the large number of components and the presence of high molecular weight molecules, it proved hard to determine the exact composition. However, a major part of the chemical composition of pyrolysis oils from different suppliers has been revealed in a few thorough studies [18, 90, 112]. It is clear that largely the same components are identified in the different oils, but that their quantities can deviate significantly. The variation in composition depends on many factors, including biomass type, feedstock pretreatment, process conditions and condensing parameters [96, 145]. The oil’s age and storage temperature have influence as well, since the liquid is not in thermodynamic equilibrium due to rapid quenching of the vapors released during pyrolysis [15, 42]. The composition of this biofuel is therefore not well-defined. Nevertheless, it can be stated that all fast pyrolysis oils derived from biomass have very different properties with respect to fuels derived from fossil sources. This is illustrated by Table 1.1, which compares typical properties of wood-derived pyrolysis oil and No. 2 diesel. As some of these properties have impact on the processes occurring in spray combustion applications, major problems can be expected when pyrolysis oil is used in existing combustion installations.

1.3 The application of pyrolysis oil in gas turbines

An attractive way of generating power and heat from pyrolysis oil is via combustion in gas turbines. Stationary gas turbines such as shown in Fig. 1.2 are widely used for converting energy in both large and small scale power plants around the world. In a gas turbine, heat is added to a compressed air stream by burning fuel in one or more internal combustion chambers. The mixture of hot combustion products and excess air is subsequently directed to a turbine, where the gas flow expands while producing shaft work. A large part of this mechanical power is used to drive the compressor, while the remaining power is used to drive a generator for electricity production. Depending on the combustor design, a gas turbine can operate on gaseous or liquid fuels. In the latter case, the fuel is sprayed into the chamber using an atomizer and evaporates in the hot combustion environment. The fuel vapors released from the droplets mix with air and are ignited by recirculated combustion gases in order to sustain a stable flame.

Figure 1.2: The OPRA OP16 all-radial, single-shaft industrial gas turbine rated at 1.9 MW_e [115].

The combustion sections of existing gas turbines are carefully designed for a specific range of petroleum-based fuels with similar properties. Alternative fuels which do not comply with the standard specifications are hence likely to cause problems related to the spray formation, the evaporation or the combustion kinetics. This holds in particular for pyrolysis oils, which have multiple physical and chemical properties that together tend to have an adverse effect on all of these key processes in a gas turbine [22, 39, 90, 91]. The most important differences with standard fuel oils in this regard include the high water and oxygen contents, wide volatility distribution and high viscosity.

From the abovementioned properties, only the viscosity can be adapted without changing the composition of the raw product, thereby adding significant cost. As for any other liquid, the viscosity of pyrolysis oil is a strong function of temperature and therefore can be reduced simply by preheating. A low viscosity is required to produce a fine spray, because viscous forces dissipate the instabilities induced by the atomizer and by aerodynamic forces to break up the fuel stream into small droplets. As the spray characteristics control the evaporation time as well as the mixing of fuel and air in the combustion zone, the viscosity is a key parameter in liquid fuel combustion. Unfortunately, there are two factors that restrict the maximum temperature of pyrolysis oil. In the first place, it is known that strong preheating sets off polymerization reactions as the oil is in a non-equilibrium state [15, 42, 90, 111, 126]. At elevated temperatures, the oil becomes increasingly reactive due to its high oxygen content. Secondly, the presence of water and components with a low boiling point can result in vapor formation in the fuel line at high oil temperatures [90, 143]. Since these phenomena may lead to problems with the fuel supply, pyrolysis oil is generally preheated in the fuel line to a maximum temperature of 80–90 °C in order to avoid any undesired changes in physical and chemical state [32, 67]. At such temperatures, pyrolysis oils can still exceed the standard viscosity levels for gas turbine injection systems.

The poor thermal stability should also be highlighted as a major complicating factor once the pyrolysis oil is sprayed into the combustor. Solid matter can be formed inside the droplets during the evaporation process [31, 126, 143], which results in char particles that require long burnout times and potentially cause damage to certain turbine components. However, previous studies [31, 126] showed that the char-forming tendency of the droplets reduces with higher evaporation rates. This implies that, despite the unfavorable viscosity of the oil, fine atomization must be achieved to minimize the presence of solid particles in the combustion gases. A well-atomized spray furthermore decreases the risk of coke formation on the combustor walls due to incomplete evaporation of the fuel.

Pyrolysis oil combustion experiments in gas turbines or stand-alone combustors have been performed by a small number of researchers. Modifications to the fuel supply and injection systems were often required to account for the lower calorific value, increased viscosity, acidity and potential solids content. In general, it was shown that unmodified burners normally used for diesel do not allow for efficient operation on this biofuel [10, 11, 32, 138]. Reported issues included high emissions of carbon monoxide (CO) and unburned hydrocarbons (UHC) as well as burning particles leaving the combustor as sparks. Furthermore, carbon-rich deposits were found on the combustor walls, see Fig. 1.3, and on the turbine blades. In one of the test campaigns, it proved impossible to sustain combustion even when the pyrolysis oil was mixed with an alcohol and besides preheated to improve its properties [118]. Experiments with modified combustion chambers showed far more promising results. Pure pyrolysis oil was successfully applied in an industrial gas turbine rated at 2.5 MW_e after redesigning the flame tubes, the fuel supply system and the atomizer

Figure 1.3: Typical fuel residues found in an unmodified combustion chamber after burning pyrolysis oil [11, 118].

[97, 122]. Strong preheating of the oil was still required, though, and the build-up of deposits could not be prevented. An online cleaning system using crushed nut shells was installed to remove the deposits from the hot section components during operation. In another study [10], it was found the combustion efficiency drastically improved by removing the wall film cooling, providing a larger combustion volume and by changing the air split to obtain higher temperatures in the primary zone. No fuel sediments were observed on the combustor walls after these modifications.

The experimental campaigns with (mixtures of) pyrolysis oil are essential for the progress in combustor development. Nevertheless, the phenomena that occur in these experiments are complex and depend on many parameters. To get a more profound understanding of the burning behavior of biofuels such as pyrolysis oil, there is a need for more knowledge and experience regarding the effect of certain fuel properties on the combustion.

1.4 Research objectives

The work presented in this thesis is part of the BE2.O program [144]. This joint program of the Province of Overijssel, the University of Twente and regional companies aims to accelerate the use of bioenergy by stimulating innovation. In one of the research projects, the University of Twente cooperated with the industrial partners OPRA Turbines and BTG-BTL in the development of gas turbines suitable for biomass-derived pyrolysis oil.

Previous test campaigns have shown that the use of pyrolysis oil in existing burners leads to poor combustion. In this thesis, the effects of typical pyrolysis oil properties on the atomization and combustion process are investigated using both numerical and experimental methods. The main purpose is to provide better insights in order to facilitate the development of new combustor designs. Two objectives have been formulated in relation to this goal.

The first objective is to describe the evaporation and flame characteristics of pyrolysis oil. This objective will be accomplished by using a numerical approach. CFD modeling is extensively used in the design and optimization of combustion installations today, but models that include the characteristics of pyrolysis oil are still in an early stage of development. This part of the thesis is closely related to the simultaneous development of combustion hardware for biofuels within OPRA.

The second objective is to determine the effect of fuel viscosity on the atomization and the combustion in a gas turbine. The limited possibility to lower the viscosity of pyrolysis oil via preheating can result in inferior atomization. However, there is insufficient knowledge about the sensitivity of the combustion process to a change in spray quality that may occur due to an increase in fuel viscosity. This question will be addressed by relating combustion tests with a micro gas turbine to the spray characteristics in the near field of the atomizer.

1.5 Thesis outline

The research performed to achieve the objectives defined in the previous section has been divided into four parts, which are each described in a separate chapter.

Chapter 2 deals with the CFD modeling of ethanol spray combustion in a modified, down-scaled diesel combustor. Ethanol has been chosen as a single-component reference fuel for combustion simulations with the multicomponent pyrolysis oil and is a suitable fuel for validation purposes.

Chapter 3 describes a CFD model for the combustion of a typical pyrolysis oil. Comparative simulations with pyrolysis oil and ethanol illustrate the differences in the evaporation and flame characteristics.

Chapter 4 presents an experimental study on the atomization of viscous liquids. A test rig has been developed to visualize sprays in the near-field of the atomizer using high-resolution imaging. The image data is used to determine the spray structure at varying liquid temperatures and pressures in a region that is relevant for combustion applications.

Chapter 5 relates the measured effect of viscosity on the spray to combustion efficiencies in a micro gas turbine. Using the same atomizer, the gas turbine is operated on fuels with varying viscosity while monitoring the exhaust gas emissions.

Chapter 6 summarizes the conclusions drawn in the previous chapters and provides recommendations for future research.

Chapter 2

CFD modeling of ethanol combustion

Abstract

The combustion of ethanol in a modified OPRA OP16 gas turbine burner has been modeled using a CFD approach. Simulations are performed in ANSYS Fluent for five different equivalence ratios. The model is based on a steady-state RANS code for the gas phase and an unsteady particle tracking method for the fuel spray. Detailed combustion chemistry is included by using the steady laminar flamelet model. Combustion tests with ethanol have been performed to obtain validation data for the CFD model and to investigate the combustion of ethanol with respect to diesel as the standard fuel. The experiments are conducted in a test rig at atmospheric pressure for a thermal input ranging from 29 to 59 kW. Exhaust gas temperature and emissions (CO , CO_2 , O_2 , NO_x) were measured at various fuel flow rates while keeping the air flow rate and air temperature constant. The temperature profile of the combustor liner has been determined by applying thermochromic paint. Visual data of the flame zone has been obtained using digital imaging with and without a CH radical filter. The CFD model provides good predictions of the air distribution over the combustor and of CO_2 and O_2 concentrations in the exhaust gas. NO_x emissions are found to be in fair agreement. Validation of the predicted evaporation rates and the spray length indicates that the discrete phase model gives acceptable results. Comparison between the burning tests with ethanol and diesel shows that CO emissions are similar, but NO_x emissions are lower for ethanol.

This chapter is adapted from the publication:

J.L.H.P. Sallevelt, A.K. Pozarlik, M. Beran, L.-U. Axelsson, and G. Brem. "Bioethanol Combustion in an Industrial Gas Turbine Combustor: Simulations and Experiments". In: J Eng Gas Turb Power 136.7 (2014).

2.1 Introduction

To reduce the consumption and emissions of fossil fuels, the interest in the application of biofuels for the generation of power and heat is growing. This trend will result in the need for gas turbine combustors that are capable of handling non-conventional fuels, which often have different physical and chemical properties from those of fossil fuels. It is therefore important to investigate how the use of such novel fuels affects the quality of combustion. Among the biofuels that are considered to be applicable in gas turbine engines, ethanol produced from biomass sources is seen as a promising alternative. Bioethanol is currently the most widely used biofuel in the world as it has been employed as a transportation fuel since many decades, in both blended and pure form [6].

In the literature, only little data is available regarding the combustion behavior of pure ethanol in gas turbines. However, the few experimental studies conducted so far confirm the technical feasibility. Tests with ethanol in a 2.5 MW_e industrial gas turbine were conducted at various loads [97, 122]. The equipment ran stably and the normalized CO and NO_x emissions were measured to be low for all conditions. Emissions of SO₂ were negligible, as sulfur is naturally absent in bioethanol. These results are in agreement with the findings of Moliere et al. [106], who carried out a preliminary characterization of the combustion of naphtha/bioethanol blends with up to 95% ethanol. All blends showed excellent combustion performances, with low NO_x emissions and virtually zero emissions of CO, UHC and SO_x.

To reduce the relatively high cost associated with anhydrous ethanol, Breaux and Acharya [20] studied the effect of elevated water content on swirl-stabilized ethanol/air flames. Their test results indicated that hydrous ethanol with up to 20% water can be used for continuous flame applications. The water reduced the peak flame temperatures and therefore also NO_x emissions, while negative effects on combustion efficiency or flame stability were measured to be insignificant.

A numerical study has been performed by Laranci et al. [80] to investigate ethanol as a fuel for a micro gas turbine with an annular combustion chamber. The ethanol enters the computational domain as droplets with a diameter of 120 μm, after which the fluid dynamics and vaporization are tracked by a Lagrangian solver. The article reports preliminary simulation results in terms of temperatures, pressures and emissions. These results have not been validated because experimental data from the combustion chamber was only available for natural gas combustion. Nevertheless, there seem to be inconsistencies in the calculated emission data, so that the reliability of the presented preliminary data can be questioned.

In the present study, the application of ethanol as a biomass-derived fuel has been examined both numerically and experimentally in modified OPRA's 2 MW class OP16 gas turbine combustor. A commercial CFD code is used to simulate the ethanol combustion process at different operating points based on reduced chemical kinetics. Experiments in an atmospheric test rig have been performed to obtain data for validation of the CFD results and to evaluate the combustion quality of ethanol

Figure 2.1: Scheme of the test rig and the location of sensors.

with respect to diesel.

2.2 Experimental methods

The experimental work has been conducted with a modified, downscaled OP16 gas turbine combustor. This reverse-flow tubular combustor is mounted in an atmospheric test rig as schematically shown in Fig. 2.1. Thermocouples are used to measure the temperature of the injected fuel, the inlet air and the exhaust gases. The pressure sensor in the top left is used to measure the pressure loss in the combustor. Continuous samples were taken from the exhaust gas to measure its composition during the tests. Concentrations of CO_2 and O_2 have been determined with an ADC 5000 analyzer, oxides of nitrogen with a Thermo Model 42C and CO levels with a Thermo Model 48C.

The experimental procedure started by establishing a stable air flow of 75 g/s at a constant temperature. After preheating of the setup by burning fuel for at least 15 min, a series of experiments have been performed at atmospheric pressure with a thermal input ranging from 29 to 59 kW. Once steady state conditions were reached at a certain fuel flow rate, all sensor data were logged using data acquisition software and emissions were read from the gas analyzer displays.

Thermochromic paint has been applied to determine the temperature profile on the liner for ethanol combustion with a fuel input of 43 kW. To assure an adequate sensitivity of the paint to temperature changes, several different types of paint have been applied. The paint colors have been visually inspected to determine the temperature range at each location on the liner surface.

The air flow, fuel flow and combustor inlet temperature were measured with

an accuracy of $\pm 0.7\%$, $\pm 2.4\%$ and $\pm 1.5\%$, respectively. The calibration sheet of the exhaust gas thermocouples reports a maximum error of $\pm 0.27\%$. However, these thermocouples were not shielded during the measurements. Comparative tests with a shielded thermocouple showed that the unshielded sensors give up to 10% higher values due to radiation from the flame. The emissions have been analyzed with an estimated accuracy of ± 0.25 pp for CO_2 , ± 0.5 pp for O_2 and ± 2 ppmv for both NO_x and CO.

2.3 Numerical methods

The numerical study has been performed by using the Euler-Lagrange approach in ANSYS Fluent [52]. In this approach, the fuel spray is considered as a discrete liquid phase travelling in a continuous gas phase. Parcels, representing fuel droplets with similar properties, are tracked throughout the domain while they interact with the surrounding gas. The RANS equations governing the gas phase are coupled with a non-premixed combustion model to include detailed flame chemistry. The models describing the gas phase, fuel spray and chemical reactions are discussed in the following sections.

2.3.1 Computational domain

In order to limit the computational cost, a 45° slice of the combustor geometry is taken as the flow domain. The combustor is not fully rotationally symmetric, however, because the number of circumferentially distributed air admission holes are not always divisible by 8 at all axial locations. Hence, the original geometry had to be modified to allow for the use of periodic boundary conditions in the CFD code. The required symmetry was achieved by changing the number of air admission channels at two locations in the nozzle from 7 to 8 and from 14 to 16, respectively. The total inlet area of these flow passages has been preserved to minimize the influence of these changes on the air split. Since the nozzle air streams are collected in shared volumes first, any differences in the local flow field inside the nozzle will be hardly noticeable at the nozzle outlet annuli. The computational domain is extended by 50 mm to reduce the effect of the outlet boundary condition in the calculations.

The domain has been spatially discretized using an unstructured tetrahedral grid with two to three layers of prisms at the flow boundaries. Three grids have been tested to examine grid dependency of the solution. The coarse, medium and fine grid respectively consisted out of 1.45, 2.60 and 3.21 million cells. In all grids, 8 to 12 cells were used across the width of a channel or hole.

Comparison of the velocity and temperature profiles showed that a cell size of 1.3% of the liner diameter is needed to capture the steep gradients near the walls, whereas twice this cell size is sufficient for the core of the domain. According to this information, a final grid consisting of 2.28 million cells (see Fig. 2.2) provides the best trade-off between resolution and computation time.

Figure 2.2: Final grid used for the simulations.

2.3.2 Gas phase

Chemically reacting turbulent flows are mathematically described by the conservation equations for mass, momentum, species and enthalpy. The density-weighted time-averaged Navier-Stokes equations are solved to obtain the solution of the mean turbulent flow field.

The Reynolds stresses and the species and enthalpy turbulent fluxes are closed using the Shear Stress Transport (SST) $k-\omega$ turbulence model. In case of swirling flows, the SST $k-\omega$ model developed by Menter [102] generally shows good performance [46] at modest computational cost. The model uses blending functions to combine the advantages of the $k-\omega$ model, which is more robust and accurate in the near-wall region, with the $k-\epsilon$ model, which is preferred in the far field zones away from the surface.

Heat transfer by nonluminous radiation has been included in the calculations by using the discrete ordinates (DO) model [52]. This type of radiation is due to presence of certain heteropolar gases, mainly carbon dioxide and water vapor. Scattering caused by gas molecules has been neglected, because it does not play a major role in radiative heat transfer [29]. The value of the absorption coefficient depends on the composition of the gas mixture and is computed using the weighted-sum-of-gray-gases model [52]. This model evaluates the local value of the radiation absorption coefficient as function of the local mass fractions of water vapor and carbon dioxide. Luminous radiation depends on the number and size of the solid particles (mainly soot) in the flame. Since soot production in the flame is not modelled, luminous radiation is neglected.

The walls of the combustion chamber participate in the internal heat transfer via both convection and radiation. It is assumed that the absorptivity of the walls is equal to the emissivity, and that the reflected and emitted radiation from the surfaces is fully diffuse.

2.3.3 Fuel spray

Despite intensive research over the past decades, the atomization process is still not well understood [103]. The physics governing the spray characteristics are very

complex and, especially in the dense spray region, are challenging to investigate with current experimental techniques. Most studies therefore start with the atomized spray by imposing a distribution of droplet sizes as an inlet condition for the simulations.

Also in this study, the most complex phenomena taking place in the dense spray region are not captured in the model. Instead, the fuel is injected into the combustor in the form of droplets according to a Rosin-Rammler distribution. Here, the Lagrangian formulation has the advantage that the representation of the imposed distribution is relatively easy, because different properties can be assigned to each parcel injected.

Once the parcels are injected in the shape of a hollow cone, only secondary breakup needs to be considered. According to Faeth et al. [50], this process can take place in different modes depending on the Weber number and Ohnesorge number:

$$\text{We} = \frac{\rho_g U_r^2 D}{\sigma} \quad \text{Oh} = \frac{\mu_l}{\sqrt{\rho_l D \sigma}} \quad (2.1)$$

where U_r is the velocity of the droplet relative to the gas, D is the droplet diameter, σ is the surface tension and subscripts g and l denote properties of the gas and the liquid phase, respectively. The Ohnesorge number is the ratio between the viscous forces and surface tension forces. Experimental research has shown that viscous forces are insignificant if $\text{Oh} < 0.1$ [50]. The estimated Ohnesorge number in the present study will be lower than this value, so that breakup is virtually not influenced by viscous damping in the liquid. The breakup mode is therefore only described by the Weber number, which determines the ratio between the disruptive aerodynamic force and the restorative surface tension force. The maximum Weber number is estimated to be 16, which means that secondary atomization might take place by means of bag breakup. Breakup at these low Weber numbers can be modelled with rather good accuracy using the TAB model developed by O'Rourke and Amsden [52].

The trajectory of a particle or droplet in a carrier fluid is predicted by integrating the force balance over a single dispersed phase particle. In case the particles concern small droplets in a gas turbine combustor, it may be assumed that the density of the droplet is much larger than that of the fluid, that the droplet size is small compared to the turbulence integral length scale and that the effect of shear on droplet motion is negligible [105]. Furthermore, gravity and buoyancy effects can be neglected compared to drag forces. The drag coefficient is calculated from the dynamic drag model, in which the drag depends on the flow regime around the droplet and the droplet shape. The random effects of turbulence on particle dispersion are included by using the discrete random walk model [52].

When modelling a particle-laden flow, it is important to examine the extent of coupling between the discrete and continuous phase [121]. In most fuel sprays, the local liquid volume fraction is close to unity near the orifice of the atomizer and

decreases downstream due to desintegration and atomization of the liquid structure [4]. According to a study by Faeth et al. [50], a pressure-atomized spray in still gases after primary breakup can be considered as a dilute environment, where effects of droplet collisions are negligible. This observation is supported by Merci et al. [103], who found that a spray becomes diluted beyond the liquid core, with liquid volume fractions less than about 1%. Following these observations the dispersed spray can be modelled using two-way coupling of turbulence, thereby disregarding any interactions between droplets.

Evaporation of the fuel is calculated using a diffusion-based model. Here, the mass flux at the droplet surface is evaluated by assuming that the partial pressure of vapor at the interface is equal to the saturated vapor pressure [52]. The diffusion coefficient of ethanol vapor in air is configured as a function of the droplet film temperature using the 1/3 averaging rule. In case a droplet hits the hot flame tube, it is assumed that the fuel is released instantaneously.

The importance of radiation absorption by fuel droplets relative to convective heat transfer depends primarily on the type of fuel, the temperature of the flame and the droplet size. Faeth [49] states that previous studies have shown that radiation effects are relatively unimportant for droplet sizes representative for most fuel sprays. This conclusion is in accordance with the results of Tseng and Viskanta [141] and Godsave [61]. Radiative droplet heating has therefore been ignored in the present study.

2.3.4 Droplet size distribution

Injection of the fuel in the form of droplets requires a definition of the initial droplet size as an input parameter. However, because atomization is a chaotic process, the droplets formed after primary breakup are not uniform in size. To account for these variations, it is assumed that the droplet size obeys a Rosin-Rammler distribution [89]:

$$1 - F = e^{-(D/\bar{D})^q} \quad (2.2)$$

where F is the volume fraction of the droplets with a diameter smaller than D . The distribution is defined by a characteristic mean diameter $\bar{D}$ and the spread parameter q . Here, $\bar{D}$ is the droplet diameter for which $1 - F = e^{-1}$ or, equivalently, $F = 0.632$. The parameter q is a measure for the spread in the droplet size.

Experimental data on the droplet size distribution of the spray produced by the prefilming airblast nozzle in the combustor are not available. Hence, empirical correlations have been used to estimate the two parameters required for defining the spray. A representative value for $\bar{D}$ can be found by first estimating the Sauter mean diameter (SMD). This parameter compares the total spray volume to the total surface area of all droplets. Research on the performance of prefilming airblast atomizers has

been conducted by El-Shanawany and Lefebvre [45]. Based on their drop size measurements using a wide variety of liquids at representative atomizing conditions for this study, they proposed a practical correlation to estimate the SMD:

$$\text{SMD} = 0.073 \left(\frac{\sigma}{\rho_a U_a^2} \right)^{0.6} \left(\frac{\rho_f}{\rho_a} \right)^{0.1} D_{pf}^{0.4} \left(1 + \frac{1}{\text{ALR}} \right) + 0.015 \left(\frac{\mu_f^2 D_{pf}}{\sigma \rho_f} \right)^{0.5} \left(1 + \frac{1}{\text{ALR}} \right) \quad (2.3)$$

where D_{pf} is the diameter of the prefilmer, U denotes the velocity and ALR is the air-to-liquid mass ratio. The subscripts f and a refer to fuel and air, respectively. Under the assumption that the variation in droplet size can be described by Eq. 2.2, the SMD is uniquely related to $\bar{D}$. The relation between these two characteristic diameters can be found in Liu [94] and reads:

$$\bar{D} = \text{SMD} \cdot \Gamma (1 - 1/q) \quad (2.4)$$

A representative value for q is estimated based on experimental data found in Lefebvre [86] for an airblast atomizer at different atomizing air velocities. Values of q varying from 3.35 to 3.6 are reported for a water spray at air speeds ranging from 54.8 to 122 m/s. Interpolation gives a spread parameter of about 3.4 at an air velocity of 60 m/s, characteristic for the atomizer conditions in the bioethanol tests. Although the effect of the differences between the properties of water and ethanol is unclear, the reported value is used as an estimation for the spread diameter of the ethanol spray.

The droplet size distribution resulting from Eqns. 2.2–2.4 differs slightly for each case in Table 2.1. As an example, the differential distribution curve for Case 3 (SMD = 44 μm) is shown in Fig. 2.3.

2.3.5 Non-premixed combustion modeling

Solving the species conservation equations for all species involved in detailed chemistry calculations rapidly exceeds computational limits. For this reason, combustion is modeled following the flamelet approach described in Appendix C. The general idea is to decompose the combustion problem into two subproblems: mixing and flame structure. The first is related to the mixing of the fuel and oxidizer streams, and therefore treats all aspects related to the flow field. The flame structure problem involves linking the mixing state to the flame variables, thus describing the combustion process. Departure from chemical equilibrium due to straining of the flame is characterized by the scalar dissipation rate at the flame location. This parameter essentially accounts for the influence of mixing on the flame structure. In addition, the effect of heat loss or heat gain on the flame temperature has been incorporated by

Figure 2.3: Calculated droplet size distribution curve for the ethanol spray in Case 3.

using non-adiabatic flamelets. The actual flame temperature is obtained by correcting the adiabatic flame temperature based on the enthalpy level as calculated from the enthalpy balance equation.

The chemical reactions have been preprocessed using a reduced mechanism for ethanol oxidation proposed by Roehl and Peters [125]. This mechanism includes 38 species and 228 reactions. The non-adiabatic, steady flamelets have been calculated for different scalar dissipation rates up to the rate at which the flame is extinguished. Average values of the flame variables are then computed and tabulated for different enthalpy levels. The variables stored in the PDF tables are temperature, species mass fraction and density. Thermal NO formation is predicted by the extended Zeldovich mechanism [52]. The species concentrations required to calculate the formation rates are obtained from the solution of the combustion model.

2.3.6 Boundary conditions

A mass flow rate and temperature condition are specified at the inlet. The air flow of 75 g/s during the combustion tests has been corrected for the leak air at the connection between the liner and the exhaust duct. The leak air was measured to be 22% of the total air flow at cold conditions. The inlet temperature corresponds to the value at which the air leaves the compressor stage in the gas turbine. It is assumed that the turbulence intensity at the inlet is 5%. This parameter can be used to determine the turbulence parameters k and ω . At the outlet, the relative static pressure is set to zero. The fuel flow rate has been varied to make a comparison at different thermal inputs. The operating conditions for the five simulated cases are defined in Table 2.1.

Table 2.1: Operating conditions in the five simulated cases.

Case	Overall ER [-]	Air flow ^a [g/s]	Fuel flow [g/s]	Power ^b [kW]
1	0.15	58.5	0.98	26
2	0.20	58.5	1.30	35
3	0.25	58.5	1.63	44
4	0.30	58.5	1.95	53
5	0.35	58.5	2.28	61

^a corrected for 22% leak air measured in the test rig.

^b based on a lower heating value of 27 MJ/kg.

The temperature on the outer surface of the liner at base conditions has been determined experimentally using thermochromic paint. Visual inspection of the colors resulted in local upper and lower temperature limits. A representative temperature profile for use in the CFD model is obtained by approximating the mean values of each range indicated by the paint. The dimensionless temperature limits and the derived profile are shown in Fig. 2.4. Although the liner temperature may vary with thermal input, this profile has been imposed on the outer liner surface in all simulations to estimate the heat flux through the flame tube. On the inner surface, a heat flux is prescribed such that the energy balance is not violated.

An emissivity of 0.7 has been assumed for the (oxidized) inner liner surface and 0.6 was chosen for the remaining surfaces [29, 88]. The walls of the outer casing are considered adiabatic to model the thick layer of insulation around the combustor in the test rig. The liner extension walls are adiabatic. To more closely approximate the open space behind the outlet, a free slip condition has been applied on the extended part of the liner.

2.3.7 Numerical procedure

The numerical solution presented in this paper has been computed using a pressure-based coupled AMG solver. Next to explicit under-relaxation factors, a pseudo transient technique has been employed as a form of implicit under-relaxation to stabilize the solver while the solution is calculated. The PRESTO! scheme has been selected as the pressure interpolation scheme.

Quantities at cell faces are interpolated from the center values using a second order upwind scheme, except for velocities. A first order scheme for the momentum equation was used in order to achieve convergence by damping out strong oscillations in the flow. The effect of this setting on the flow field has been evaluated by comparing cold flow simulations. Changing the scheme to first order did not affect the air split significantly. With respect to the second order solution, the deviation in air admission is 1% for the atomizer, 3% for the swirler, 0% for the primary air holes and 0.4% for the dilution air holes. The overall flow pattern did not change either,

Figure 2.4: Dimensionless liner temperature limits from the paint test and the profile used for CFD.

but the velocity profiles measured along the flame tube radius generally showed an underestimation of the recirculation strength. In the primary zone, however, the flow fields predicted by the different methods are in fairly good agreement. Since the phenomena of interest mainly take place in this region, the discretization error of the velocities is considered to be acceptable.

2.4 Results and discussion

In this section the results from the simulations and combustion tests with ethanol are reported and compared. In addition, the test results for ethanol are compared with the results for diesel as a reference fuel. Adiabatic flame temperatures (AFT) and compositions following from a complete combustion reaction (CCR) are included in the graphs to check the integrity of the simulations.

The experimental data have been time-averaged over more than 30 s with a sampling interval of 0.1 s. The measurement locations are indicated in Fig. 2.1. Simulation results have been obtained at the outlet of the computational domain, which is located 40 mm upstream of the position of the sensors in the test rig. The normalized overall imbalance of mass and heat in the converged solutions is found to be less than 0.002% and 3%, respectively. Here, the total mass flow and thermal input are used for normalization.

2.4.1 Flow and temperature fields

Figure 2.5 gives an impression of the droplet trajectories, the flame location and the velocity field inside the combustor. Comparison of the calculated air distribution

(a) Dimensionless temperature field (top) and velocity field (bottom).

(b) Dimensionless temperature field (top) and velocity field (bottom).

Figure 2.5: Dimensionless temperature and velocity fields in Case 3, shown on a cross section that is coincident (a) and not coincident (b) with the primary and dilution air jets.

Figure 2.6: Measured and calculated dimensionless exhaust gas temperatures as function of the overall equivalence ratio.

over the combustor shows good agreement with measurements; the deviation in air flow through the primary and dilution holes is found to be 1 and 4% of the total air flow rate, respectively. Due to the strong recirculation and swirl in the primary zone, the flame is forced to the outer region of the flame tube, close to the wall. The liner is cooled by the fresh air from the compressor on the outside and a protective air sheet originating from the swirler on the inside. It is seen that the fresh air flowing through the casing is slightly preheated due to the heat transfer through the liner, which is about 5% of the heat released by the flame.

A comparison of the dimensionless exhaust gas temperature as function of the overall equivalence ratio is shown in Fig. 2.6. The results from the CFD model are slightly lower than the adiabatic flame temperatures. In terms of heat, the differences between these numerical results ($< 4.5\%$) are in the same order as the overall energy imbalance in the CFD simulations. The temperatures measured in the test rig, however, are significantly lower than these calculated values. Also, a significant deviation between the measured temperatures for ethanol and diesel is observed, whereas the adiabatic temperatures are almost the same for both fuels. High heat loss from the combustor can be excluded as a major cause because of proper insulation. The error bars in the graph furthermore indicate that the differences only increase when correcting for the influence of thermocouple radiation (see also Sec. 2.3). Therefore, the difference must be due to the temperature gradient over the exhaust radius. This implies that the measured temperatures are strongly dependent on the position of the thermocouples in the test rig and on the flow field corresponding to that specific operating condition.

Figure 2.7: Measured and calculated CO_2 concentration as function of the overall equivalence ratio.

2.4.2 Emissions

The CO_2 and O_2 levels as function of the equivalence ratio are given in Fig. 2.7 and 2.8. The graphs illustrate a very good agreement between the calculations and the test results. The concentrations of CO, dimensionless and normalized to 15% oxygen, are plotted in Fig. 2.9. The graph shows a strong increase in CO level for overall equivalence ratios below 0.2. No data could be obtained for the ethanol flame at these lean conditions, because the flame became very unstable. The lean limit for diesel is expected to be lower due to the higher flame temperature. At equivalence ratios above 0.2, it can be concluded that diesel and bioethanol yield similar CO concentrations. The graph of the unburnt hydrocarbon content of the flue gas is omitted here, but shows the same trend.

CO emissions predicted by the CFD model are not shown in the graph because they were strongly underestimated over the entire range of operating conditions. Although the calculations show that CO is formed where combustion is in an early stage, almost all CO is consumed in subsequent reactions so that CO levels at the outlet are negligible. This deficiency is a consequence of the fast chemistry simplification behind the steady laminar flamelet model. The flame is assumed to immediately respond to the mixing state, and departure from chemical equilibrium is accounted for only as a result of aerodynamic strain. Relatively slow chemical processes such as low-temperature CO oxidation cannot be described by the current combustion model. Models that include chemical non-equilibrium due to large chemical time-scales should give more accurate results, but are unfortunately not economically feasible yet.

Figure 2.8: Measured and calculated O_2 concentration as function of the overall equivalence ratio.

Figure 2.10 shows the NO_x emissions, non-dimensionalized and normalized to 15% oxygen content, as function of the equivalence ratio. As expected, the concentration increases with the ER due to higher temperatures in the combustion chamber. Since the fuels do not contain nitrogen, these emissions are due to the formation of thermal or prompt NO_x . The test results show that NO_x emissions for bioethanol are considerably lower than for diesel, with a reduction of roughly 50% over the entire range. The CFD analysis only provides a prediction for the NO concentration. NO_2 emissions are not included in the Zeldovich mechanism, but can be estimated from the NO levels. The combustion tests have shown that NO accounts for about 75% of the total NO_x . The NO levels obtained from CFD are therefore divided by this value to make an estimation of the total NO_x levels. A fair agreement is seen when comparing the numerical and experimental data points.

2.4.3 Droplet evaporation

As can be observed in Fig. 2.5, the simulations indicate that a small amount of fuel reaches the liner surface. The larger droplets partly evaporate but eventually impinge on the liner, after which the remaining fuel is vaporized instantly in accordance with the boundary condition prescribed at these walls. In case this prediction is incorrect, there are three possible explanations: the initial droplet sizes are overestimated, the TAB model fails to describe the secondary breakup, or the evaporation model underpredicts the evaporation rate.

The first of the aforementioned explanations is unlikely, because the correlation of

Figure 2.9: Measured dimensionless CO concentration as function of the overall equivalence ratio, normalized to 15% O₂.

Figure 2.10: Measured and calculated dimensionless NO_x concentration as function of the overall equivalence ratio.

Figure 2.11: Calculated droplet diameter as function of residence time for Case 3.

El-Shanawany yields relatively small droplet sizes compared to those obtained using other empirical correlations for prefilming airblast atomizers [58, 85]. The droplet life time is highly sensitive to the initial droplet size, so the use of a different SMD correlation will generally increase the impingement of droplets significantly. The second explanation can also be rejected based on the relatively low SMD used for the spray definition. According to the model, the Weber number remains under the critical value for breakup since the initial droplet size is generally smaller than $100\text{ }\mu\text{m}$ (see Fig. 2.3). This finding is in agreement with the work of Gepperth et al. [58]. They showed that droplet sizes very close to the edge of an airblast atomizer can be several hundreds of microns, and that the SMD predicted by Eq. 2.3 can only be representative when secondary breakup has already occurred to a large extent.

To get more insight into the evaporation process itself, the evolution of the droplet diameter as function of time is shown in Fig. 2.11. The graph reports tracking data for 10 different parcel diameters in the spray. It can be seen that droplets with an initial diameter larger than $80\text{ }\mu\text{m}$ are not completely evaporated before reaching the wall.

Evaluation of droplet temperature data over time shows that the droplets are quickly heated up to a certain equilibrium temperature. At this temperature, the heat transfer towards the droplet is equal to the evaporative cooling. Since the diffusion coefficient is high in the hot combustor environment and the heat of vaporization of ethanol is relatively large, the droplet temperature does not reach the boiling point. This finding is confirmed by experimental data found in Maqua et al. [99] and Lavieille et al. [81].

In Fig. 2.12, the square of the droplet diameter is shown as function of time. The graph illustrates a predominantly linear relation between these parameters, which means the evaporation process can be approximated using the D^2 -law:

Figure 2.12: Calculated square droplet diameter as function of the droplet travel time in Case 3.

$$D^2 = D_0^2 - K \cdot t \quad (2.5)$$

where D_0 is the initial droplet diameter, t is the droplet residence time and K is the evaporation constant. The D^2 -law is widely used to describe the evaporation of single component, spherical droplets. The evaporation constant in the current simulations can be determined from Fig. 2.12 and varies between 1.2 and 1.5 mm²/s for the droplets larger than 50 μm. Measurements on burning ethanol droplets in quiescent air have shown that K is between 0.81 and 0.86 mm²/s [61, 62, 151], but data for higher Reynolds numbers (i.e. $Re = 10 - 100$) has not been found. The relatively high values for K seen in the CFD model can be expected due to the effect of convection around the droplets, but more data on droplet evaporation in convective flows is required to properly verify the evaporation model in this case.

The thermochromic paint does not indicate unexpected liner temperatures in the primary zone (Fig. 2.4) due to the possible impact of the fuel spray. Nevertheless, this result should not be regarded as conclusive, since the simulations show that only a small fraction of the total fuel flow impinges on the liner and the location of the spray was rather unsteady due to the swirling motion. It is besides not obvious that a strong relation exists between droplet impingement on the inside and the temperature on the outside.

The model result was further supported by visual inspection of the flame tube from the rear side during combustion experiments with this burner, which strongly indicated that the spray indeed impacted on the liner. The spray path was marked by the bright, blue colored part of the low-soot ethanol flame, primarily due to the

Figure 2.13: Image of the ethanol flame without and with CH*-filter in front of the camera.

chemiluminescence of CH radicals. Using a bandpass filter to isolate the emission from this specific reaction intermediate, it was shown that the decomposition of fuel occurred from the atomizing lip up to the liner surface.

In an effort to verify the droplet behaviour in a different way, the flame was visualized from the rear side during the combustion experiments as shown in Fig. 2.13. The spray path is marked by the bright, blue-colored part of the low-soot ethanol flame, primarily due to the chemiluminescence of CH radicals (CH*). The CH radical is a good indicator of the reaction zone due to its short lifetime and is mainly present at the fuel-rich side of this zone [77, 147]. Figure 2.13b has been obtained by using a bandpass filter (430 ± 2 nm) to isolate the emission from this specific reaction intermediate. The image confirms that the decomposition of fuel starts at the atomizing edge and occurs up to the liner surface. Closeups of the flame zone taken without the CH*-filter shown in Fig. 2.14 also indicate that some droplets are reaching the flame tube wall.

Based on the discussion above, it can be concluded that the present approach for modeling the fuel spray leads to acceptable results. The calculated droplet evaporation rates are plausible and the predicted spray length is fairly accurate.

Figure 2.14: Closeups of the ethanol flame during combustion tests in the modified, down-scaled diesel combustor.

2.5 Conclusions

In this work, the combustion of ethanol has been studied in a modified, downscaled burner of the OPRA OP16 industrial gas turbine. CFD simulations and combustion tests have been performed for a thermal input ranging from 29 to 59 kW. The burning tests with ethanol have been compared with results from the model and with the combustor performance on diesel fuel. The ethanol test data show a high combustion efficiency for all evaluated conditions. CO emissions are found to be similar to those for diesel combustion, but NO_x levels are considerably lower.

The CFD model is able to correctly describe the air distribution over the different zones in the combustor. Concentrations of CO₂ and O₂ in the exhaust gas are also in good agreement with theory and experiments. The trend of the NO_x emissions is captured with fair accuracy. The current model is however incapable of predicting CO emissions. A significant deviation is observed between the predicted and the measured exhaust gas temperatures. This is attributed to incomplete mixing of flue gases at the outlet of the combustor. When compared to adiabatic flame calculations, the temperatures provided by the CFD model show a close match.

The simulations show that the ethanol spray is not completely evaporated before reaching the liner. This finding is supported by images from the flame zone obtained during the combustion experiments. Furthermore, it is found that the calculated evaporation rates are plausible when compared to experimental data from ethanol droplet studies. The current approach for modeling the fuel spray is therefore considered to be adequate.

Chapter 3

A computational model for pyrolysis oil combustion

Abstract

The growing demand for the use of biofuels for decentralized power generation initiates new developments in gas turbine technology. Recently, new combustors for low-calorific fuels have been designed and tested. This chapter discusses the use of CFD techniques for modeling the combustion of pyrolysis oil in a new burner geometry from OPRA Turbines. Pyrolysis oil contains many different compounds, which are represented by a discrete fuel model consisting of seven components. The components and their initial fractions approximate the volatility, water content, elemental composition and heating value of a typical fast pyrolysis oil. Simulations have been carried out for both the multicomponent pyrolysis oil and, as a reference, ethanol, a single-component biofuel with a higher volatility. The numerical analysis is mainly focused on the evaporation and the flame characteristics of the two biofuels. Comparative simulations have been performed to evaluate different evaporation and combustion models, and to examine the influence of the initial droplet size.

3.1 Introduction

Fast pyrolysis oil is a renewable biofuel produced from biomass waste materials that can potentially be used as a fuel for industrial gas turbine engines [11, 32, 39, 67, 76, 97]. It is composed of a large number of oxygenated compounds that are formed during the thermal decomposition of biomass in the pyrolysis process. The chemical and physical properties of pyrolysis oil are markedly different from conventional fossil fuels. Regarding spray combustion applications, the high water content, high viscosity and high coking tendency are particularly challenging. Several test campaigns have indicated that these properties can cause incomplete combustion and fouling [10, 32, 118, 138]. It is generally concluded that modification of the combustion equipment is required to achieve acceptable operating performance with this biofuel.

The development of new combustors for this purpose can be facilitated by models that describe the evaporation and burning characteristics of pyrolysis oil with respect to other fuels. Especially CFD models can be useful to gain insight into the interactions between the pyrolysis oil spray and the surrounding air in a combustion chamber. However, the numerical analysis of these phenomena has received little attention so far. The few models [21, 69, 83, 100, 153] that have been proposed to approximate the behavior of pyrolysis oil droplets in a high temperature environment are shortly discussed in Appendix B. Since most of these models are restricted to the evaporation process, the characterization of the entire combustion process using numerical methods still needs to be explored.

This chapter presents a CFD approach for modeling pyrolysis oil spray combustion in an industrial gas turbine. The commercial code ANSYS Fluent has been employed to model the vaporization and combustion of pyrolysis oil in the low-calorific fuel combustor that was recently developed by OPRA for the application of biofuels in their OP16 gas turbine [12]. The aim is to capture the main burning characteristics of pyrolysis oil in order to contribute to the development of suitable combustion systems. The results for pyrolysis oil have been compared to simulations with ethanol, a single-component biofuel which is used as a reference. Additional computations have been performed to verify the sensitivity of the results to the evaporation model, the initial droplet size and to the combustion model.

3.2 Droplet evaporation theory

The vaporization of the various pyrolysis oil constituents is one of the essential modeling tasks. This section gives a summary of the classical theory [49, 87, 128, 136, 149] that forms the basis of the evaporation models used in this work. The gas and liquid phase equations are briefly discussed here for single-component fuels. However, essentially the same theory can be applied for modeling the evaporation of multicomponent liquids such as pyrolysis oil. In such cases, each individual species contained in the liquid will evaporate at a different rate depending on its properties

and concentration at the surface. This requires to account for the property variations between the different constituents of the liquid.

3.2.1 Gas phase

The equations describing the mass and heat transfer at the droplet surface are derived by considering spherically symmetric vaporization of a single-component droplet in a quiescent atmosphere. In the earliest formulation suggested by Maxwell, the rate of evaporation for a static droplet is modeled by only considering diffusive transport:

$$\dot{m} = 4\pi R_d D_v \rho (Y_{v,s} - Y_{v,\infty}) \quad (3.1)$$

where R_d is the droplet radius, D_v is the diffusion coefficient of the fuel vapor, ρ is the total density of the mixture of gas and fuel vapor in the vicinity of the droplet, and $Y_{v,s}$ and $Y_{v,\infty}$ are the fuel vapor mass fractions at the surface and in the far field. From Eq. 3.1 and the corresponding energy equation, it follows that the Sherwood (Sh) and Nusselt (Nu) numbers for a static droplet are given by:

$$\text{Sh} = \text{Nu} = 2 \quad (3.2)$$

In case the droplet is moving, a correction should be applied to account for the influence of the convective flow around the droplet. Theoretical analysis of the boundary layer shows that the general form of this modification can be written as:

$$\text{Sh} = \text{Sh}_0 + \beta_c \text{Re}^{1/2} \text{Sc}^{1/3} \quad \text{Nu} = \text{Nu}_0 + \beta_c \text{Re}^{1/2} \text{Pr}^{1/3} \quad (3.3)$$

where the subscript 0 denotes the value for a static droplet and the correction factor β_c is to be determined empirically. The parameters Re, Sc and Pr are respectively the Reynolds, Schmidt and Prandtl numbers.

Equation 3.1 is only valid for low evaporation rates, however, since it ignores the convective flow of fuel vapor away from the droplet surface. The outward vapor flow induced at high evaporation rates is referred to as Stefan flow and impedes the transfer of mass and heat at the droplet surface.

A more general formulation for quasi-steady droplet evaporation that includes this effect has been developed in the 1950s [61, 137]. Starting from the continuity equations for mass and species, it was derived that the evaporation rate can be described by:

$$\dot{m} = 4\pi R_d D_v \rho \ln(1 + B_M) \quad (3.4)$$

where B_M is the Spalding mass transfer number defined as:

$$B_M = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}} \quad (3.5)$$

When assuming a Lewis number equal to unity, an equivalent expression for the rate of droplet mass loss can be obtained from the energy balance:

3.2. Droplet evaporation theory

$$\dot{m} = \frac{4\pi R_d k_g}{C_{p,v}} \ln(1 + B_T) \quad (3.6)$$

where k_g is the thermal conductivity of the gas, $C_{p,v}$ is the specific heat capacity of the vapor and B_T is the Spalding heat transfer number:

$$B_T = \frac{C_{p,v}(T_\infty - T_s)}{L_{\text{eff}}} \quad (3.7)$$

The parameter L_{eff} in this equation is the effective latent heat of vaporization, defined as:

$$L_{\text{eff}} = L + (|\dot{Q}_d|/\dot{m}) \quad (3.8)$$

where L is the specific latent heat and $\dot{Q}_d$ is the conductive heat transfer rate at the surface used to heat the droplet interior.

By further evaluating Eq. 3.4 and 3.6, it is found that the Sh and Nu numbers are now expressed by:

$$\text{Sh} = 2 \frac{\ln(1 + B_M)}{B_M} \quad \text{Nu} = 2 \frac{\ln(1 + B_T)}{B_T} \quad (3.9)$$

In the limit of low evaporation rates, $B_M \rightarrow 0$ and $B_T \rightarrow 0$ such that the solution of Maxwell given by Eq. 3.2 is obtained. For a moving droplet, the value of 2 is substituted by the corrected value calculated from Eq. 3.3.

For droplets that are surrounded by a flame, the theory for a non-reacting atmosphere can be extended to obtain the burning rate of a drop in an oxidizing gas. The rate of mass loss of a burning droplet is given by Eq. 3.6, with a modified mass transfer number to account for the heat release near the drop surface:

$$B_{T,c} = \frac{C_{p,v}(T_\infty - T_s) + (Y_{O,\infty}/\sigma_O)Q_c}{L_{\text{eff}}} \quad (3.10)$$

where the subscript c refers to combustion, Q_c is the heat of combustion and σ_O is the stoichiometric mass ratio of fuel and oxidizer.

In case a constant droplet temperature is assumed, or if the droplet is in thermal equilibrium after an initial heat-up period, the classical theory predicts that the square of the droplet diameter decreases linearly with time. This leads to the well-known D^2 -law:

$$D^2(t) = D_0^2 - K \cdot t \quad (3.11)$$

where D_0 is the initial diameter of the droplet and K denotes the evaporation or burning rate constant. From the Maxwell equation, it follows that the value of K is given by:

$$K = \frac{8k_g}{\rho_l C_{p,v}} (Y_{v,s} - Y_{v,\infty}) \quad (3.12)$$

The rate constant in the Spalding model for evaporating droplets, K_v , and burning droplets, K_c , are described by:

$$K_v = \frac{8k_g}{\rho_l C_{p,v}} \ln \left(1 + \frac{C_{p,v}(T_\infty - T_s)}{L_{\text{eff}}} \right) \quad (3.13)$$

$$K_c = \frac{8k_g}{\rho_l C_{p,v}} \ln \left(1 + \frac{C_{p,v}(T_\infty - T_s) + (Y_{O,\infty}/\sigma_O)Q_c}{L_{\text{eff}}} \right) \quad (3.14)$$

The linear relation between D^2 and time has been confirmed by many experimental observations with single-component liquids. Note that this principle does not hold for multicomponent liquids, since the value of K is not constant when the properties of the liquid and of the vapors leaving the droplet are changing.

3.2.2 Liquid phase

Transport processes in the liquid phase are usually not resolved in practical spray combustion simulations to reduce the computational demand of the evaporation problem. A widely used approach in CFD codes is to assume that the liquid temperature is uniform in space but varying in time. The change in droplet temperature over time is then computed by solving a global heat balance [3]:

$$mC_p \frac{dT}{dt} = 4\pi R_d^2 h(T_\infty - T) - \dot{m}L \quad (3.15)$$

where the heat transfer coefficient, h , is calculated from the Nusselt number.

3.3 Pyrolysis oil fuel model

Considering the large number of compounds present in pyrolysis oil, the composition was simplified using a discrete component approach. To capture the most relevant properties for the evaporation and combustion behavior, a surrogate fuel was developed that represents the volatility, water content, elemental composition and heating value of a typical pyrolysis oil.

The pyrolysis oil devolatilization characteristics reported by Branca et al. [18] were used as a guideline in selecting the components for the fuel model. On basis of thermogravimetric analysis (TGA) of four different pyrolysis oils (BTG, Dynamotive, Ensyn and Pyrovac), they proposed to divide the devolatilization curve into six main temperature zones. It was shown that the measured weight loss in the zones could be correlated with the mass fractions of the compounds identified in the oil samples of which the boiling points fell within the corresponding temperature ranges. In the surrogate fuel developed for the current study, the total weight loss in each of the six temperature zones is lumped into a single organic compound that is typically found in pyrolysis oils. Water has been selected as an additional species, because it is the most abundant constituent of pyrolysis oil and highly influences the evaporation

3.3. Pyrolysis oil fuel model

Table 3.1: Specification of the discrete fuel model used as a surrogate for pyrolysis oil. The temperature zones have been adopted from Branca et al. [18]. T_b and Y_{init} denote respectively the boiling point and the initial mass fraction.

Zone	Oil temp. (K)	Component	Formula	T_b (K)	Y_{init} (%)
1	< 360	Methanol	CH ₃ OH	338	10
2	360 – 400	Water	H ₂ O	373	25
		Acetic acid	CH ₃ COOH	391	10
3	400 – 450	Acetol	C ₃ H ₆ O ₂	419	10
4	450 – 500	Phenol	C ₆ H ₅ OH	455	10
5	500 – 550	Eugenol	C ₁₀ H ₁₂ O ₂	527	15
6	> 550	Levoglucosan	C ₆ H ₁₀ O ₅	623	20

curve due to its high latent heat of vaporization. This approach resulted in the fuel model specified in Table 3.1. The surrogate fuel has an elemental composition of C 40% H 9% O 51% by weight and a lower heating value (LHV) of 15.6 MJ/kg, both of which are typical for fast pyrolysis oils [17, 31, 113, 126]. Properties of the individual components in the model can be found in Appendix A.

The initial mass fractions of the components have been estimated by evaluating TGA data reported in the literature. Branca et al. [18] determined devolatilization curves for the abovementioned pyrolysis oils using a heating rate of 5 K/min to a final temperature of 600 K. The measured weight loss in each of the six temperature zones was compared to their prediction based on the mass fractions and boiling points of the oil constituents. For the Dynamotive and BTG oils, the TGA data obtained from these experiments are listed alongside the predictions in Table 3.2. Both oils were produced from softwood and obtained by collecting the entire liquid from the pyrolysis reactor. Due to differences in the feedstock and the production process, the Ensyn and Pyrovac oils were considerably less volatile and therefore excluded from the present discussion. Table 3.2 also shows the TGA results reported by Van Rossum et al. [126]. These experiments were performed with pyrolysis oil produced from forest residue by VTT using a heating rate of 50 K/min up to a temperature of 823 K.

The weight losses of the Dynamotive and BTG oils measured by Branca et al. deviate considerably from the predictions, especially in the lowest temperature zones. It was stated that these differences were mainly caused by the low heating rate used for the analysis. The slow process presumably allowed the oil constituents to largely evaporate already before their respective boiling points were reached. A reasonable agreement between the measurements and predictions for the individual oils was however observed by comparing the total weight loss over the first three zones, which cover the evaporation of water and all relatively light compounds.

A comparison of the TGA data obtained for the two oils shows that the BTG oil is more volatile than the Dynamotive oil in the lower temperature regions. The

Table 3.2: Weight loss in wt.% for the different temperature zones as measured using TGA and predicted on basis of composition and boiling points. Data reproduced from Branca et al. [18] for the Dynamotive and BTG oils and from Van Rossum et al. [126] for the VTT oil.

Zone	Oil temp. (K)	Weight loss (wt.%)				
		Dynamotive ^a		BTG ^b		VTT ^c
		TGA	Pred.	TGA	Pred.	TGA
1	< 360	16.7	7.8	27.6	7.9	28.0
2	360 – 400	13.3	33.2	16.6	44.4	18.4
3	400 – 450	13.7	8.4	13.1	6.5	9.6
4	450 – 500	9.7	2.9	8.3	1.6	7.0
5	500 – 550	8.9	4.7	5.7	3.1	5.0
6	> 550	6.0	7.2	4.2	4.9	16.0
1 – 2	< 400	30	41	44	52	46
1 – 3	< 450	44	49	57	59	56
1 – 6	Full range	68	64	76	68	84

^a Dynamotive oil, 21% water, heating rate 5 K/min up to 600 K.

^b BTG oil, 30% water, heating rate 5 K/min up to 600 K.

^c VTT oil, 24% water, heating rate 50 K/min up to 823 K. Predictions are not available for this oil.

primary reasons for the higher volatility are the higher water content (30 vs 21 wt.%) and the lower pyrolytic lignin fraction (8 vs 25 wt.%) of the BTG oil. The TGA curve obtained for the VTT oil with a water content of 24 wt.% is generally similar to that of the BTG oil, though the heating rate was ten times as high. A large difference is seen in the highest temperature zone, however, presumably because the VTT sample was heated to a higher final temperature.

Since the heating rates in a gas turbine combustor are several orders of magnitude higher (typically $\geq 10^5$ K/min), the actual evaporation curve of a droplet in the spray is expected to follow the predicted values according to the boiling points more closely than seen in Table 3.2. This presumption is supported by TGA measurements at different heating rates conducted by Van Rossum et al. [126]. In Table 3.3, the measured weight loss of the VTT oil in each zone is reported for heating rates of 1–100 K/min up to 1073 K on basis of the sample cup temperature. The data cannot be directly compared to the values given in Table 3.2 because the temperature of the pyrolysis oil itself is unknown, but the results indicate that the release of volatiles is shifted towards higher temperatures in case the heating rate is increased. It therefore seems plausible that the evaporation behavior at high heating rates will be strongly correlated with the oil composition and the boiling points of the various components.

Following these considerations, the initial weight fractions for the lowest three temperature zones given in Table 3.1 ($T < 450$ K) have been chosen based on the

3.3. Pyrolysis oil fuel model

Table 3.3: Weight loss in wt.% of the VTT oil at different heating rates as measured using TGA up to 1073 K. The temperatures are those of the sample cup. Data reproduced from Van Rossum et al. [126].

Zone	Cup temp. (K)	Weight loss (wt.%)		
		1 K/min	10 K/min	100 K/min
1	< 360	28	18	7
2	360 – 400	15	17	17
3	400 – 450	11	14	16
4	450 – 500	8	9	10
5	500 – 550	4	8	9
6	> 550	16	18	26
1 – 6	< 1073	82	84	85

predicted values reported in Table 3.2. The total mass fraction represented by these zones was constrained to 55%, which is the average value of the predictions for the Dynamotive and BTG oils. After setting the water content to 25 wt.%, the average value of all three oils considered in the table, the remaining mass was divided over the other three components in these zones.

For the higher temperature zones ($T > 450$ K), the data in Table 3.2 cannot be used as a reliable basis for the present fuel model. Firstly, the chemical characterization of the oils was incomplete regarding the heavier species. It can be seen that the predicted values do not sum up to 100%, which is mainly because the nonvolatile fractions were excluded from the analysis [19]. Secondly, the TGA results obtained at such temperatures are not representative because the liquid phase chemistry is sensitive to the heating rate. At low heating rates (1–100 K/min), pyrolysis oils show a high tendency to form nonvolatile material under influence of polymerization reactions once the water and light components have evaporated [126]. This polymerization process typically results in a large amount of secondary char at the end of a TGA experiment, as can be seen from the total weight loss data given in Tables 3.2 and 3.3. In several studies, however, it was observed that the charring tendency of pyrolysis oil is strongly reduced by increasing the heating rate. Evaporation experiments with small droplets resulted in a char yield as low as 4% [126] and 1% [31] of the original pyrolysis oil mass. The heating rates in these experiments were estimated to be 10^6 and above 10^5 K/min, respectively. In spray combustion experiments only 0.1% of the original mass was obtained as char [143], although it must be noticed that the hot product gases were not quenched so that part of the char could have been consumed via surface reactions. Nevertheless, these studies clearly show that TGA underpredicts the mass release in the upper temperature regions.

Given the low char yield under typical spray combustion conditions, a solid phase was not included in the fuel model. The small amounts of char that remain

from the droplets may have implications for the soot emission and the service life of certain engine components, but are not expected to significantly influence the general combustion characteristics currently studied. Consequently, the initial mass fractions chosen for the components in zones 4–6 in Table 3.1 account for the evaporation of volatiles with a high boiling point as well as the cracking of the nonvolatile pyrolysis oil constituents. As the content of nonvolatiles (pyrolytic lignin, sugars, extractives) is very significant in most oils [90, 112, 113], the mass fractions are increasing towards higher boiling points. However, it remains uncertain if the assumed fractions accurately describe the evaporation curve in this region because appropriate reference data is not available.

3.4 Numerical methods

The combustion of pyrolysis oil and ethanol in an industrial gas turbine burner has been numerically investigated by using the Euler-Lagrange approach in ANSYS Fluent 14.5 [3]. Details on the computational domain and the models used to describe the processes taking place in the gas and the liquid are provided in the following paragraphs. The numerical setup for ethanol combustion is partly based on the modeling approach used to simulate the combustion of ethanol in a diffusion-mode burner for conventional fuels (see Chapter 2).

3.4.1 Computational domain

Figure 3.1 shows a schematic of the combustion chamber that is considered in this study. This reverse-flow tubular combustor has recently been developed by OPRA Turbines to efficiently burn low-calorific fuels in the OP16 gas turbine rated at 1.9 MW [11]. Compared to the standard combustor used for burning fossil fuels in diffusion mode, the new design has a larger volume to provide enough residence time for complete burnout. The distribution of air was furthermore changed to ensure sufficient burning rates of the low-calorific fuels. Another major difference is the flame stabilization technique, which is now provided by a radial swirler only. Fuel is injected using a prefilming airblast nozzle.

The simulations have been performed using a 45 degree section of the combustor to reduce the computational cost. Still, due to the large combustor volume, meshing the entire flow path resulted in an infeasible amount of elements for combustion simulations. The computational domain used for the reacting flow cases therefore only included the flame tube, the swirler and the nozzle. Boundary conditions for the flow field and turbulence parameters imposed on the inlets of the domain were extracted from the nonreacting flow simulations, which were performed with a 45 degree slice of the complete geometry.

Both domains have been discretized using an unstructured tetrahedral grid with boundary layer elements. Local refinements were used to fill the width of a channel or hole with a minimum amount of 10 cells. The grid dependency study for the

Figure 3.1: Sketch of the biofuel combustor developed by OPRA Turbines [12]. The arrows indicate the flow field according to the current simulations.

nonreacting flow domain included a coarse, medium and fine mesh, which were constructed with a global cell size of respectively 8, 6 and 4 mm. After comparison of the results, a final mesh was created consisting of 7.4 million elements. The grid dependency for the reacting flow domain was studied using 9 different grids. In the finest grid, used as a reference, the global cell size was set to 2 mm. Smaller global sizes were not investigated, because they led to an impractical amount of elements. Temperature and velocity profiles were evaluated at various locations to find the optimum configuration. The analysis resulted in a final mesh containing 3.4 million cells, with local refinements near the atomizer, in the flame region and adjacent to the liner. Although considerably less elements were used compared to the 2 mm reference mesh, it was observed that velocity and temperature profiles at different sample lines along the combustor axis did not deviate more than 6%.

3.4.2 Gas phase modeling

The gas phase is described by the steady-state RANS equations. Favre-averaged conservation equations for mass, species, momentum and enthalpy have been solved to obtain the mean field quantities, while effects of turbulent fluctuations are modeled using the SST $k-\omega$ formulation as available in Fluent [3]. The density and heat capacity of the gas are computed from respectively the ideal gas law and a mixing law. Correlations for air are used to approximate the thermal conductivity and viscosity of the gas as function of temperature. Radiative heat transfer inside the combustor has not been included in the model.

3.4.3 Fuel spray definition

In the discrete phase model, the fuel spray is considered as a collection of parcels representing individual droplets with the same properties. A transient solver tracks the parcels in a Lagrangian frame of reference while they exchange mass, heat and

momentum with their surroundings. These processes are incorporated in the governing equations for each of the two phases by including source terms (two-way coupling). Since fuel sprays in gas turbines are typically characterized as dilute, any droplet-droplet interactions are unlikely to occur and can be neglected [50].

The fuel is introduced into the domain in the form of parcels with a predefined diameter. This approach avoids modeling the complex breakup phenomena occurring when the high-speed atomizing air rips off droplets from the fuel film at the edge of the prefilmer. To provide an acceptably smooth distribution of the fuel in circumferential direction, the parcels are released at 40 equally spaced injection locations at each time step of the discrete solver. The time step is configured such that the number of particles represented by each parcel is limited to typically 10–75, depending on the droplet size. This ensures that the discrete phase is also well distributed in the direction of the spray.

The droplet size distribution of the sprays produced by the prefilming airblast nozzle is unknown. Several empirical correlations for estimating the mean droplet size exist in the literature, but the predictions from these correlations show large differences. For the purpose of this study, it was therefore assumed that the droplets in the fuel sprays are uniform in size, i.e. 30 or 50 μm . Although such sprays are hypothetical and generally do not represent the real case, the uniformly-sized sprays give a clear indication of the relation between the flame and the drop size. Nevertheless, to illustrate the influence of the spread in the drop sizes observed in practical sprays, comparative simulations have been performed using a Rosin-Rammler distribution, see Eq. 2.2. Following the approach described in Chapter 2, the characteristic diameter was derived from an estimated Sauter mean diameter (SMD) using the correlation proposed by El-Shanawany and Lefebvre [45], while a typical value for the spread parameter was obtained from experimental data for water sprays [86]. For $q = 3.45$, this approach results in a distribution with an SMD of 42 μm and a $\bar{D}$ of 54 μm . The differential and cumulative curves of the distribution are shown in Fig. 3.2.

Secondary breakup as well as radiative droplet heating have been neglected. The error caused by these simplifications is acceptable since, for the small droplets considered here, the Weber number is typically lower than 10 and convection is reported to be the dominant heat transfer mechanism [50, 141].

3.4.4 Interphase transport

Once the parcels have been released, the parcel trajectories are computed from the drag force exerted by the flow. The drag coefficient for a parcel is approximated by that of a spherical particle. Other forces acting on the parcels, such as virtual mass and pressure gradient forces, are negligible compared to the aerodynamic drag. The effect of turbulent velocity fluctuations on the droplet trajectories has been taken into account using the discrete random walk model [3].

Heat and mass transfer between the phases is described by the classical evaporation theory discussed in Sec. 3.2. The influence of the Stefan flow has been investi-

Figure 3.2: Differential and cumulative curves of the droplet size distribution used in this study.

gated by performing simulations with both the Maxwell and the Spalding vaporization model. Evaporation rates in these models are based on the Sherwood numbers in respectively Eq. 3.2 and Eq. 3.9, which are both corrected for external convection using Eq. 3.3 with $\beta_c = 0.6$. For the simulations with pyrolysis oil, these equations are solved for each fuel component listed in Table 3.1. Vapor concentrations at the droplet surface are computed from Raoult's law under the assumption of an ideal mixture in vapor-liquid equilibrium. The diffusion coefficients have been evaluated at a film-averaged temperature using the 1/3-rule recommended by Hubbard et al. [71].

3.4.5 Liquid phase modeling

The selective evaporation of the various constituents of a multicomponent fuel can lead to significant mass and temperature gradients within the droplet. Consequently, the influence of internal transport on the evaporation process can be more pronounced than in case of pure liquids [1, 135]. Simulation results are hence expected to be sensitive to the model used for describing the liquid phase transport mechanisms. However, solving transport equations inside each droplet requires large computational effort. The current CFD code therefore relies on the rapid mixing assumption, which is in line with the work of Hallett and Clark [69] and Zhang and Kong [153]. It is accordingly assumed that the droplet is spatially uniform in temperature and composition. The temperature change in time is computed from the global heat balance given by Eq. 3.15. The validity of the rapid mixing assumption for the fuels and conditions studied here is reviewed in Appendix D.

3.4.6 Combustion modeling

The pyrolysis oil flame is described using a combustion model based on thermodynamic equilibrium since a reaction mechanism is not available. Under the assumption that species react toward their equilibrium state over a characteristic time, the mean reaction rate for species i can be modeled as [3]:

$$R_i = \rho \frac{Y_i^{\text{eq}} - Y_i}{\tau} \quad (3.16)$$

where ρ is the mixture density, Y_i is the mean mass fraction as obtained from the species conservation equation, Y_i^{eq} is the local equilibrium mass fraction and τ denotes a characteristic time scale. The characteristic time is equated to the turbulent time-scale, which is described by the turbulence model:

$$\tau = \tau_{\text{turb}} = \frac{k}{A\epsilon} \quad (3.17)$$

where k is the turbulent kinetic energy, ϵ is the eddy dissipation rate and A is a model constant equal to 4 by default. This model will be referred to as the relaxation-to-equilibrium (RTE) model.

The RTE model has also been applied in the simulations with ethanol to facilitate comparisons with the pyrolysis oil cases. For modeling the ethanol flame, however, alternative methods incorporating combustion kinetics can be used because suitable reaction mechanisms exist. The sensitivity of the temperature field to the chosen chemistry model is therefore evaluated by performing additional simulations with ethanol using the non-adiabatic steady laminar flamelet model [3]. The laminar ethanol flamelets were calculated on basis of a reaction mechanism developed by Röhl and Peters, including 38 species and 228 reactions [125]. The average temperature, density and species mass fractions in the turbulent flame were subsequently computed and stored in multidimensional look-up tables of the form:

$$\tilde{\phi} = \tilde{\phi}(\tilde{Z}, \widetilde{Z'^2}, \tilde{\chi}_{\text{st}}, \tilde{H}) \quad (3.18)$$

where $\tilde{\phi}$ is the quantity of interest, $\tilde{Z}$ is the mean mixture fraction, $\widetilde{Z'^2}$ is the mixture fraction variance, $\tilde{\chi}_{\text{st}}$ is the stoichiometric scalar dissipation rate, and $\tilde{H}$ is the mean enthalpy level. The mean enthalpy is incorporated to account for heat losses due to droplet evaporation, which requires adjustment of the adiabatic quantities. However, the influence of heat loss on the species composition under non-equilibrium conditions (i.e. $\tilde{\chi}_{\text{st}} \neq 0$) is neglected. A more detailed description of the flamelet model is given in Appendix C.

3.4.7 Boundary conditions and case specification

Air enters the domain with a total flow rate of 300 g/s at a temperature equal to the compressor discharge temperature in OPRA's OP16 engine. The thermal input is set

Table 3.4: Overview of the models used for the reacting flow simulations.

Case	Fuel	Combustion	Evaporation	Droplet size
E.1	Ethanol	RTE	Maxwell	Uniform, 50 μm
E.2	Ethanol	RTE	Spalding	Uniform, 50 μm
E.3	Ethanol	RTE	Maxwell	R-R distribution
E.4	Ethanol	RTE	Maxwell	Uniform, 30 μm
E.5	Ethanol	Flamelets	Maxwell	Uniform, 50 μm
PO.1	Pyrolysis oil	RTE	Maxwell	Uniform, 50 μm
PO.2	Pyrolysis oil	RTE	Spalding	Uniform, 50 μm
PO.3	Pyrolysis oil	RTE	Maxwell	R-R distribution
PO.4	Pyrolysis oil	RTE	Maxwell	Uniform, 30 μm

to 280 kW in all simulations, which corresponds to a fuel flow rate of 10.5 g/s for ethanol and 17.9 g/s for pyrolysis oil. A pressure condition is applied at the outlet. The combustor walls are assumed to be adiabatic. Impingement of droplets on the liner is described by the wall-jet boundary condition [3]. The wall-jet model predicts the trajectory of a droplet after impacting a high-temperature wall where no liquid film is formed.

The combustion model, evaporation model and droplet size distribution have been varied to study the influence of these settings on the solution. Table 3.4 gives an overview of the settings used in the reacting flow simulations. A more detailed description of these models can be found in Secs. 3.4.3 and 3.4.6, and in Sec. 3.2.

3.4.8 Solution method

The system of equations was solved using a pressure-based AMG solver with a pressure-velocity coupling algorithm. Values on the cell faces were computed using the second-order upwind scheme. Explicit as well as implicit under-relaxation was used to stabilize the solver. The PRESTO! scheme has been selected for the pressure interpolations.

Figure 3.3: Comparison of the temperature fields for ethanol (top) and pyrolysis oil (bottom) combustion (Case E.1 vs PO.1).

3.5 Results and discussion

This section presents the results obtained from the reacting flow simulations listed in Table 3.4. The results for ethanol and pyrolysis oil combustion using the same model configuration are discussed first. Subsequently, it is examined to what extent the flame and spray characteristics are sensitive to the evaporation model, the droplet size and the combustion model. Temperatures and velocities have been made dimensionless through division of the values by a certain constant reference value.

All simulations were converged satisfactorily, unless stated otherwise. The overall mass and heat imbalance were respectively below 0.01% of the total mass flow rate and below 0.3% of the heat of combustion ($280 \text{ kW} \pm 0.5\%$). The predicted air distribution over the combustor zones agrees well with measurements performed by OPRA [11], with an error of less than 1% of the total flow.

3.5.1 Temperature field and evaporation behavior

Figure 3.3 shows the temperature contours for ethanol (Case E.1) in the top half and for pyrolysis oil (Case PO.1) in the bottom half, together with the corresponding fuel sprays. In these simulations, the chemistry is predicted by using the RTE model, and the evaporation of the $50 \text{ }\mu\text{m}$ droplets is computed using the Maxwell equation (see Table 3.4). The peak temperatures for the ethanol case in Fig. 3.3 are reached near the atomizer pintle and near the combustor axis further downstream. The temperatures in these regions are in close agreement with the adiabatic flame temperature of

Figure 3.4: Impression of the subsequent evaporation of species in the pyrolysis surrogate, based on the rate of mass loss. The plots are obtained with a uniform droplet size of $50\ \mu\text{m}$ (Case PO.1).

2353 K. In the pyrolysis oil case, the peak temperature is observed close to the liner and is only 2140 K. This temperature is significantly lower than the adiabatic flame temperature of 2287 K for the pyrolysis oil surrogate fuel. However, it is very well possible that the maximum temperature of the pyrolysis oil flame does not correspond to the adiabatic value because the fuel components are not released simultaneously. The differences in molecular formulas of the vaporizing components make that a wide range of local C-H-O ratios are possible. In practice, the flame temperatures for both fuels are expected to be slightly lower than predicted by the model, primarily since radiative heat losses are neglected. The total amount of energy required for evaporating the fuel is more than twice as high for pyrolysis oil as for ethanol, i.e. 20.5 kW compared to 9.5 kW. As illustrated by Fig. 3.3, the evaporating pyrolysis oil droplets therefore cause a large decrease in gas temperature near the spray.

It is also observed that the pyrolysis oil spray penetrates considerably further into the combustor. A qualitative impression of the subsequent evaporation of fuel species can be found in Fig. 3.4. To get detailed insight into the evaporation process, Fig. 3.5 reports the square of the nondimensional diameter and the temperature of the droplets in the ethanol and pyrolysis oil spray as function of time. The small dots indicating the current state of each droplet show a significant degree of scattering due to the modeled effect of turbulent velocity fluctuations (see Sec. 3.4.4). For the sake of convenience, this discussion will only consider averaged values at each point of time, which are indicated by the solid curves for ethanol and the dashed curves for pyrolysis oil.

The figure shows that the evaporation curve for ethanol approximates the D^2 -law given by Eq. 3.11. After a short heat-up period the temperature tends to stabilize between 338 and 351 K, whereby the exact value varies with the conditions of the

Figure 3.5: Comparison of the square of the nondimensional droplet diameter and the droplet temperature as function of time for the ethanol (solid) and pyrolysis oil (dashed) spray (Cases E.1 and PO.1).

Table 3.5: Comparison of evaporation constants for vaporizing or burning ethanol droplets.

Author(s)	Method	D_0 (μm)	T_{gas} (K)	U_{rel} (m/s)	K (mm^2/s)
Current	Num.	50	800 – 1800	0 – 55	0.98
Godsave [61]	Exp.	1500	T_{flame}	quiescent	0.81
Goldsmith [62]	Exp.	1500 – 1800	T_{flame}	quiescent	0.86
Maqua et al. [99]	Exp.	105	1140	5 – 6	0.81
			1260	4 – 5	0.71
			1270	2 – 4	0.73

droplet surroundings. The evaporation rate constant in Eq. 3.11 can be determined from the average slope of the diameter curve from this point ($t \geq 1$ ms) and is found to be $0.98 \text{ mm}^2/\text{s}$. In Table 3.5, this result is compared to experimental values reported in the literature for vaporizing or burning ethanol droplets. The somewhat higher value found in this work is probably related to the velocity of the droplets relative to the gas, U_{rel} , which is generally much higher in the current simulations. According to the correlation that accounts for the effects of gas phase convection on the evaporation rate, Eq. 3.3, the external velocity can have major impact on the vaporization rate via the Reynolds number. Nevertheless, since measured values for higher relative velocities or typical Re numbers (5–20) have not been found in the literature, the accuracy of the predicted evaporation curve for these conditions cannot be fully confirmed.

The dashed curves in Fig. 3.5 show the evaporation of the multicomponent py-

rolysis oil surrogate. A rapid increase in temperature is again observed within the first millisecond, where already part of the methanol escapes from the drop surface. The temperature curve then levels off while the remaining methanol, the water and part of the acetic acid vaporize. The D^2 -curve shows that the evaporation rate constant is only $0.36 \text{ mm}^2/\text{s}$ at this stage, which is largely due to the high latent heat of the water. This adds to the effect of the relatively high density of the surrogate fuel, increasing from 1050 kg/m^3 to 1317 kg/m^3 over the droplet lifetime.

When practically all the water has been released around $t = 3.5 \text{ ms}$, the temperature curve steeply increases up to the final value just above 600 K , where the levoglucosan evaporates in an equilibrium state. The heating rate in this latter part of the curve is an important indicator for the formation of char inside the droplet. From this model, it follows that the mean heating rate is $8 \cdot 10^6 \text{ K/min}$. This result suggests a low tendency of the droplets to form solid residue according to earlier studies (see Sec. 3.3). The average evaporation rate constant after $t = 3.5 \text{ ms}$ is changing to $1.0 \text{ mm}^2/\text{s}$. In this time range, however, the evaporation rate is also influenced by a rapid increase in temperature of the surrounding gas. Whereas the droplet surrounding is typically around 1000 K up to this point, temperatures up to 2000 K are reached at the end of the curve.

Experimental data to validate the pyrolysis oil results are hardly available, but some valuable measurements have been performed by Shaddix and Hardesty [130]. For poplar and switchgrass oil droplets with an initial diameter of $350 \text{ }\mu\text{m}$, they found that the burning rate “ranged from $\approx 0.3 \text{ mm}^2/\text{s}$ (shortly after the droplet heat-up period) to $0.5\text{--}0.6 \text{ mm}^2/\text{s}$ at later residence times”. An important note is that the square of the nondimensional droplet diameter in these measurements did not reach values lower than 0.75 and 0.85 for respectively the poplar and switchgrass oil due to the occurrence of microexplosions. Nevertheless, these data suggest that the model predicts a representative surface regression rate for the first part of the evaporation curve. The total lifetime of a pyrolysis oil droplet is roughly 60% longer than that of an ethanol droplet. If compared to the evaporation time for No. 2 diesel, even larger differences can be expected since reported burning rates for diesel are slightly higher than for ethanol under similar conditions [61, 130]. This outcome underlines the need for large combustion chambers and fine atomization for burning pyrolysis oil successfully.

3.5.2 Comparison of the evaporation models

To investigate the sensitivity of the droplet life to the evaporation model, additional simulations have been performed with the Spalding evaporation model (Eq. 3.4) instead of the Maxwell equation (Eq. 3.1). The results of Cases E.2 and PO.2 in Table 3.4 are shown in Fig. 3.6. This figure can be compared to the results obtained with the Maxwell equation given in Fig. 3.3. From the difference in spray length between the two cases, it is clear that the evaporation rates predicted by the Spalding model are significantly lower. In the pyrolysis oil simulation, this results in a completely dis-

Figure 3.6: Comparison of the temperature fields for ethanol (top) and pyrolysis oil (bottom) combustion using the Spalding evaporation model instead of the Maxwell equation (Cases E.2 vs PO.2).

torted temperature field since a major part of the spray impinges on the liner. The flame has become detached from its original location and the fuel burns in the rear half of the combustor. Poor solver stability was seen in this case. Flame detachment is not observed in the ethanol case because of the higher volatility, but the evaporation process is much slower for the ethanol spray as well.

A quantitative evaluation of the difference in vaporization rate is given in Fig. 3.7 by comparing the two ethanol cases E.1 and E.2 (note the change in temperature scale). The figure shows that the evaporation rate constant predicted by the Spalding model is only $0.53 \text{ mm}^2/\text{s}$, which results in a 65% increase in average droplet lifetime. Although it is expected that the Spalding model predicts lower evaporation rates than the Maxwell equation as noted in Sec. 3.2, such long evaporation times are highly unlikely considering the measured regression rates listed in Table 3.5. This indicates that the droplet should be regarded as burning rather than evaporating when using the Spalding theory under these conditions. In other words, more accurate results can be expected from the droplet combustion model given by Eq. 3.6 in combination with Eq. 3.10. Calculations performed by Shaddix and Hardesty [130] show that the burning rate predicted by Eq. 3.14 is typically 1.5–2.0 times higher than the evaporation rate obtained from Eq. 3.13 for diesel and pyrolysis oil droplets. This ratio between K_c and K_v agrees well with the difference between the measured and predicted surface regression rates for ethanol as observed in this study.

From the models considered in the present simulations, the Maxwell equation is thus observed to give the most credible results. A possible explanation is that

Figure 3.7: Comparison of the square of the nondimensional droplet diameter and the droplet temperature as function of time in case of ethanol combustion, computed using the Maxwell equation (solid) and the Spalding evaporation model (dashed) (Case E.1 vs E.2).

the adverse effect of Stefan convection at the drop surface is compensated by the flame surrounding the droplet. The over-simplified Maxwell equation, in which both these effects are not included, may therefore still be capable of providing reasonable estimations for the droplet lifetime.

3.5.3 Influence of the initial droplet size

As explained in Sec. 3.4.3, the uniform droplet size used in this study does not reflect the diameter variations observed in practical fuel sprays. The possible influence of this simplification on the results has been examined by performing an additional simulation with ethanol and pyrolysis oil, in which the uniform size was replaced by the Rosin-Rammler distribution shown in Fig. 3.2. This section also discusses the results for a uniform droplet size of 30 μm instead of 50 μm , simulating extremely fine atomization.

Figure 3.8 shows the spray and the temperature field for ethanol combustion using a size distribution (top) and a uniform size of 30 μm (bottom) (Case E.3 vs E.4). The results for these two cases can be compared to the base case with a uniform size of 50 μm , shown in the top half of Fig. 3.3. Aside from the differences in spray penetration, the figures show very similar temperature fields for all three cases. This also holds for the velocity fields, although the velocity contours are omitted here. The results for ethanol combustion are hence found to be remarkably insensitive to the exact size distribution of the droplets specified at the injection location.

In case of pyrolysis oil combustion, the influence of the droplet size on the temperature field is more pronounced. This is illustrated by Fig. 3.9, which compares the

Figure 3.8: Comparison of the temperature fields for ethanol combustion using the Rosin-Rammler distribution shown in Fig. 3.2 (top) and using a uniform drop size of 30 μm (bottom) (Case E.3 vs E.4).

Figure 3.9: Comparison of the temperature fields for pyrolysis oil combustion using the Rosin-Rammler distribution shown in Fig. 3.2 (top) and using a uniform drop size of 30 μm (bottom) (Case PO.3 vs PO.4).

results for a nonuniform drop size (top) to those for a uniform size of 30 μm (bottom) (Case PO.3 vs PO.4). For both cases, the temperature field is significantly different with respect to the base case with a uniform size of 50 μm , shown in the bottom half of Fig. 3.3. An important difference with ethanol is that most of the energy in this fuel is released after the evaporation of the water. When using the Rosin-Rammler distribution (Case PO.3) instead of a uniform size of 50 μm (Case PO.1), a significant part of the fuel reaches this stage in the evaporation process relatively soon due to the presence of small droplets in the spray. This causes the flame temperature to rise faster in the first case. On the other hand, the largest droplets in the distribution do not fully evaporate before impacting the combustor liner. A small fraction of the fuel is therefore burning along the liner wall, where it forms a thin, hot film of product gases.

Impingement of drops on the liner is found to occur for initial diameters larger than 65 μm . This diameter should hence be considered as the maximum desirable droplet size to avoid possible coke formation on the inner liner walls. However, since droplet diameters up to 100 μm are common in practical fuel sprays, it is likely that the spray is partly impacting the liner. This scenario has been confirmed by test runs with pyrolysis oil in OPRA's atmospheric test rig [11], after which some droplet traces were observed on the liner wall around the impact location. Furthermore, it explains why the removal of film cooling on the liner inner wall resulted in a considerable decrease of sediments in preliminary tests with the down-scaled standard combustor [10, 11]. At engine conditions, however, spray impingement is hardly expected to occur because the atomization quality is known to improve at higher pressures.

Changing the droplet size in the pyrolysis oil cases not only influences the temperature field, but also affects the flow field close to the atomizer. When either using a size distribution (Case PO.3) or a very fine spray (PO.4), an additional circulation region is formed in front of the nozzle pintle. It is remarkable, however, that the flow pattern remains unchanged when varying the droplet size in the simulations with ethanol. Figure 3.10 compares the flow fields and sprays of the ethanol and pyrolysis oil simulations using 30 μm as the drop size (Case E.4 vs PO.4). The top half of the figure represents the ethanol case and shows the strong curvature in the flow near the pintle as seen in most of the simulations. In the bottom half, it can be seen that the curvature has turned into a separate vortex. The temperature in this zone is significantly lower compared to the previous situation (typically by 150–300 K), since the new circulation contains part of the atomizing air that otherwise would have followed the swirler air in outward direction. The vortex can thus have adverse consequences for the evaporation and ignition of the fuel, and might affect the performance of the combustor in practice.

The temperature field in the 30 μm pyrolysis oil case is further influenced by the altered spray path as seen in the bottom half of Fig. 3.10. The small droplets are carried in a more forward direction compared to the path of the 50 μm shown in Fig. 3.3, such that the fuel is largely located at the inner side of the bulk flow

Figure 3.10: Comparison of the velocity fields for ethanol (top) and pyrolysis oil (bottom) combustion using a uniform drop size of $30\text{ }\mu\text{m}$ (Case E.4 vs PO.4). An additional circulation region is formed in case of pyrolysis oil. The colors are based on the velocity magnitude.

originating from the nozzle and the swirler. This reduces the mixing of hot product gases on the outer side and therefore results in a lower temperature in the circulation region adjacent to the dome. In combination with the relatively cold vortex in front of the nozzle, the temperature on both sides of the spray has become lower and the combustion heat is more concentrated in the core region of the burner at some distance from the nozzle (see Fig. 3.9).

3.5.4 Comparison of the combustion models

The flame characteristics for pyrolysis oil were calculated by employing the RTE model, in which the gas phase reacts towards thermodynamic equilibrium with a finite reaction rate (see Sec. 3.4.6). In case of ethanol, however, intermediate reactions could be incorporated in more detail by using the flamelet model because reaction mechanisms are available. To evaluate the effect of kinetics on the ethanol flame in these simulations, it is interesting to compare the results obtained with the RTE model on the one hand and the flamelet model on the other hand (Case E.1 vs E.5).

A good impression of the burning process is given by the CO_2 mole fraction contours shown in Fig. 3.11. By comparing the contours for the RTE model in the upper half to those for the flamelet model in the bottom half, it can be seen that the overall reaction towards CO_2 proceeds slower in case of the flamelet model. As a consequence, this model predicts a more distributed release of combustion heat over the combustor volume.

Figure 3.11: Comparison of the CO_2 fields for ethanol combustion using the RTE model (top) and the flamelet model (bottom) (Case E.1 vs E.5).

In the flame zone, where fuel and air mix in a high-velocity flow, the deviation in overall reaction rate is a combined effect of various factors. Given that the velocity fields are very similar but not identical, the local fuel-air ratios in certain regions are different between the both cases. The equilibrium state as well as the influence of turbulence on the chemistry are furthermore calculated in a different manner. On top of that, the RTE model does not account for flame strain. Generally, it can be said that the mixture fraction variance and the scalar dissipation rate strongly reduce the temperature in this zone. When assuming that the more advanced flamelet model gives more accurate results, it is advisable to decrease the overall reaction rate in the RTE model by the lowering the model constant A in Eq. 3.17.

In the post-flame zone, towards the combustor centerline, the effect of the mixture fraction variance and the scalar dissipation rate diminishes. The fuel-air ratio shows only little variation here, and is close to the stoichiometric value. In the figure, it is seen that the CO_2 contours predicted by the two models become similar in this region. However, small concentration differences for species such as CO still result in local temperature deviations of 20–100 K.

Despite the abovementioned differences between the models, it seems that the relatively simple RTE model is suitable for obtaining a good estimation of the flame characteristics. Comparative simulations with ethanol show that the RTE model and the flamelet model are in excellent agreement when A is decreased to a value of 2, but even the default value of 4 leads to fairly similar results. This suggests that the RTE model may also be used to obtain adequate predictions for the pyrolysis oil flame as long as detailed combustion kinetics are not available. The value of A should then

Table 3.6: Predicted and measured CO₂ emissions and outlet temperatures. The model predictions in this table are flow-averaged values in the dry gas. Experimental values have been provided by OPRA. The temperatures are non-dimensional and the concentrations have been normalized to 15% oxygen.

Case	CO ₂ (%)	T_{out} (-)	Case	CO ₂ (%)	T_{out} (-)
E.1	4.27	3.21	PO.1	5.34	3.16
E.3	4.27	3.21	PO.3	5.34	3.15
E.4	4.27	3.21	PO.4	5.32	3.15
E.5	4.19	3.17			
Exp.	4.27	2.79	Exp.	5.45	2.86

be optimized based on experiments.

3.5.5 CO₂ emissions and outlet temperatures

The CO₂ concentrations and dimensionless temperatures at the outlet are given in Table 3.6. The table includes predictions from the CFD model as well as experimental data obtained by OPRA at similar operating conditions [11]. The normalized CO₂ concentrations correspond to the theoretical values based on the atomic ratios of the two fuels and are in good agreement with the measured values. This is an important validation of the overall credibility of the model. Regarding the temperatures, however, the measured values are considerably lower than predicted by the model due to the non-uniform temperature profile at the outlet. Similar deviations have been observed in Chapter 2, where CFD results were compared to experiments in OPRA's conventional fuel burner and adiabatic temperature calculations.

The table furthermore shows that, for the same model configuration, the predicted outlet temperature for pyrolysis oil combustion is slightly lower compared to the ethanol case (Cases PO.1 and E.1). This temperature difference is mainly caused by the higher total mass flow rate in the first case. The lower temperature and CO₂ concentration reported for Case E.5 is due to the high CO level predicted by the flamelet model used in this simulation.

3.6 Conclusions

The combustion of ethanol and fast pyrolysis oil in OPRA's low-calorific fuel burner has been modeled using a the Euler-Lagrange method in ANSYS Fluent. Given the complex, multicomponent nature of pyrolysis oil, a surrogate fuel has been developed to obtain a feasible implementation of its properties in the CFD code. The composition of the light fraction ($T_b < 400$ K) could be derived from experimental data. However, the heavy fraction of the oil was modeled with more uncertainty, be-

cause there is limited knowledge about the composition as well as the evaporation behavior of this fraction at high rating rates.

Comparing the results obtained for pyrolysis oil and ethanol burning, it is found that the peak combustion temperature is relatively low in the pyrolysis oil case. The difference cannot be fully explained by the lower adiabatic flame temperature of pyrolysis oil, and is therefore also related to the multicomponent evaporation and mixing. In addition, it is observed that the pyrolysis oil spray cools down the recirculated gases more strongly because more than twice the amount of heat is required for evaporating the fuel. The total lifetime of a 50 μm pyrolysis oil droplet is approximately 60% longer than that of an ethanol droplet of the same size. For this particular combustor, pyrolysis oil droplets larger than 65 μm are seen to impinge on the combustor liner. These findings underline the importance of a large primary zone and of fine atomization for the combustion of this biofuel. The numerical results are in reasonable agreement with the experimental data available, but further research is needed to validate the simulations in more detail.

The consequences of changing the evaporation model, the initial droplet size or the combustion model on the results have also been discussed. It is concluded that the Maxwell equation gives more credible predictions for the evaporation process than the Spalding evaporation model. Regarding the spray modeling, it is seen that results for ethanol are insensitive to the initial droplet size defined at the injection location in the investigated diameter range. In case of pyrolysis oil, however, changing the droplet size leads to differences in both the temperature and the velocity field. The ethanol flame has been predicted using two different combustion models. Comparative simulations have shown that a model based on thermodynamic equilibrium gives similar predictions as the flamelet model, which is based on chemical equilibrium. This suggests that the general characteristics of a pyrolysis oil flame can be predicted with fair accuracy, even if a reaction mechanism is not available.

Chapter 4

Characterization of viscous biofuel sprays in the near field region

Abstract

The atomization of biodiesel, vegetable oil and glycerin has been studied in an atmospheric spray rig by using digital imaging (PDIA). Images of the spray were captured in the near field of the atomizer and processed to automatically determine the size of both ligaments and droplets. The effect of the spray structure in this region is of major interest for the combustion of biofuels in gas turbines. The sprays were produced by a pressure-swirl atomizer that originates from the multifuel micro gas turbine (MMGT) setup. Various injection conditions have been tested to investigate the influence of viscosity on the spray characteristics and to assess the overall performance of the atomizer. The spray measurements have been compared to combustion experiments with biodiesel and vegetable oil in the micro gas turbine at similar injection conditions. The results show that the primary breakup process rapidly deteriorates when the viscosity is increased. A higher viscosity increases the breakup length, which becomes visible at the measurement location in the form of ligaments. This effect leads to an unacceptable spray quality once the viscosity slightly exceeds the typical range for conventional gas turbine fuels. It was found that the penetration depth of ligaments can have major impact on the combustion process, and that the mean droplet size cannot fully represent the spray quality in the near field. The measured delay in primary breakup at increased viscosity shows that pressure-swirl atomization is unsuitable for the application of pure pyrolysis oil in an unmodified gas turbine engine.

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4.1 Introduction

Pyrolysis oil can be produced from a variety of forest and agricultural biomass waste materials [104] via thermochemical decomposition in absence of oxygen. The dark brown, combustible liquid that results from this process with a yield of 65–75 wt.% is considered as a promising alternative for fossil fuels in industrial applications. However, the presence of a large amount of oxygenated compounds gives pyrolysis oil markedly different properties compared to conventional petroleum-derived fuels. The difference in fuel properties has led to a number of technical hurdles that need to be addressed before application in combustion devices can be successful on the long term.

An interesting possibility is the use of pyrolysis oil in gas turbine engines. Gas turbines are relatively fuel-flexible and are capable of generating power on both large and small scales, suiting the demands of the future energy system. Pyrolysis oil combustion in gas turbines has therefore been subject of a few experimental studies in the past years [10, 95, 97, 122, 138, 143]. These studies, conducted in both scientific and industrial test rigs, have shown that the use of pure pyrolysis oil often leads to major problems. Reported issues include high CO emissions, flame instability, fuel deposits in the hot section and unburned particles in the exhaust gas.

The poor burning characteristics of pyrolysis oil are related to its low volatility, low heating value and limited stability, but can also be attributed to the fuel spray quality. Pyrolysis oil has a high viscosity with respect to the conventional fuels, which causes the atomization process to be less effective [89]. Preheating the oil in order to reduce the viscosity to an acceptable level is only allowed to a limited extent, because certain reactive compounds tend to polymerize at elevated temperatures. Whereas the atomization of pyrolysis oil can be problematic for this reason, it is essential to deliver very fine sprays to cope with the adverse combustion properties of this biofuel. Improving the atomization is not only required to restrict the evaporation time, but can also largely prevent the formation of carbon-rich particles which are sometimes seen as sparks during combustion tests. Previous studies have shown that the amount of solid residue after evaporation decreases with the drop size, since polymerization reactions are suppressed at high heating rates [31, 126].

For these reasons, it is important to measure and compare the quality of sprays under different conditions. Information on the influence of fuel properties helps to further define biofuel specifications and atomization requirements for combustion applications. Spray measurements are furthermore essential for understanding some of the phenomena that occur during test campaigns with various viscous biofuels, i.e. to separate the effects of spray characteristics from those of chemical kinetics.

The literature concerning the atomization of pyrolysis oil or other viscous fuels for gas turbine applications is scarce. Only few studies on this topic have been found, which consider a variety of atomizers, liquids, test conditions and sample locations. Detailed information on the spray in the near field region is not often reported in these studies, presumably due to measurement difficulties. However, the

spray characteristics close to the atomizer are of special interest for evaporation and mixing, and besides most relevant as input data for spray combustion models in CFD.

Krumdieck and Daily [76] were among the first researchers to study the atomization of pyrolysis oil. They tested internally and externally mixed air-assist atomizers for use in spray combustion experiments with this biofuel. The authors concluded that the internally mixed atomizer performed much better, but did not describe the spray quality in terms of droplet size.

López Juste and Salvá Monfort [95] studied the general appearance of a pyrolysis oil spray produced by a pressure-swirl atomizer in preparation for combustion tests. To obtain a viscosity below 10 cP, the pyrolysis oil was preheated to 115 °C. They found that the spray angle decreased from the standard value of 60° for diesel to only 20° for pyrolysis oil. The cause of this remarkable change was not identified. Since the researchers wanted to avoid any major modifications to their injection system, the combustion tests were carried out using a mixture of pyrolysis oil and ethanol to lower the viscosity. Figures defining the spray quality were not discussed.

Significant work on pyrolysis oil atomization has been done by García-Pérez et al. [55]. Their study includes drop size measurements in sprays of pyrolysis oil (at 80 °C), No. 2 diesel (at 25 and 40 °C) and water (at 25, 60 and 80 °C). The sprays were produced by two different Delavan pressure-swirl atomizers (type A and W) at varying injection pressures. Droplet sizes between 2 and 197 µm were measured 50 mm downstream of the atomizer using Malvern Mastersizer equipment, which is based on laser diffraction technology. Within the tested range of injection pressures, the Sauter mean diameter (SMD) of the pyrolysis oil sprays was 45–75 µm for atomizer type A, and 35–70 µm for atomizer type W. These values were typically 10–20 µm higher than those measured in the diesel and water sprays. The difference was attributed to the relatively high viscosity of the pyrolysis oil, which was still 17 cP despite preheating to 80 °C.

Atomization studies related to other viscous biofuels than pyrolysis oil can provide useful insights as well. Crayford et al. [37] investigated the pressure-swirl atomization of a bio-oil derived from the food industry. Details about the viscosity of the bio-oil are not given, but a temperature of 27.5 °C was indicated as the melting point. The researchers used phase Doppler anemometry (PDA) to record the droplet size and velocity simultaneously at a specified point, while backlight photography was employed for providing information on the general spray structure. The global SMD of the full cone bio-oil spray, derived from local measurements at 6 axial and 9 radial positions, decreased from 59 to 55 µm when preheating the fuel from 60 to 80 °C. At 80 °C, the global SMD and structure of the bio-oil spray and the benchmark gas-oil spray were similar. However, the authors underline that characterization of an entire spray using a single drop diameter is problematic. Close to the atomizer, 25 mm downstream, a preheat temperature of only 70 °C would be necessary to match the SMD measured in the gas-oil case.

Panchasara and Agrawal [116] examined straight vegetable oil (VO) sprays pro-

duced by an airblast atomizer at different oil temperatures and air-to-liquid ratios (ALR). Laser sheet visualization was used to capture spray images for qualitative analysis. Quantitative, pointwise measurements of droplet diameters and gas phase velocities in the full cone were performed with a phase Doppler particle analyzer (PDPA) system. It was found that an increase in oil temperature and ALR both improve the atomization, especially in the outer region of the spray. However, with a maximum SMD of only 60 μm for a VO viscosity of 28 cP, good atomization was achieved even at low oil temperature and low ALR. In the near field, 20 mm downstream, the SMDs were below 42 μm at all conditions.

Recently, interesting results have been presented on the atomization of viscous fuels using a novel method referred to as ‘flow-blurring’ [24, 133, 134]. In this concept, air penetrates the fuel flow in a region close to the orifice to create a turbulent two-phase mixture. The air bubbles contained in the fuel rapidly expand when exiting the nozzle, thereby disintegrating the liquid structure. This technique has been shown to deliver superior atomization performance compared to conventional airblast atomization methods and is suggested to have an advantage over effervescent atomization regarding the flow stability inside the atomizer. Droplet size measurements using PDPA in reacting glycerol sprays and in non-reacting vegetable oil and diesel sprays produced by a flow-blurring atomizer have been reported by Simmons and Agrawal [132, 133]. Without preheating the liquids, they obtained SMDs of typically 25–40 μm in the glycerol spray (100 mm downstream) and 35–55 μm in the near field of the vegetable oil spray (20 mm downstream). Such SMDs are exceptionally low, considering the viscosities of respectively 930 and 50 cP. The flow-blurring atomizer is still in the research phase and not (commonly) used in practical combustion applications yet.

In this work, the effect of viscosity on spray quality has been assessed by using an economically attractive high-resolution particle imaging technique (PDIA). Sprays of three different liquids were visualized at varying injection conditions in the region near the atomizer to investigate the primary atomization process. The size of the droplets captured on the images was then determined via automated analysis. Also the effect of ligaments in the proximity of the atomizer was taken into account, showing the significance of a proper primary breakup process. The investigated sprays were produced by the pressure-swirl atomizer from the multifuel micro gas turbine (MMGT) setup at the University of Twente. The droplet size data resulting from this study can therefore be compared with exhaust gas emissions measured in combustion experiments (see Chapter 5).

4.2 Research method

The droplet size measurements in the present study have been performed using a non-intrusive optical technique referred to as particle/droplet image analysis (PDIA) [73]. In this method, the spray is first visualized by capturing shadow images of the

droplets. The spray images are then analyzed on a computer using a Matlab script for automatic recognition and sizing of the droplets.

Among the methods available for sizing droplets, direct imaging has until recently been an uncommon technique for the characterization of sprays used in combustion applications. Limitations in resolution and sensitivity made photography unreliable or too costly for sizing the small droplets in the range 10–100 μm , typical for fuel sprays. Thanks to great progress in digital imaging technology, however, PDIA has proven to be a robust, accurate and cost-effective tool for research on fuel atomization [27, 73]. The method has besides an important advantage over other techniques, such as PDA, since it delivers a visual impression of the spray structure. This allows for detecting liquid fragments of any shape and gives good insight into the breakup process as shown in several studies [5, 26, 58, 59, 75, 78, 82].

In this section, the experimental setup that was developed for capturing high quality images of the spray will be explained first. Subsequently, details are given about the methods used for analyzing the images to evaluate the spray quality.

4.2.1 The spray imaging setup

The spray imaging setup has been designed to visualize individual droplets in a spray at different pressures and temperatures. Following the principle of shadowgraphy, a downward spray is exposed to a light source on one side, providing background illumination for a camera that is located on the opposite side. As the droplets reflect or deflect the majority of the incident backlight, they are seen as dark spots on the image when crossing an imaginary measurement volume defined by the position and optical characteristics of the camera. This configuration is schematically illustrated in the setup overview shown in Fig. 4.1. The position of the light source in the setup is fixed, while the camera position can be adjusted electronically to shift the focal plane towards the desired location in the spray. The location of the camera is horizontally and vertically measured with micrometer accuracy using a linear encoder system.

A frequency-doubled Nd:YAG laser serves as the light source for the measurements. The laser emits light with a wavelength of 532 nm, a pulse duration of 6 ns and a maximum pulse energy of 1 J. These pulses were short enough to avoid any motion blur and sufficiently intense to obtain good contrast in the images. However, direct use of the laser spot results in a highly disturbing speckle pattern due to mutual interference of the single-frequency light waves. Hence, after entering the spray chamber, the laser beam penetrates a glass flow cell with a fluorescent dye solution. The light emitted by the dye covers a wider spectral range and provides high quality, uniform illumination of the image background. A ground glass diffuser is placed just in front of the flow cell to obtain a more uniform laser spot for excitation of the dye.

The droplets in the spray are captured using a digital camera (Nikon D5200) with a resolution of 6000×4000 pixels. The images on the sensor are formed by

Figure 4.1: Schematic overview of the spray imaging setup.

a micro lens (Tamron 180 mm F3.5 Macro 1:1) and a teleconverter (Kenko DG MC 3X PRO300), which together achieve a maximum reproduction ratio of 3:1. This combination resulted in an optical system with sufficient magnification and resolution to capture the droplets at a suitable focal distance. All three components are mounted vertically in a box to protect the system against the spray. Images are captured through a glass window in the bottom of the protection box and via a silver-coated mirror underneath. The camera is remotely controlled and sends the images directly to the computer.

The timing of the laser Q-switch and the camera shutter is managed by a delay generator. By activating the triggering scheme programmed in the delay generator, the image capturing is performed automatically with a total cycle time of 2 seconds per image.

An external fuel supply system is used to control the liquid flow. This system is able to supply liquid to the atomizer at pressures up to 60 bar and temperatures up to 100 °C. The liquid temperature is measured close to the atomizer using a K-type thermocouple in the flow.

In order to prevent accumulation of mist inside the setup, the air inside the spray chamber is ventilated by using a centrifugal air extractor. The air inlets are located in the side walls to minimize interactions between the air flow and the spray.

Figure 4.2: Process flow diagram of the image analysis script.

4.2.2 Digital image analysis

The images captured in the experimental setup are automatically analyzed using a Matlab script. The script is developed to recognize spherical as well as non-spherical liquid objects in the image and rejects any objects of which the size cannot be determined accurately. The output data contain the relevant geometric properties of all accepted objects, which are used to calculate the overall spray characteristics.

First of all, the quality of the raw image data is assessed by checking the intensity of the background illumination. Since the object recognition method is based on contrast, the results from the script are rather sensitive to variations in background intensity. Images with insufficient overall contrast are therefore removed from the raw data set. Very few images were rejected, however, as the exposure was generally constant during the measurements.

The remaining images are then analyzed by the script, following the procedure that is schematically shown in Fig. 4.2. The procedure starts by converting the raw RGB image to grayscale and enhancing the contrast. The enhanced image is then reduced to a binary image in black-and-white (B/W) using a certain threshold value. The binary image is the input for the Canny edge detection [25], of which the result is

improved by a cleanup process. Edges with single-pixel gaps (equivalent to $1.47\ \mu\text{m}$) are closed, whereas edges with larger gaps are discarded. Closed edges mark the contours of objects in the image.

After identifying the objects, their pixel regions are used to determine the relevant geometric properties. Here, the effective diameter is derived from the surface area to increase the linear accuracy. Objects that are smaller than the chosen size threshold are removed, because the sizing method becomes inaccurate if an object contains only a few pixels.

The objects are then classified as either droplets or ligaments based on the roundness parameter $4\pi A_c / p^2$, where A_c is the cross section area and p is the perimeter. This parameter is unity if the cross section of the object is perfectly circular, and goes towards zero if the shape deviates from a circle. In this study, objects are marked as non-spherical if the parameter is below the threshold of 0.25. Droplets or ligaments containing considerable cavities are removed after hole detection. Holes in an object lead to errors, since the objects are identified on basis of the outer edge and cavities would be considered as part of the liquid phase.

Subsequently, it is essential to determine if the detected objects are in focus. The sizing of objects that are located partly or entirely out of the measurement volume is unreliable due to a lack of contrast with the background. The out-of-focus detection in the script is based on the approach described by Lee and Kim [84], who propose to use a combination of two parameters. The first is the gradient intensity (GI), evaluating the average normal gradient at the object boundary. The second parameter is the value of contrast (VC), which is defined as the normalized maximum contrast between the object and the background. The VC can be more effective for testing small objects. The droplet and ligaments are considered in focus only if both the GI and VC criteria are satisfied.

Converting the geometric object properties from pixels to micrometers gives the final output data for the individual droplets and ligaments. These data contain the surface area, the perimeter and, in case of droplets, the effective diameter. However, when the overall spray quality is evaluated by calculating a mean diameter, the droplet data needs to be corrected for differences in the depth of field. The depth of field (DoF) of the optical system is here defined as the depth of the imaginary measurement volume around the focal plane, in which objects are photographed acceptably sharp for measuring their size with good accuracy. This optical property depends on the size of the object to be captured, see Fig. E.3 in Appendix E.1. Similar trends were found by Lee and Kim [84] and by Castanet et al. [26]. Since the depth of field starts to decrease when the object size falls below a certain limit, the method is naturally biased towards large droplets and ligaments. The depth of field correction that has been applied to compensate for this effect is described in Sec. 4.3.2.

In the analysis procedure described above, certain input parameters need to be defined that have influence on the final result. As can be seen in Fig. 4.2, the script uses several threshold values as well as a conversion factor between pixels and micrometers. Furthermore, a depth of field correction is used to obtain a more realistic

result for the spray quality. To minimize the measurement error and optimize the setup's capabilities, the most influential input values have been defined by measuring the system characteristics and by calibration. The results from these activities are described in Sec. 4.3 and Appendix E.1.

4.3 Optimization of the method

The characteristics of the optical arrangement are mainly expressed by the focus distance, field of view, reproduction ratio, exposure and depth of field. These properties are largely determined by the hardware, but are also influenced by the zoom and aperture setting. A parameter study was therefore performed to optimize the system settings for the droplet size measurements. The optical characteristics are furthermore required to define and optimize the input values for the image analysis script as described in Sec. 4.2.2.

4.3.1 Optimization procedure

To measure the reproduction ratio and the depth of field at different settings, a Patterson globe reticle [119] was used as a reference. The 10 circles with different diameters that are printed on the glass surface cover the size range representative for the droplets to be measured. Figure 4.3 shows the circles as captured by the camera in the spray imaging setup. Here, the circle diameter decreases from 450 μm on the left to 18 μm on the right.

Figure 4.3: Circles on the reticle as captured in the setup.

The reproduction ratio is found by capturing the reticle in the focal plane. The circle diameters in terms of pixels as measured using the analysis script are then compared to their real sizes. This ratio directly gives the pixel-to-micron conversion factor, which is equivalent to the reproduction ratio. Once the conversion factor is known, the depth of field can be determined by photographing the circles at varying distance from the focal plane until they appear completely blurred. The threshold values in the script that govern the in-focus criteria are then adapted such that the measurement error is acceptable for each size (see Fig. 4.4). Since changing the threshold values also affects the conversion factor, these parameters have been optimized in an iterative process.

Figure 4.4: Relative measurement error as function of the GI.

4.3.2 System characteristics and accuracy

On basis of the results from the parameter study, the zoom setting was chosen as a trade-off between focus distance, reproduction ratio and depth of field. The aperture setting followed from balancing the exposure and depth of field. For this optimized configuration, the conversion factor is measured to be $1.47 \mu\text{m}/\text{px}$. The associated field of view is about $8.8 \times 5.9 \text{ mm}$ as a consequence of the sensor resolution.

The input parameters of the analysis script were adjusted such that the measurement error is restricted to an acceptable level. From the results of the depth of field analysis given in Appendix E.1, it can be concluded that the gradient intensity (GI) parameter is effective for controlling the error by rejecting the out-of-focus objects of any size. The percentual measurement error relative to the circle size is shown as function of the GI in Fig. 4.4. By choosing a GI of 0.25, as indicated in the figure, the maximum relative error in the investigated size range from 18 to 450 μm is kept under 12% of the object diameter.

The value of contrast (VC) parameter has a nearly constant value of 1 for all circles larger than 40 μm due to the fact that even blurry objects have a very dark area in the center. Therefore, the VC is generally unsuitable as a selection criterium in this case. A useful relation between the VC and the distance from the focal plane is only observed for the smallest circle of 18 μm , but also for this size the GI is found to be more strict so that the VC is completely overridden.

The graphs shown in Appendix E.1 also illustrate that the depth of field increases with the object size. According to Fig. E.1, the depth of field ranges from 400 μm for the 18 μm circle to 1050 μm for the 450 μm circle when the GI is set to 0.25. The markers in Fig. 4.5 indicate the depths of field measured for the sample diameters

Figure 4.5: Relative depth of field as function of the object size.

considered in the analysis, relative to the depth of field for the largest circle (450 μm). To construct a curve over the entire range, the markers are connected using linear segments. The depth of field correction applied in the script is performed by dividing the number of detected droplets of a certain size by the corresponding value prescribed by Fig. 4.5. This way, the relative depth of field is virtually restored to 100% for all object sizes.

An effective object diameter of 15 μm is chosen as the lower detection limit of the method. This diameter, represented by 10 pixels on the image sensor, is adopted as the size threshold in the analysis script (see Fig. 4.2).

4.4 Test conditions

4.4.1 Atomizer specification

The sprays in the atomization tests were produced by the pressure-swirl atomizer that originates from the multifuel micro gas turbine (MMGT) setup at the University of Twente. A drawing of this atomizer is given in Fig. 4.6. The atomizer produces a hollow cone spray with an angle of 90–100° and is characterized by a flow number of $41 \cdot 10^{-8} \text{ m}^2$. The flow number was experimentally determined and can be used to accurately describe the mass flow rate through the atomizer via the following relation [89]:

$$\dot{m} = \text{FN} \sqrt{\rho_l \Delta p} \quad (4.1)$$

where FN is the flow number, ρ_l is the liquid density and Δp is the applied pressure difference.

Figure 4.6: Drawing of the tested pressure-swirl atomizer: 1 - swirl chamber housing, 2 - gasket, 3 - pressure piece, 4 - nozzle screw, 5 - nozzle body, 6 - filter, 7 - housing, 8 - gasket, 9 - gasket, 10 - nozzle cap, a - swirl chamber inlet, b - cooling air inlet, c - fuel inlet. Reproduced from [57].

4.4.2 Properties of the tested liquids

The spray characteristics have been studied for three different liquids: biodiesel (BD), vegetable oil (VO) and glycerin (GL). These liquids have been selected to investigate the effect of mainly viscosity on the average spray quality. Together with the density and surface tension of the liquid, the viscosity is seen as one of the relevant properties in pressure atomization [89]. Since the density and surface tension are much weaker functions of temperature, preheating primarily influences the viscosity of the liquids. This is illustrated by Table 4.1, where the properties of interest are given for the three liquids at the minimum and maximum temperature used in the experiments.

Table 4.1: Variation in biodiesel, vegetable oil and glycerin properties over the tested temperature ranges. Viscosities were measured, densities and surface tensions were obtained from [8, 48, 60].

Property	Unit	Biodiesel		Vegetable oil		Glycerin	
		20	60	50	100	60	100
Density	kg/L	0.87	0.84	0.90	0.87	1.18	1.15
Surface tension	mN/m	32	28	31	28	62	58
Viscosity	cP	6.3	2.3	17.9	4.9	17.0	4.8

Figure 4.7: Measured viscosity of the three tested liquids as function of temperature.

The properties of biodiesel at 60 °C are equal to those of No. 2 diesel at room temperature. The spray characteristics for biodiesel at this temperature should therefore be representative for operation at standard diesel fuel. The liquid referred to as vegetable oil here is actually a mixture of straight vegetable oils that is characterized by a high viscosity. The density of this oil mixture is slightly higher compared to biodiesel, whereas the surface tension is nearly the same within the respective temperature ranges. Both these fuels were recently tested in the MMT setup to measure the effect of fuel viscosity on the exhaust gas emissions (Chapter 5). The spray quality measured in the present study can therefore be compared to emission data obtained from the combustion tests.

The glycerin is a 77 wt.% glycerol/water mixture, which is chosen as a test liquid to investigate the influence of viscosity when also the density and surface tension are considerably higher than those of the standard fuels. Testing with a high surface tension is relevant because values up to 40 mN/m have been measured for pyrolysis oil at room temperature [130], whereas the typical value for diesel is 28 mN/m. The surface tension for the glycerin is even higher than for pyrolysis oil, however, so that the effect of this property will be exaggerated. The density of the glycerin is in good agreement with that of pyrolysis oil.

Since the study is focused mainly on the influence of viscosity in relation to atomization quality, this fluid property was measured as function of temperature using a Brookfield DV-II + Pro viscometer. The results are shown in Fig. 4.7, where regression curves indicate the viscosity outside of the measurement range.

Figure 4.8: Impression of the size and location of the focal plane in the spray.

4.4.3 Operating conditions

An overview of the atomizer operating conditions is shown in Table 4.2. All images have been captured 18 mm downstream of the atomizer, see Fig. 4.8. This sample location corresponds to the height where the primary breakup process is just completed in the biodiesel spray at 10 bar and 20 °C. The optical system was configured as defined in the optimization procedure. However, the ISO value was adjusted to compensate for a reduction in camera exposure at higher injection pressures, presumably caused by a higher spray density or a slight increase in spray cone angle.

The images are uncorrelated snapshots of a quasi-steady spray. Since it is a matter of coincidence which part of the spray is present in the measurement volume, a sufficient number of images are required to determine the average spray characteristic at the sample location. Preliminary image data has shown that the mean droplet size indeed fluctuates for each image but converges to a constant value by including more images in the dataset. To ensure a converged result, 80 to 100 images were captured at each injection condition. The convergence of the SMD for different sprays at 10 bar and 30 bar is illustrated in Appendix E.2.

Table 4.2: Overview of the atomizer operating conditions.

Liquid	Pressures (bar)	Temperatures (°C)
Biodiesel	10, 20, 30	20, 30, 40, 60
Vegetable oil	10, 20, 30	50, 60, 70, 80, 90, 100
Glycerin	10, 20, 30	60, 70, 80, 90, 100

4.5 Results and discussion

Objects detected in the image analysis procedure are marked as either spherical or non-spherical. This feature allows to evaluate the atomization quality for combustion applications on basis of droplets as well as ligaments. Information on both types of objects is reported by expressing the results in terms of three different parameters that are used as spray quality indicators: the normalized ligament area (NLA), the mean ligament size (MLS) and the Sauter mean diameter (SMD). The influence of pressure and temperature on these indicators is shown for successively the biodiesel, vegetable oil and glycerin sprays. Figure axes have been fixed for convenient comparison of results for the different liquids. The experimental data are subsequently compared to the combustion performance as measured in the MMGT setup (see Chapter 5). Implications for pyrolysis oil combustion in the MMGT setup will be considered at the end of this section.

4.5.1 Spray quality indicators

In pressure-swirl atomization, the liquid leaves the nozzle orifice in the form of a thin, conical sheet. Instabilities in the liquid cause the sheet to disintegrate into elongated structures or ligaments, which then break up further to form droplets [4]. This process is usually referred to as primary breakup. The droplets may then split up further due to interactions with its surroundings during secondary breakup. Images containing ligaments thus show that the primary breakup process was incomplete or that secondary breakup of big drops is occurring at the measurement location. In this study, the capturing of ligaments formed during primary breakup is promoted by measuring close to the atomizer.

The content of non-spherical objects in the measurement data has been quantified by calculating the normalized ligament area (NLA). This parameter is defined as the total area represented by ligaments, normalized with the total area of both ligaments and droplets as measured in the images:

$$\text{NLA} = \frac{\sum A_{c,\text{lig}}}{\sum A_{c,\text{lig}} + \sum A_{c,\text{drop}}} \quad (4.2)$$

where A_c refers to the cross-sectional area.

The NLA can be used as an indicator for primary breakup, though also secondary breakup has influence on its value. In the latter case, however, the elongated shape is not representing a ligament directly originating from the liquid film, but defining the contours of a heavily distorted droplet. Such objects are typically smaller than ligaments and are beneficial for the spray quality due to their higher surface-to-volume ratio. They are besides likely to break up into even smaller droplets in the next moment, which evidently leads to faster evaporation. Poor atomization is hence indicated only by the considerably larger ligaments formed during primary breakup. Therefore, in case the NLA of a spray is substantial, it is relevant to determine the

size of the ligaments as well. To this end, an additional parameter expressing the mean ligament size (MLS) is defined as the total ligament area divided by the total number of ligaments:

$$\text{MLS} = \frac{\sum A_{c,\text{lig}}}{N_{\text{lig}}} \quad (4.3)$$

The NLA and MLS parameters together give essential information about the atomizer performance at certain injection conditions. It must be noted, however, that flawless detection of ligament boundaries is more challenging than resolving droplet boundaries. The most complex shapes are therefore not always properly recognized, so that some of the ligaments can be missing in the data set. Still, despite this deficiency, the ligament data is useful for indicating the trends.

The Sauter mean diameter (SMD or D_{32}) is used as a third indicator of the atomizer performance to compare the droplet size distributions obtained from the image data. Examples of such distributions can be found in Appendix E.3. The SMD is a suitable measure for the mean droplet size in the spray when evaporation is important as it compares the total spray volume to the total surface area. The definition of the SMD is given by Eq. 4.4, where D_{drop} is the calculated effective diameter of the droplet based on its area. Non-spherical objects are not taken into account here, because their volumetric shape is rather arbitrary.

$$\text{SMD} = \frac{\sum D_{\text{drop}}^3}{\sum D_{\text{drop}}^2} \quad (4.4)$$

4.5.2 Results for biodiesel

Figure 4.9 shows the NLA as function of pressure for the biodiesel sprays at 20 to 60 °C. Recall that the axes have been scaled in conformity with the figures showing data for the other liquids. Considering the low values, the primary breakup process can be assumed to be complete at all conditions. The graph also shows that the temperature has no significant effect. Apparently, the changes in biodiesel properties over the temperature range are relatively small in relation to atomization.

By raising the pressure, however, the NLA is observed to slightly increase. This trend can be mainly attributed to secondary breakup of large droplets. A larger pressure drop over the orifice results in stronger instabilities propagating in the liquid, which can be dominant over the surface tension forces that tend to restore the spherical shape. In such cases, the liquid elements are detected as ligaments instead of droplets. The secondary breakup process leads to a better spray quality, since the volume-to-surface ratio of a stretched droplet is more favorable and some of the large droplets will split up. Another possible explanation is the higher exit velocity at the atomizer orifice. Since the measurement location is fixed in space, the available breakup time becomes shorter when increasing the pressure and breakup might

Figure 4.9: Normalized ligament area as function of pressure for biodiesel.

have not taken place yet for a small part of the ligaments. Given the fact that the MLS is not increasing with pressure, however, this effect is most likely not significant here.

The SMD as function of pressure is reported in Fig. 4.10 for the different temperatures. Increasing the pressure from 10 to 30 bar leads to a considerable reduction in SMD, roughly from 80 down to 60 μm . Again, no clear effect of temperature is observed. It can therefore be concluded that the spray quality at the sample location is insensitive to variations in viscosity between 2 and 6 cP.

4.5.3 Results for vegetable oil

The physical properties of straight vegetable oil are quite similar to those of biodiesel, except for the viscosity. Vegetable oil is therefore suitable to nearly isolate the effect of increased viscosity on the spray quality. Any influence of temperature on the atomization performance is consequently assumed to be caused by viscous effects.

In contrast to the biodiesel cases, preheating was required to achieve an acceptable degree of atomization. An evident relation between the spray and the oil temperature was hence already seen during the measurements in the experimental setup. This relation is further illustrated in Fig. 4.11, showing the NLA for the vegetable oil sprays at temperatures between 50 and 100 °C. It can be seen that the NLA is clearly reduced by increasing the temperature until it reaches a certain minimum value. This reduction indicates that ligaments appear less frequently as the primary breakup is enhanced at lower viscosities. The temperature at which the minimum NLA is reached depends on the pressure. The detected ligament area is reduced between 50 and 90 °C at a pressure of 10 bar, while at 30 bar it is redundant to preheat

Figure 4.10: SMD as function of pressure for biodiesel.

to temperatures above 60 °C. It can thus be concluded that the effect of temperature is more pronounced at lower pressures.

The minimum NLA that can be reached slightly increases towards higher pressures. Such a trend was also observed in the biodiesel results described earlier (see Fig. 4.9) and can be attributed to secondary breakup. Here, it is important to note the similarity in viscosity of both liquids at these conditions, as can be seen in Fig. 4.7.

Since a significant portion of the spray volume is represented by ligaments at some of the investigated conditions, the mean ligament size is considered in addition to the NLA. In Fig. 4.12, the MLS is given as function of pressure for the temperatures at which the NLA exceeds 3%. A consistent trend is observed towards smaller ligaments with increasing pressure and temperature. The graph illustrates that the influence of the injection conditions is in fact stronger than suggested by the NLA data in Fig. 4.11. Raising pressure or temperature does not only reduce the breakup time of ligaments but also decreases their average size, thereby promoting the heat transfer to the spray in two different ways.

Figure 4.13 presents the SMD of the droplets in the vegetable oil sprays at temperatures between 50 and 100 °C. Considering the strong influence of temperature on the primary breakup process, it is noteworthy that such a clear dependency is not observed in the results for the mean droplet size. Variations with temperature are only noticed at a pressure of 10 bar, where the SMD fluctuates between 66 and 74 μm, though the relation between temperature and droplet size is inconsistent. Possibly, only the thin ligaments were disintegrated, while the thicker ones are still largely intact at this pressure. Since ligaments are not included in the SMD calculation, higher viscosity might lead to a lower droplet size in some cases. Increasing the

Figure 4.11: Normalized ligament area as function of pressure for vegetable oil.

Figure 4.12: Mean ligament size as function of pressure for vegetable oil.

Figure 4.13: SMD as function of pressure for vegetable oil.

pressure causes a slight reduction in SMD.

The mean droplet sizes shown in the figure are similar to those measured in the biodiesel cases, see Fig. 4.10. The results for vegetable oil in comparison to biodiesel therefore suggest that the droplets formed during primary atomization are not responsible for any major combustion issues. Instead, the problematic combustion behavior of a fuel with such a high viscosity is more likely caused by the tendency of ligaments to persist. As the breakup of ligaments is delayed or even prevented due to viscous dissipation, a high temperature or more atomization energy is required to restore the spray quality.

4.5.4 Results for glycerin

Regarding atomization, the physical properties of the glycerin are different from those of biodiesel in every aspect (see Table 4.1). It must therefore be kept in mind that the trends for glycerin may describe effects of surface tension and density next to viscosity. Considerable differences are also observed with respect to the vegetable oil properties, although the viscosities of both liquids are in the same range. In the following discussion of the results for glycerin, the differences with respect to the vegetable oil data are occasionally illustrated by figures comparing two images taken of the sprays. In each of these figures, both images have been obtained for the same injection pressure and liquid viscosity.

Measurements with glycerin were performed at temperatures starting from 60 °C to avoid capturing the liquid film that leaves the atomizer orifice. In Fig. 4.14, however, high NLA levels show that the primary breakup is still incomplete at temperatures under 80 °C. A typical image taken from the 10 bar glycerin spray at 60 °C is

Figure 4.14: Normalized ligament area as function of pressure for glycerin.

given in Fig. 4.15. The snapshot of the glycerin spray is shown next to a representative image taken from the vegetable oil spray for the same pressure and viscosity. The ligaments visible in each image confirm the deterioration of the atomizer performance at such conditions. By studying all images captured from the two sprays in a qualitative manner, it is found that the sprays are quite similar regarding the frequency and size of the ligaments.

At high pressure, however, this similarity is not observed anymore. Compared to the vegetable oil spray, the ligaments in the glycerin spray at 30 bar are generally larger and besides seen more frequently. The difference in size is illustrated in Fig. 4.16, where the two images show the largest ligament found in respectively the glycerin and the vegetable oil spray. This insight is also provided by considering the NLA data for both sprays. The upward trend of the NLA with pressure in Fig. 4.14 is indeed opposite to the trend seen in Fig. 4.11 for the vegetable oil spray. Since the viscosity is the same in these cases, the deviating trend for glycerin must be related to the combination of high surface tension and increased liquid density.

(a) GL, 10 bar, 60 °C

(b) VO, 10 bar, 50 °C

Figure 4.15: Example images of a glycerin spray (a) and vegetable oil spray (b) at low pressure and low temperature. The viscosity of both liquids is about 17 cP.

(a) GL, 30 bar, 60 °C

(b) VO, 30 bar, 50 °C

Figure 4.16: Example images of a glycerin spray (a) and vegetable oil spray (b) at high pressure and low temperature. The viscosity of both liquids is about 17 cP.

Figure 4.17: Example images of a glycerin spray (a) and vegetable oil spray (b) at high pressure and high temperature. The viscosity of both liquids is 4.8 cP

When the glycerin temperature is 80 °C or above, the primary breakup occurs upstream of the measurement location. Although the NLA in Fig. 4.14 is indeed expected to decrease due to reduced viscosity, the graph shows exceptionally low values at all pressures. This behavior is a consequence of the surface tension, which quickly forces the liquid elements into a spherical form once primary breakup has occurred. Since ligaments are distinguished from droplets based on their roundness, virtually all objects detected in the images are identified as droplets. The strong shape-preserving tendency also suppresses further breakup of the droplets. The slight increase in NLA with pressure, measured for biodiesel and vegetable oil at such low viscosities (see Figs. 4.9 and 4.11), is therefore not observed here. Manual inspection of the images confirm that secondary breakup does hardly occur. The difference in droplet shape between glycerin and vegetable oil sprays is visually illustrated by the images in Fig. 4.17.

Figure 4.18 shows that the average size of the ligaments detected in the glycerin sprays is decreased by raising the pressure. This trend agrees with the results for vegetable oil given in Fig. 4.12 and confirms that the breakup of ligaments is improved when more atomization energy is transferred to the liquid.

The SMD of the sprays in the temperature range 60 to 100 °C is given in Fig. 4.19. A comparison with the data for biodiesel and vegetable oil in Figs. 4.10 and 4.13, respectively, indicates that the glycerin droplets are significantly larger at all conditions. The difference is highest at 10 bar, where the SMD of glycerin is 100–110 μm against 70–80 μm for the other two liquids. Even though the primary atomization

Figure 4.18: Mean ligament size as function of pressure for glycerin.

Figure 4.19: SMD as function of pressure for glycerin.

is complete at 80 °C and above, such large droplets are not likely to evaporate fast enough in a conventional gas turbine combustor. The mean droplet size can be reduced by increasing the atomization energy via the pressure, but a pressure of 30 bar is needed to obtain similar SMD values as measured in the vegetable oil sprays at only 10 bar. Again, the SMD does not show a consistent relation with temperature. For this reason, the atomization quality at the sample location cannot be derived from the droplet data only.

4.5.5 Comparison with combustion experiments

The biodiesel and vegetable oil used in the present study have also been tested in the MMGT setup. This setup was employed to investigate the influence of viscosity on the burning performance of the two biofuels in a micro gas turbine, as described in detail in Chapter 5. Since the fuel spray was produced by the same atomizer in both studies, it is interesting to compare the results from the combustion experiments with the measured spray characteristics reported above.

In combustion tests with vegetable oil in idle mode, the exhaust gas contained a significant amount of unburned fuel in the form of blue smoke when the viscosity exceeded 9 cP. The smoke was assumed to be caused by incomplete evaporation of the fuel, creating fuel-rich zones in which the fuel is partly cracked instead of combusted. In such case, the poor breakup should be recognizable in the spray characteristics at such conditions. Given that the injection pressure during these tests was 13 bar and that the combustion chamber pressure was 2.0 to 2.5 bar, the pressure difference over the atomizer was approximately the same as in the 10 bar cases in the present study.

As mentioned in Sec. 4.5.3, the vegetable oil spray quality is most likely determined by the ligaments observed in the spray. Therefore, the viscosity limit that followed from the burning tests is to be compared with the NLA as function of viscosity, shown in Fig. 4.20 for a pressure of 10 bar. The figure indicates that the delay in primary breakup becomes visible in the images when the viscosity exceeds 7 cP. This turning point is in fairly good agreement with the combustion tests. The small difference of 2 cP can be related to a few uncertain factors that could have promoted the breakup in the combustion chamber. Firstly, the flame might have been located slightly downstream of the sample location, which would give ligaments more time to break up before entering the flame. Secondly, the atomizer cooling flow and swirling air flow enveloping the spray may have caused additional instabilities. According to Lefebvre and Ballal [89], also the higher air density in the combustor can lead to a shorter breakup length. For these reasons, it is well possible that the adverse effects of ligament formation were slightly suppressed in the combustor with respect to the current measurements in the spray rig.

Another result from the combustion tests is the relation between viscosity and CO emissions as shown in Fig. 4.21. For both biodiesel and vegetable oil injected at 12 to 13 bar, the CO concentration in the exhaust gas was found to increase linearly

Figure 4.20: Normalized ligament area as function of viscosity at a pressure of 10 bar.

Figure 4.21: CO emissions at 15 vol.% O₂ as function of viscosity for No. 2 diesel, biodiesel and vegetable oil.

with viscosity in the range 2 to 9 cP. Figure 4.22 reports the SMD of the investigated 10 bar sprays with viscosities up to 10 cP. The graph shows that the assumed relation between viscosity and droplet size in this range cannot be confirmed. In fact, the SMD is quite insensitive to viscosity, which suggests that the decrease in CO emissions is primarily related to the breakup length of the spray, see Fig. 4.20. Figure 4.23 shows a slight increase in SMD with viscosity for the 30 bar sprays, but this effect is small compared to the influence of pressure.

In Figs. 4.22 and 4.23, it is seen that the SMDs for glycerin are relatively large with respect to those for biodiesel and vegetable oil. These graphs therefore show that liquids with high density and surface tension are atomized less efficiently, irrespective of the viscosity. The influence of density with respect to surface tension has not been investigated in the present study. However, it is noteworthy that the density is usually considered as the least significant among the three liquid properties affecting the spray structure [86]. The relative variation in density between the tested liquids is besides considerably lower than the relative difference in surface tension, see Table 4.1. Therefore, it can be expected that the surface tension plays a more important role here by inhibiting the formation of additional surface area.

4.5.6 Implications for pyrolysis oil combustion

The results obtained in the present study can be used to estimate the technical feasibility of burning pure pyrolysis oil in a gas turbine by employing pressure-swirl atomization. As outlined in the introduction, fine atomization is a critical aspect considering the adverse properties of this biofuel compared to conventional fuels. The experiments with biodiesel, vegetable oil and glycerin are therefore valuable for predicting the atomizer performance with pyrolysis oil by comparing the liquid properties, among which the surface tension and viscosity are most important.

The surface tension of pyrolysis oil at room temperature can be as high as 40 mN/m, but mostly varies between 29 and 36 mN/m [16, 32, 56, 95, 130, 142, 150]. These values are higher than those of conventional gas turbine fuels at room temperature, such as No. 2 diesel (28 mN/m). However, the difference becomes small if the pyrolysis oil is preheated. Values between 24 and 32 mN/m have been reported for pyrolysis oil at a temperature of 80 °C [16, 56, 142, 150], which are very similar to those of biodiesel and vegetable oil in this study (see Table 4.1). The surface tension should therefore not form a significant obstacle for the atomization of preheated pyrolysis oil in most cases.

An evaluation of the viscosity, however, makes clear that pressure-swirl atomizers are generally unsuitable for the application of pyrolysis oil in gas turbines. The viscosity limit obtained from the combustion experiments in the MMSGT setup is 9 cP. The high sensitivity of the pressure-swirl method to this property also follows from the present atomization study. Although the viscosity of pyrolysis oil is not well-defined since it depends on the feedstock, the production process and the oil's age, the typical values reported in the literature vary between 5 and 30 cP for a temper-

Figure 4.22: SMD as function of viscosity at a pressure of 10 bar.

Figure 4.23: SMD as function of viscosity at a pressure of 30 bar.

ature of 80 °C [15, 95, 104, 114]. Higher temperatures should be avoided because of the chemical instability of this biofuel [15]. It is hence likely that pyrolysis oil, even preheated, will exceed the range for which a pressure-swirl atomizer produces sprays of sufficient quality.

In the best case scenario, when the viscosity is under 7 cP, the pyrolysis oil spray has a short breakup length as indicated by Fig. 4.20 and an SMD similar to those measured for biodiesel and vegetable oil. Still, this is by no means a guarantee for an acceptable combustion quality. The composition of pyrolysis oils is very different from that of biodiesel and vegetable oil, in such a way that the evaporation and combustion processes are slower. Also, various pyrolysis oil fractions tend to form char inside the droplets during evaporation. These solid droplet residues burn very slowly and may damage the combustor or turbine blades, depending on their temperature history [40, 54]. To minimize the evaporation time and the formation of char, pyrolysis oil combustion requires a finer spray than typically sufficient for light fossil fuels. Earlier studies have shown that the char formation is significantly reduced by lowering the SMD down to approximately 30 μm [126, 150]. The graph in Fig. 4.23 illustrates that, even at a pressure of 30 bar, the tested atomizer is incapable of delivering sprays for which the SMD is below 50 μm . It is therefore expected that the combustion of pure pyrolysis oil in the MMGT setup is not feasible when using a pressure-swirl atomizer. To greatly improve the atomization performance and make the breakup length less sensitive to viscosity, it is strongly recommended to use a more effective type of atomizer. Recent studies discussed in Sec. 4.1 indicate that certain twin-fluid atomizers are promising alternatives.

4.6 Conclusions

The atomization of biodiesel, vegetable oil and glycerin has been studied in an atmospheric spray rig by using digital imaging (PDIA). Images were captured 18 mm downstream of the atomizer to investigate the spray structure in the primary breakup region. The images were processed to automatically determine the size of ligaments and droplets. The sprays were produced by a pressure-swirl atomizer that originates from the MMGT setup. Various injection conditions have been tested to investigate the influence of mainly viscosity on the spray characteristics and to assess the overall performance of the atomizer. The spray measurements have been compared to combustion experiments with biodiesel and vegetable oil in the micro gas turbine at similar injection conditions.

The results show that the primary breakup process rapidly deteriorates when the viscosity is increased. A higher viscosity increases the breakup length, which becomes visible at the measurement location in the form of ligaments. This effect leads to an unacceptable spray quality once the viscosity slightly exceeds the typical range for conventional gas turbine fuels. Only biodiesel was atomized without problems at all test conditions, which covered viscosities in the range 2–6 cP. In case of veg-

etable oil, a decrease in atomizer performance was measured for viscosities above 7 cP. This value is in reasonably good agreement with the upper limit of 9 cP found during combustion experiments in the MMGT setup. In the images of the glycerin sprays, ligaments started to appear at viscosities between 8 and 12 cP.

Regarding the SMD of the sprays, no significant effect of viscosity is observed in the range 2–10 cP. The decrease in combustion efficiency measured over this viscosity range therefore cannot be explained by the average drop sizes in the primary breakup region. Instead, the delayed breakup of ligaments is considered as the main issue when burning viscous fuels. The results from the glycerin sprays indicate that a high surface tension causes an appreciable increase in SMD.

The current findings show that pressure-swirl atomization is unsuitable for the application of pure pyrolysis oil in an unmodified gas turbine engine, mainly due to the formation of persistent ligaments at increased viscosity.

Chapter 5

The impact of viscosity on the performance of a micro gas turbine

Abstract

The relation between spray quality and combustion performance in a micro gas turbine has been studied by burning a viscous biofuel at different fuel injection conditions. Emissions from the combustion of a viscous mixture of straight vegetable oils have been compared to reference measurements with No. 2 diesel. The effect of fuel viscosity on pollutant emissions is determined by adjusting the injection temperature. The measurements confirm that a reduction in fuel viscosity improves the spray quality, resulting in faster droplet evaporation and more complete combustion. CO emission levels were observed to decrease linearly with viscosity in the tested range. For the pressure-swirl atomizer used in the tests, the upper viscosity limit is found to be 9 cP. Above this value, droplet evaporation seems to be incomplete as the exhaust gas contains a considerable amount of unburned fuel. The influence of increased injection pressure and combustor temperature is evaluated by varying the load. Adding more load resulted in improved combustion when burning diesel. In case of vegetable oil, however, this trend is less consistent as the decrease in CO emissions is not observed over the full load range. The outcome of this study gives directions for the application of pyrolysis oil in gas turbines, a more advanced biofuel with high viscosity.

This chapter is based on the publication:

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5.1 Introduction

5.1.1 Background

Gas turbines can play a major role in the transition to a more sustainable energy supply. Gas turbines offer some important advantages over other conversion technologies, including high power-to-weight ratio, high reliability, high flexibility and low pollutant emissions [67]. The scalability of gas turbines furthermore allows for the production of heat and power in a decentralized manner. With overall energy efficiencies above 80% in cogeneration plants, this technology is considered to be promising for distributed applications [44, 109].

When it comes to application of liquid biofuels, the relatively robust burning characteristics in gas turbines is of particular interest. While reciprocating engines are very sensitive to problems such as clogging and delayed ignition, gas turbines have shown good potential to cope with alternative fuels. Experimental studies have shown that most common biofuels, such as bioalcohols and biodiesel, can already be burned in pure form in standard or slightly modified combustor designs without any major problems [13, 97, 101, 107, 122]. Nevertheless, in view of the overall efficiency and sustainability including fuel production, it is preferable to focus on second generation biofuels derived from biomass residues. In this class of biofuels, fast pyrolysis oil is considered as a promising example [39, 51, 67, 96].

Due to the rather low feedstock quality and the random nature of the decomposition reactions, the properties of pyrolysis oil are very different from those of conventional fossil fuels. For this reason, pyrolysis oil is not directly suitable for use in combustion devices, including gas turbines. The few attempts that have been made revealed major problems as incomplete combustion, flame instability and coke formation on combustor walls [10, 95, 97, 122, 138, 143]. Therefore, it is generally concluded that fuel blending or thorough modification of the gas turbine is required for successful application.

The poor combustion behavior of pyrolysis oil is partly a result of its unfavorable chemical properties. For instance, the low heating value and the presence of non-volatile matter slow down the mass and heat transfer inside a combustion chamber considerably. Researchers have been trying to improve the quality of pyrolysis oil for several decades by optimizing the production process or upgrading the raw product [39, 104, 154]. Unfortunately, these studies did not yet result in a feasible method for obtaining pyrolysis oil with properties similar to fossil fuels. For this reason, more research has been initiated with a focus on adapting existing combustion devices to operate on pyrolysis oil in its present form.

In the development of such fuel flexible combustion systems, it is of crucial importance to look into the influence of fuel properties on the spray quality. The atomization process governs the evaporation and distribution of fuel inside the combustion chamber and is therefore closely related to the combustion performance [89]. In case of pyrolysis oil, most of the conventional atomization techniques tend to deliver

a fuel spray of poor quality. This issue is mainly attributed to the high viscosity of the oil, which has a dampening effect on the fuel breakup mechanism [37, 55]. Since the time required for complete evaporation is considerably higher when the fuel is poorly atomized, some fraction of the fuel may impinge on the liner. The increased evaporation time can be a major cause for the aforementioned problems that were encountered in pyrolysis oil burning tests.

Aside from the effect on the evaporation process, atomization also has a significant influence on the combustion kinetics of pyrolysis oil. Due to the chemical instability of this biofuel, polymerization reactions at elevated temperatures lead to the formation of non-volatile matter inside the droplets during their flight in the combustor [40, 54, 130, 143, 152]. Research on individual droplets has revealed that these undesired reactions are suppressed in case the droplet heating rate is very high [31, 126]. As the heating rate is highly dependent on droplet size, small droplets are required to avoid deterioration of the pyrolysis oil quality during evaporation. Hence, given the current properties of raw pyrolysis oil, improved atomization can be seen as a key factor towards efficient combustion.

Due to the adverse effect of high viscosity on spray quality, viscous fuels are normally preheated to a temperature at which the flow properties are acceptable. However, in case of pyrolysis oil, the allowable preheating temperature is limited to around 80 °C because of the chemical instability as explained above. This limitation implies that the viscosity of pure pyrolysis oil cannot always be lowered to a level that is typical for distillate fuel oils. As a consequence, the spray characteristics might be affected even if the oil is preheated, so that the combustion of pure pyrolysis oil in gas turbines can be problematic irrespective of the combustion kinetics.

5.1.2 Aim of the study

In this work, the effect of viscosity on the combustion efficiency in a micro gas turbine is investigated by changing the injection temperature of a viscous fuel. Here, the fuel viscosity at the pressure-swirl atomizer is used as measure for the spray quality, while CO emissions indicate the combustion efficiency. The main goal is to determine the sensitivity of the combustion process to an increase in fuel viscosity and to identify a typical maximum viscosity for which the atomization is still acceptable.

Straight vegetable oil has been used as the fuel for the experimental test campaign. This biofuel is selected to capture the effect of viscosity, while excluding the complex chemistry effects associated with pyrolysis oil. The stability of vegetable oil allows for preheating up to high temperatures, such that a wide range of viscosities can be tested. The experiments with vegetable oil have been compared to reference measurements with diesel. Next to viscosity effects, also the influence of load has been examined. The results from this study can be useful in formulating practical guidelines for good atomization of pyrolysis oil as a first and very important requirement.

5.1.3 Previous work

The literature on straight vegetable oil combustion in gas turbines is scarce; only few works have been found that are similar or closely related to the present study. Habib et al. [68] tested several vegetable oil-based biodiesels (soy, canola and recycled rapeseed), an animal-derived biofuel and their 50% blends with Jet A fuel in an unmodified 30 kW gas turbine. Engine performance and emissions are reported for all biofuels except for the pure animal fat biofuel due to its high sooting potential. However, no information is given about the injection system and fuel injection temperature.

Cavarzere et al. [28] investigated the performance of a Solar T-62T-32 micro gas turbine fed by blends of diesel and straight vegetable oils in different concentrations. The researchers were able to gradually increase the vegetable oil content up to 100% without running into any particular problems. Unfortunately, the authors did not report the injection temperatures used during the test runs, while they mention that the fuel tanks for vegetable oil blends were heated to reduce the viscosity.

Significant work was published by Chiaramonti et al. [34], who performed experiments with diesel, biodiesel and vegetable oil in a Garrett GTP 30-67 micro gas turbine equipped with a pressure-swirl atomizer. It was found that the combustion of pure vegetable oil and its blends with diesel required preheating of the fuel to at least 120 °C. At idle conditions, combustion could not be sustained even at this temperature. However, the results generally showed that preheating the fuels reduced CO emissions. The effect of fuel temperature was measured to be more pronounced at partial load. Also, it is concluded that the combustion efficiency for vegetable oil at 120 °C is very similar to that of diesel at standard conditions.

These conclusions are confirmed by field tests with a slightly modified Capstone C30 conducted by Prussi et al. [120]. In this micro gas turbine, straight vegetable oil was injected by air-assist atomizers at three different temperatures. CO emissions decreased with higher preheating temperatures, especially at low load conditions, and were nearly the same as for diesel in case of maximum load. Considering the strong influence on the engine performance, viscosity was identified as the most important parameter to be controlled. Comparison of the data obtained by Prussi et al. with other studies will only be possible to a limited extent, however, because the fuel temperatures are not reported explicitly.

The experimental work discussed above indicates that the research on this topic is in an early stage. Straight vegetable oil has been applied in gas turbines only few times, with varying degrees of success, and it can be said that little results have been reported on the quantitative relation between combustion efficiency and viscosity for this fuel.

5.2 Experimental setup

The combustion experiments have been conducted with the multifuel micro gas turbine (MMGT) setup at the University of Twente. This setup is developed for testing alternative fuels, or biofuels in this case, at varying fuel injection temperatures and loads. It consists of five main modules: a micro gas turbine, a generator, a fuel supply system, a resistive load and a control unit. Various sensors are used to collect data during the experiments. The gas turbine, the fuel supply system and the measurement equipment are discussed in the following subsections.

5.2.1 Micro gas turbine with generator

The micro gas turbine selected for the test setup is a DG4M-1, which was formerly used as an auxiliary power unit. Thanks to its simple, radial design, the DG4M-1 is relatively robust to alternative fuels and easily accessible in case modifications are required. As shown in Fig. 5.1, it features a single stage, centrifugal compressor and turbine on a single main shaft. The power shaft, which is driven by the main shaft via a gearbox, is connected to a generator to produce electricity. The electrical power is supplied to three 15 kW fan heaters that can be switched on individually to vary the load condition. The fuel is burnt in a single silo, reverse-flow combustion chamber equipped with a pressure-swirl atomizer. This atomizer produces a hollow cone spray with an angle of $90\text{--}100^\circ$. The specifications of the gas turbine are listed in Table 5.1 [57].

Figure 5.1: Functional overview of the DG4M-1 gas turbine: 1 - compressor, 2 - diffuser, 3 - combustion chamber, 4 - turbine nozzle, 5 - turbine [57].

Table 5.1: Specifications of the DG4M-1 micro gas turbine with generator [57]. Fuel consumption data are based on No. 2 diesel.

Property	Unit	Value
Rotational speed of main shaft	rpm	27 600
Rotational speed of power shaft	rpm	6000
Maximum power	kW _e	47
Compression ratio	–	2.3–2.6
Air consumption	m ³ /s	1.2
Fuel consumption at no load	L/h	48
Fuel consumption at full load	L/h	82

5.2.2 Fuel supply system

In the original configuration, the fuel supply was controlled mechanically and preheating was achieved by leading the fuel line through the exhaust. However, both the fuel control and preheating design were unsuitable for biofuel combustion. The standard feeding system was hence disconnected and replaced by a newly designed fuel supply system (FSS). This new system can be used to operate the gas turbine over a wide range of operating conditions and to switch between standard fuel and biofuel during a run. In addition, the fuel preheating capacity has been increased considerably to handle viscous fuels.

A flowsheet of the FSS is given in Fig. 5.2. The diesel fuel, alternative fuel and cleaning fuel are stored in separate tanks. Cleaning fuel is only used for flushing the fuel lines and the atomizer. Diesel fuel is required for the startup and shutdown of the MMGT. After startup, the operator can decide to continue on diesel or switch to the alternative fuel, depending on the type of experiment. The fuel from all three tanks are led through can filters to prevent clogging in the atomizer. A small waste tank is used to drain contaminated fuel during the tests.

The fuel switching is achieved by using two pressurized circuits, one for diesel and one for the alternative fuel. These circuits are separated by a four-way valve that controls which fuel is recirculated and which fuel is supplied to the atomizer. In both circuits, the pressure is controlled by adjusting a needle valve in a bypass line. The pressure level is chosen such, that the thermal input after switching is similar and therefore the rotational speed of the MMGT is hardly influenced. Besides the fuel pressure, also the temperature is adjusted before switching to minimize the risk on a blowoff. The alternative fuel, which is a viscous biofuel in this research, is preheated in the tank and then further heated in the fuel line by two cartridge heaters that are located near the atomizer (not shown in Fig. 5.2).

Figure 5.2: Flowsheet of the fuel supply system.

5.2.3 Measurement equipment

The operating conditions of the setup are monitored by measuring pressures, temperatures and rotational speed. The pressure in the combustion chamber is measured using a GE PMP 1400 sensor with an accuracy of $\pm 2\%$ of its range 0–16 barg, including errors due to thermal effects. Two RS Type 461 sensors measure the pressure in the fuel line, one in the alternative fuel circuit of the FSS (see Fig. 5.2) and one just in front of the atomizer. These sensors work with an accuracy of $\pm 0.25\%$ in their range 0–100 barg and have been calibrated using a GE Druck DPI 104. All pressure sensors are connected to analog ports of the NI USB-6009 data acquisition device.

Temperatures are measured in the fuel tanks, in the fuel line close to the atomizer and in the exhaust using K-type thermocouples. These thermocouples have an accuracy of $\pm 2.2^\circ\text{C}$ or $\pm 0.75\%$ of the measured value. The acquisition of temperature data is performed by an NI 9213 module with a maximum error of $\pm 1.2^\circ\text{C}$ in the temperature range 0–500 $^\circ\text{C}$. The combined accuracy of the sensor and measurement hardware is therefore $\pm 3.4^\circ\text{C}$ for temperatures under 300 $^\circ\text{C}$, but increases to $\pm 5.0^\circ\text{C}$ at a temperature of 500 $^\circ\text{C}$.

The gas composition in the exhaust is measured using several analyzers to cover a wide range of species and to reduce measurement uncertainty. An rbr-ecom KD electrochemical analyzer measures dry gas concentrations of O_2 , CO and NO . In addition, a set of analyzers composed of a Siemens Oxymat 61 and a Maihak Multor 610 is used to measure O_2 , CO_2 and CO in a conditioned gas sample stream. The Oxy-

5.3. Fuel properties

Table 5.2: Specifications of the gas analyzing equipment.

Analyzer	Species	Range	Uncertainty
ecom KD	O ₂	0–21 vol. %	±0.3 vol. %
	CO	0–400 ppm	±20 ppm
		400–4000 ppm	±5% of value
	NO	0–2000 ppm	±5 ppm or 5% of value
Oxymat	O ₂	0–25 vol. %	±1% of range
Multor	CO ₂	0–20 vol. %	±2% of range
	CO	0–2000 ppm	±2% of range

mat determines the O₂ concentration based on the paramagnetic alternative pressure method. The Multor uses infrared absorption to detect CO₂ and CO. The measurement ranges and uncertainty levels for these analyzers are given in Table 5.2. In some of the experiments, the conditioned gas sample was also led through a Gasmet CX-4000 Fourier Transform Infrared (FTIR) analyzer to determine the concentration of unburned hydrocarbons (UHC). The hydrocarbons included in the FTIR library were methane, ethane, ethylene, propane, hexane and formaldehyde.

5.3 Fuel properties

The fuels tested in the present study are No. 2 diesel and vegetable oil. Diesel is the standard fuel for the gas turbine and was therefore selected as the reference fuel. Vegetable oil was used to investigate the influence of fuel viscosity on the combustion process. The fuel referred to as vegetable oil here is a mixture of plant-derived oils, commercially available as liquid frying fat. Typical fuel properties important for spray combustion are listed in Table 5.3.

Although the application of pyrolysis oil is the ultimate goal, there have been reasons to perform the experiments with vegetable oil instead. Firstly, the evaporation behavior as well as the combustion kinetics of vegetable oil and diesel fuel are similar. The differences in fuel composition will therefore have only minor effects, as was concluded by Panchasara et al. [117] after experiments in an atmospheric pressure burner. This leaves the atomization quality as the main factor influencing the combustion of this biofuel, which is dominated by the viscosity in the tested fuel temperature range [34, 120]. It is hence most important that the viscosity of vegetable oil is representative for pyrolysis oil.

As indicated in Table 5.3, this property highly varies between the different pyrolysis oils because it very much depends on the feedstock and the production process [114]. Furthermore, once the oil is produced, its viscosity can change over time due to aging reactions [15]. Although a comparison is not so straightforward for these reasons, it is clear that the vegetable oil mixture is sufficiently viscous to make it a

Table 5.3: Properties of the two tested fuels and pyrolysis oil. Data obtained from the EN 590 norm and from the literature [32, 48, 67, 114, 146]. Viscosities of diesel and VO have been measured (see Fig. 5.3).

Property	Unit	No. 2 diesel	Vegetable oil	Pyrolysis oil
Lower heating value	MJ/kg	42–43	38–39	16–19
Density ^a	kg/L	0.82–0.84	0.92	1.1–1.3
Surface tension ^b	mN/m	28	31–34	30–36
Flash point	°C	> 55	> 230	> 40
Viscosity	cP			
at 20 °C		3.5	56	> 60
at 40 °C		2.1	25	> 17
at 80 °C		1.1	7.7	> 5

^a Density at 20 °C.

^b Surface tension at 25 °C.

good substitute for this research. The viscosity of most types of pyrolysis oil at a temperature of 80 °C, considered as the upper temperature limit for pyrolysis oil, can be matched by vegetable oil in the tested temperature range of 20–120 °C. This is also illustrated in Fig. 5.3, where the viscosity of diesel, vegetable oil and a number of pyrolysis oils are compared as function of temperature. The data shown for the first two fuels, indicated with solid markers, have been measured using a Brookfield DV-II+Pro viscometer. Viscosity data for the pyrolysis oils, indicated with open markers, are taken from the literature [16, 56, 95, 104, 150].

5.4 Test conditions and procedure

To experimentally investigate the influence of spray quality on the combustion process, reference experiments with diesel have been compared to experiments with vegetable oil. The experiments were performed under varying load conditions and fuel injection temperatures while recording the exhaust emissions. An overview of the investigated test conditions is shown in Table 5.4. Note that some of the experiments are overlapping to check the repeatability of the results.

The test procedure starts by preheating the alternative fuel in the tank and by setting the correct pressures of the two fuel circuits in the FSS. After startup of the MMGT on diesel, the operating conditions are adjusted to match the planned test case. Once the values reported by all sensors seem to be constant, the measurement continues for at least another minute to be sure that stationary conditions have been reached. The MMGT ran stably at all tested conditions and no flame extinction occurred during the series of experiments.

Continuous gas samples are taken from the exhaust and led to the gas analyzers ecom KD, Oxymat, Multor and sometimes also the FTIR. These analyzers together measure concentrations of O₂, CO₂, CO, NO and UHC. Especially the CO level is im-

Figure 5.3: Dynamic viscosity of No. 2 diesel, vegetable oil and pyrolysis oil as function of temperature. Pyrolysis oil data is taken from the literature [16, 56, 95, 104, 150].

portant as it indicates incomplete combustion due to poor atomization, bad mixing or cold spots inside the combustor. CO can therefore be regarded as a good measure for the efficiency of the combustion process. NO is an indicator for the (maximum) temperature in the reaction zone.

5.5 Results

This section presents the results of the experiments as described in Sec. 5.4. Firstly the results of the reference measurements with diesel will be discussed. These measurements give information about the performance of the MMGT fired on its standard fuel. Subsequently the results of the vegetable oil combustion tests are reported and compared to the reference cases.

The measurement uncertainties of the gas analyzers reported in Sec. 5.2.3 are indicated in the graphs by error bars, except for very small errors that would be almost invisible. In case normalized gas concentrations are shown, the measured values have been normalized to 15 vol.% O₂ as follows:

$$[\text{CO}]_{\text{norm}} = [\text{CO}]_{\text{meas}} \cdot \frac{[\text{O}_2]_{\text{amb}} - 15\%}{[\text{O}_2]_{\text{amb}} - [\text{O}_2]_{\text{meas}}} \quad (5.1)$$

where the subscripts 'norm', 'amb' and 'meas' indicate normalized, ambient and measured values. It must be noted that, strictly speaking, the normalized values come with larger relative error bars than the measured values because of the propagated uncertainty of the oxygen measurement (see Table 5.2). Nevertheless, as will

Table 5.4: Overview of the test conditions in the performed experiments.

Exp. No.	Fuel ^a	Load (kW _e)	Fuel temperature (°C) ^b
1	Diesel	0, 15, 30, 47	31 ^c
2	Diesel	40 ^c	31, 42, 59, 70, 80
3	Diesel	40	17, 18, 21, 30, 40
4	VO	0	73, 80, 83, 117
5	VO	0	74, 80, 90, 107, 121, 125, 127
6	VO	18	73, 78
7	VO	28	86, 109
8	VO	46 ^c	91, 108
9	VO	0	92, 112
10	VO	30	92, 110
11	VO	46 ^c	90, 108

^a Diesel = No. 2 diesel, VO = vegetable oil.

^b Fuel temperature at injection location.

^c A fluctuation of ± 1 was observed during the tests.

be explained in Sec. 5.5.1, the oxygen measurements are found to be very accurate, so that it is justified to only reckon with the uncertainty of the measured concentration to be normalized (i.e. $[\text{CO}]_{\text{meas}}$ in Eq. 5.1).

The O₂ and CO concentrations measured by the ecom KD on the one hand and the Oxymat–Multor combination on the other hand were found to correspond well, taking into account their ranges of uncertainty. For the sake of readability of the figures, however, only O₂ and CO data from the Oxymat and Multor are reported, unless stated otherwise.

5.5.1 Diesel – Tests at varying load

In Exp. 1, diesel has been combusted at different load conditions without preheating. This test gives insight into some general characteristics of the MMGT running on standard fuel, but also shows the combustion efficiency at varying load. The fuel consumption is estimated using the following relation:

$$\dot{V} = \text{FN} \sqrt{\frac{\Delta p}{\rho_l}} \quad (5.2)$$

where $\dot{V}$ is the volume flow rate, FN is the flow number of the atomizer, Δp is the differential pressure and ρ_l is the liquid density. The flow number of the atomizer was measured to be around $41 \cdot 10^{-8} \text{ m}^2$ prior to the tests.

The injection pressure as well as the estimated fuel consumption during the test are given as function of the load in Fig. 5.4. The graph shows that the fuel consumption increases linearly with the load from 48 to 82 L/h for idle and 47 kW_e, respectively. This linear trend was also observed in diesel combustion tests performed by

Figure 5.4: Fuel injection pressure and estimated fuel consumption as function of load for diesel combustion (Exp. 1).

Chiaramonti et al. [34] using a similar micro gas turbine. The fuel consumption data together with the intake air flow rate given in Table 5.1 define the fuel–air equivalence ratio (ϕ) at the different load conditions. Using a stoichiometric air–fuel ratio of 14.7 for diesel, the overall equivalence ratio varies from 0.11 when idling to 0.18 at 47 kW_e . These ratios indicate that the combustor operates under very lean conditions and that the turbine inlet temperature will be relatively low.

Figure 5.5 shows the concentrations of O_2 and CO_2 as function of the load. The exhaust gas temperatures (EGT) measured in these experiments are reported in Fig. 5.6. The linear decrease in $[\text{O}_2]$ and linear increase in both EGT and $[\text{CO}_2]$ confirm the consistency of the measurements. After normalization to 15 vol.% O_2 using Eq. 5.1, the concentration of CO_2 is found to be 4.3–4.4 vol.% for all load conditions. These values are in close agreement with the ideal combustion theory, given the fact that the H/C-ratio of diesel is typically around 1.9. It can therefore be stated that the Oxymat data are sufficiently accurate to neglect the propagating uncertainty of the oxygen measurements in the normalization.

Normalized emissions of CO are given in Fig. 5.7. The graph shows that the normalized CO concentration decreases significantly with increasing load. More complete combustion of the fuel is indeed expected, since combustor temperatures increase with load. Improved atomization due to higher injection pressures and hence faster evaporation can also play a major role here. It must be noted that, in absolute sense, the CO emissions from this gas turbine are quite high compared to typical values for modern designs. Such high emission levels have also been reported by Chiaramonti et al. [34] and are the result of the simple design and large air excess. The measurement data are however merely used to capture trends in this study, so

Figure 5.5: Measured O₂ and CO₂ emissions as function of load for diesel combustion (Exp. 1).

Figure 5.6: Measured exhaust gas temperature as function of load for diesel combustion (Exp. 1).

Figure 5.7: Normalized CO emissions as function of load for diesel combustion (Exp. 1).

that the absolute values are of minor importance.

The normalized NO emissions were found to be rather low, with concentrations increasing from 7 ppm at idle condition to 32 ppm at full load. This indicates that the temperature in the flame tube is relatively low, which can be expected seeing the low overall equivalence ratios reported above. The reliability of the NO measurements is limited, however, because of the relatively high measurement uncertainty at such low concentrations (see Table 5.2).

5.5.2 Diesel – Tests at varying fuel temperature

The influence of the injection temperature is investigated in Exps. 2 and 3. In these experiments, the temperature was varied between 17 and 80 °C while all other parameters were held constant. Although the viscosity of diesel is already low at room temperature, it still decreases by almost 3 cP over this range (see Fig. 5.3).

The normalized CO concentration as function of the injection temperature is shown in Fig. 5.8. The CO levels are only little affected at temperatures above 40 °C, where the viscosity of diesel is below 2 cP. When going towards lower temperatures from this point the CO concentration seems to increase substantially, but the trend is not fully consistent. The unexpectedly low concentrations at 17 and 18 °C can be explained by looking at the rotational speed of the MMGT, indicated by the combustion chamber pressure (CCP) in this figure. It can be seen that the CCP has a strong inverse effect on the CO concentration, possibly caused by improved swirl and mixing. This effect can also explain the slight deviation between the two data points around 30 °C, which should ideally fall on top of each other. To make a fair comparison between the emissions at different temperatures, the measured concentrations

Figure 5.8: Normalized CO emissions and combustion chamber pressure (CCP) as function of injection temperature for diesel combustion with 40 kW_e load (Exp. 2 and 3).

should be corrected for changes in the CCP. However, since the exact dependence of CO emissions on the pressure is unknown, any suggestion for a correction method would be speculative. Nevertheless, when only considering the data in the temperature range 20–80 °C, the CO graphs in Fig. 5.8 show a consistently decreasing trend. The CO emissions are reduced by about 21% over this temperature range. To avoid any influence of combustion chamber pressure fluctuations, the rotational speed was controlled more precisely in the subsequent experiments. Therefore, a strong effect of the CCP on the presented results for vegetable oil can be ruled out.

Some comparisons with the results from Exp. 1 can be made to validate the repeatability of the measurements. In Exps. 2 and 3, two tests were performed with a fuel temperature of around 30 °C. This setpoint corresponds to the temperature condition in Exp. 1. The data shown in Fig. 5.8 around 30 °C can therefore be compared to the CO emissions given in Fig. 5.7 at a load of 40 kW_e. It can be seen that the values are in good agreement. The normalized NO concentrations detected in Exps. 2 and 3 fluctuated in the range 24–31 ppm for all temperature conditions. This result is very similar to the NO emissions measured in Exp. 1 at higher loads. Emissions of UHC, measured with the FTIR during Exp. 2, were found to be insignificant.

5.5.3 VO – Tests at varying load

Although the effect of fuel temperature has been determined prior to the influence of load, the experimental results for vegetable oil at varying load will be discussed first to make the structure of the results section consistent. As reported in Table 5.4, always two temperature setpoints have been evaluated when running on vegetable oil with a certain load. The required injection pressures were about 10% higher com-

Figure 5.9: Normalized CO emissions as function of injection temperature for VO combustion (Exp. 5–11). Exp. 9–11, shown in gray, have been performed to verify Exp. 5, 7 and 8, shown in black. The marker symbol denotes the load condition.

pared to those for diesel, which is a combined effect of the lower heating value and higher density of vegetable oil (see Table 5.3).

In Fig. 5.9, the normalized CO emissions are reported for various load conditions. Different symbols are used to denote the load applied in the experiment. As is the case for diesel combustion, the influence of load addition is clearly more pronounced than the effect of injection temperature. The reduction can be attributed to the higher combustor temperatures and improved atomization at higher injection pressures. Also, the slopes of the graphs indicate that the sensitivity of CO emissions to fuel temperature diminishes with increasing load.

A further decrease in CO emissions can be expected when the load is increased from 28 to 46 kW, but the data from Exps. 7 and 8 show no significant differences. Apparently, there is a certain lower limit for the CO emissions when burning vegetable oil in this gas turbine. Such unexpected behavior is not observed in case of diesel combustion at varying loads (see Fig. 5.7). To verify this outcome, a new series of test runs, consisting of Exps 9–11, have been performed at approximately the same test conditions. The results of these validation experiments are plotted in gray in Fig. 5.9 and generally confirm the values obtained in the previous tests. Possibly, there is an influence of the penetration length of the spray since the initial droplet velocity rises with pressure. In such case, the favorable effect of a higher injection pressure on the atomization and combustor temperature can be counteracted by quenching of the fuel vapors near the liner.

Figure 5.10: Fuel injection temperature along with dimensionless emissions of CO and C_2H_4 as function of time. Raw measurement data for VO combustion without load (Exp. 4).

5.5.4 VO – Tests at varying fuel temperature

Experiments with vegetable oil at various temperatures have been performed to investigate the effect of fuel viscosity on the combustion process. High viscosity can lead to poor atomization, which in turn causes incomplete combustion or even blowoff. The fuel injection temperatures were varied between 73 and 127 °C, but the fuel switch from diesel to vegetable oil was always conducted at a temperature of 90 °C to prevent a blowoff. The influence of fuel temperature on the injection pressure was observed to be insignificant. Indeed, variations in density in the tested temperature range are rather low, and the thermal input is only proportional to the square root of the density according to Eq. 5.2. Since fuel viscosity did not change the atomizer flow number, the inviscid flow assumption made in this equation is confirmed.

Figure 5.10 shows raw measurement data obtained from Exp. 4 using the Mulator and the FTIR. The figure illustrates the evolution of the fuel injection temperature along with nondimensionalized concentrations of CO and C_2H_4 against time. The FTIR was used to measure several hydrocarbons (see Sec. 5.2.3), but only ethylene (C_2H_4) was found in significant concentrations. CO was measured by both the FTIR and the Mulator. Note that the emission graphs are slightly shifted with respect to the temperature graph due to the time lag of the analyzers. In the experiment, the fuel temperature was adjusted in a high–low–high pattern, which has resulted in an inverse pattern for the concentration of both CO and C_2H_4 in the exhaust gas. Obviously the two species show the same trend, but only C_2H_4 approaches zero at high injection temperatures. The CO emission levels measured by the Mulator and FTIR are in fair agreement.

Figure 5.11: Normalized CO emissions as function of injection temperature for VO combustion without load (Exp. 4 and 5).

Normalized CO concentrations acquired in Exps. 4 and 5 are given as function of the fuel injection temperature in Fig. 5.11. It can be concluded that the fuel temperature has considerable influence on the combustion efficiency; an increase in temperature from 73 to 127 °C has resulted in a CO reduction of 28%. The normalized NO concentrations were 6–7 ppm for all test conditions. Emissions of NO were therefore identical to the diesel case without load and can be considered as insignificant.

An important result is that the appearance of the exhaust gas changed from highly transparent to slightly opaque at fuel temperatures lower than approximately 70 °C. At such low temperatures, bluish gray smoke was observed because the poorly atomized fuel stream did not fully evaporate anymore. The vegetable oil then starts to break down into glycerol and free fatty acids, which is known to give a bluish smoke [127]. The observation of smoke in the exhaust gas prescribed the lower temperature limit in this parameter study.

The improved combustion efficiency at higher fuel temperatures is caused by enhanced atomization at lower fuel viscosities. To illustrate the effect of viscosity on the CO emissions more directly, these two parameters have been plotted against each other in Fig. 5.12. The graph shows a linear relation between CO and viscosity in the tested range. Also, it is seen that the normalized CO level for diesel and vegetable oil is similar when the viscosity is matched. The viscosity of vegetable oil at 120 °C is close to 3 cP, which almost corresponds to the viscosity of diesel at 31 °C in Exp. 1 (see Fig. 5.3). In both cases, the normalized CO concentration is approximately 1300 ppm.

The influence of fuel preheating on the evaporation curve of the droplets should also be considered in this discussion. Preheating adds energy to the fuel and, as a

Figure 5.12: Normalized CO emissions as function of fuel viscosity for VO combustion without load (Exp. 4 and 5).

result, increases the volatility of the droplets when they are injected into the combustion chamber. Compared to the total evaporation time, however, the heat-up time of a droplet is relatively short and the wet bulb temperature is reached quickly [49]. The preheating temperature is therefore expected to have little effect on the total evaporation time of the fuel droplets.

The relation between CO emissions and injection temperature or viscosity presented in this section are confirmed by additional tests performed with biodiesel. The results from the biodiesel tests are reported in Appendix F and show similar trends as seen from the experiments with No. 2 diesel and vegetable oil.

5.6 Implications for pyrolysis oil combustion

This study provides useful insights for burning pyrolysis oil in gas turbines, a more advanced biofuel with relatively low impact on the environment. Atomization problems due to high viscosity form a major obstacle for clean burning of this biofuel according to earlier studies. From the tests with vegetable oil, it appears that the maximum dynamic viscosity at which the spray can still be evaporated is 9 cP. This value is in close agreement with the preliminary norm for pyrolysis oils as described by Oasmaa et al. [114], which sets the maximum kinematic viscosity at 7 cSt (8 cP) for application in gas turbines. However, in case pyrolysis oil is to be combusted in the MMGT, it is expected that the viscosity requirement must be more strict because of the lower volatility and slower kinetics compared to vegetable oil. The viscosity limit prescribed by the norm may therefore be too optimistic if pressure-swirl atom-

ization is used for pyrolysis oil combustion in a conventional combustion chamber.

In some cases, this condition for viscosity cannot be met only by preheating pyrolysis oil to the temperature limit of 80 °C (see Fig. 5.3). To further reduce the viscosity, the oil can be blended with another fuel that has good flow properties [33, 72]. Here, it is worth mentioning the experimental work performed by Pander [118], who tested the combustion of diesel/butanol/pyrolysis oil mixtures in the same gas turbine as used in this study. Blends with the percent compositions 50/40/10 and 5/50/45 by mass, with respective viscosities of 3.4 and 7.0 cP measured at 23 °C, were successfully combusted at partial load without preheating. A third mixture, with percent composition 0/30/70 and a viscosity of 29 cP at 23 °C, failed to combust even after preheating up to 60 °C.

For applications of pure pyrolysis oil, it is strongly recommended to improve the spray quality by using other atomization methods. Twin-fluid atomizers are promising alternatives, because their performance is known to be less sensitive to changes in fuel viscosity compared to pressure-swirl atomizers. The potential of such atomizers for the combustion of a viscous, wood-derived biofuel has been demonstrated by Seljak et al. [129]. In this research, preheated liquified wood with a viscosity of around 100 cP could be burned in a jet engine combustor using air-assist atomization.

5.7 Conclusions

Combustion of a viscous biofuel has been studied in a multifuel micro gas turbine setup. The effect of viscosity on the combustion performance is investigated by changing the fuel injection temperature. Successful experiments have been conducted with a viscous mixture of straight vegetable oils. The results were compared to reference measurements with No. 2 diesel.

Comparing the results for diesel and vegetable oil, it is found that the CO emission is similar when the viscosity is the same. This implies that the viscosity is the dominant fuel property, and that the slight difference in molecular structure is of minor importance. The measurements with vegetable oil have revealed a linear relation between viscosity and CO emissions. CO concentrations were reduced by 28% when decreasing the viscosity from 9 to 3 cP. The same effect is observed in case of diesel combustion, with a CO reduction of 21% when the viscosity was lowered from 3 to 1 cP. These findings confirm that a reduction in fuel viscosity improves the spray quality, which results in faster evaporation and more complete combustion. The influence of fuel temperature and viscosity on the CO emissions observed in the results for diesel and vegetable oil is confirmed by additional tests with biodiesel. At viscosities above 9 cP, the exhaust gas contained considerable amounts of unburned fuel, presumably caused by incomplete evaporation.

Combustion experiments at different loads have shown that the CO levels also strongly depend on the equivalence ratio. In case of diesel, increasing the load re-

sulted in reduced emissions over the full range from 0 to 47 kW_e. This trend was not in full agreement with the results for vegetable oil, where no further decrease in CO level was observed above a load of 28 kW_e.

The experimental campaign with vegetable oil gives directions for the application of pyrolysis oil in gas turbines, a more advanced biofuel with high viscosity. Irrespective of the difference in burning characteristics between these biofuels, the use of pyrolysis oil in the present configuration can be rejected based on the limited tolerance to higher fuel viscosity.

Chapter 6

Conclusions and recommendations

This chapter summarizes the main findings from the research described in the previous chapters. The first part of this chapter discusses the insights gained regarding the modeling of ethanol and pyrolysis oil spray flames in industrial gas turbines. The second part presents the conclusions from the experimental work on the atomization and combustion of viscous fuels. Practical guidelines that could be derived from these studies are discussed in the third part. Lastly, a number of recommendations are provided for future research in this field.

6.1 Spray combustion modeling

A CFD model based on the Euler-Lagrange approach was used to simulate the combustion of ethanol and pyrolysis oil sprays. The gas phase was described by solving the steady-state RANS equations, combined with the Shear Stress Transport (SST) $k-\omega$ turbulence model. The fuel was injected in the form of droplet parcels with a uniform or a Rosin-Rammler distribution. A transient solver was used to track the parcels throughout the domain.

The CFD model was first applied to simulate the combustion of ethanol in a modified, downscaled diesel burner from the OPRA OP16 gas turbine. Non-adiabatic flamelets were used to describe the reactions based on a reduced mechanism. The model provided good predictions of the air distribution over the combustor and the major species in the exhaust gas. The calculated flow-averaged outlet temperatures were in close agreement with the theoretical values based on complete combustion, but the outlet temperatures measured in experiments were significantly lower (100–200 K). These deviations could not be explained by heat losses from the combustor or from the thermocouples to the environment, and were therefore mainly caused by the nonuniform temperature profile at the measurement location in the test rig. To

obtain average gas temperatures, the thermocouples should be placed much further behind the dilution air inlets.

It was observed that a minor part of the ethanol spray impacted on the liner. To validate this result, the predicted evaporation rates were first compared to empirical data from ethanol droplet studies in the literature. Data for droplets with high slip velocities are not available, but the research on quiescent droplets indicated that the predictions are plausible. Further validation of the spray modeling was done via combustion experiments in the test rig. Even though a thermochromic paint measurement did not reveal local hot spots on the outer liner wall, there was a strong indication that the fuel spray could reach the liner based on visual analysis. The discrete phase model was therefore found to predict the spray length with sufficient accuracy. Secondary breakup did not occur for droplets smaller than 100 μm , because the Weber number remained under the critical value.

The model was further developed to simulate the combustion of pyrolysis oil in an enlarged, full-scale combustor developed by OPRA for burning biofuels in the OP16 engine. The complex composition of pyrolysis oil was simplified to a mixture of seven components: methanol, water, acetic acid, acetol, phenol, eugenol and levoglucosan. The combustion of this surrogate fuel was modeled on basis of local thermodynamic equilibrium calculations, whereby the reaction rates were limited by a characteristic time scale dependent on the turbulence. Ethanol was used as the reference fuel. The simulations indicate that the peak temperature in the combustor is typically 200 K lower for pyrolysis oil than for ethanol. Since the adiabatic flame temperature of the pyrolysis oil surrogate is only 66 K lower with respect to ethanol, the difference in combustion temperature is largely due to the multicomponent nature of the fuel. It is furthermore predicted that the pyrolysis oil spray causes a stronger decrease in temperature in the region close to the injection location, because more than twice the amount of heat is required for evaporating the fuel. Moreover, the majority of the combustion heat is released during the latter half of the droplet lifetime, after the water has fully evaporated. Ignition and combustion in the proximity of the atomizer are thus expected to proceed at a lower rate. During experiments with pyrolysis oil in the full-scale burner, this effect has been observed as a decreased flame stability.

Comparative simulations with ethanol have shown that a model based on thermodynamic equilibrium gives similar predictions as the flamelet model, which is based on chemical equilibrium. This finding suggests that the pyrolysis oil flame characteristics can be predicted with reasonable accuracy without having a reaction mechanism available. However, the characteristic time scale used in the thermodynamic equilibrium model may require some adjustment for each fuel. The proper setting for pyrolysis oil combustion must be determined from experimental data.

Regarding the spray modeling, it is seen that the results for ethanol are insensitive to the initial droplet size defined at the injection location. In case of pyrolysis oil, however, changing the droplet size leads to differences in both the temperature and the velocity field. The time required for evaporation of a 50 μm pyrolysis oil

droplet was shown to be roughly 60% longer than that of an ethanol droplet, mainly due to the higher density and the high water content (25 wt.%). As a consequence, pyrolysis oil droplets larger than 65 μm were predicted to impinge on the combustor liner. Given that droplet diameters up to 100 μm are not uncommon in typical fuel sprays, this issue remains a point of concern. Some droplet markings at the fuel impact location and minor coke deposits at the inner liner found after the burning tests with pyrolysis oil were confirmative at this point. However, it must be noted that the burning tests were conducted at atmospheric pressure, and that the airblast atomizer performs better at engine pressure. A slight amount of fuel reaching the liner might furthermore be acceptable, as long as the inner surface temperature is high enough to avoid accumulation on the walls. Still, the results from both the model and the experiments clearly underline the importance of a fine spray, preferably with an SMD of about 30 μm . For the initial droplet sizes considered in the simulations ($D < 100 \mu\text{m}$), the model predicts heating rates of 10^6 – 10^7 K/min after evaporation of the water. Such high heating rates indicate that, in well-atomized sprays, secondary char formation is largely avoided. This finding was supported by experiments with pyrolysis oil in case of airblast atomization, since hardly any sparks were observed in the exhaust. As far as the model predictions could be verified by experimental data, it seems that the main trends are described with reasonable accuracy. The present model is therefore promising as a tool for new combustor developments, but further research is needed to validate the simulations in more detail.

6.2 Relating spray quality to combustion efficiency for viscous fuels

Pyrolysis oil is more viscous than standard gas turbine fuels, which can deteriorate the performance of the atomizer. The influence of viscosity on the spray and on the combustion was therefore studied using an atomization test rig and a micro gas turbine setup.

In the atomization test rig, the spray structure of liquids with varying viscosity was investigated in the near field of a pressure-swirl atomizer using high-resolution digital imaging. Images were captured 18 mm downstream of the atomizer and processed to determine the average size of droplets and ligaments. The optical system was able to capture droplets as small as 15 μm with minor error. Biodiesel and straight vegetable oil were chosen as the test liquids to cover a sufficiently wide range of viscosities while keeping other variables relatively constant. Glycerin was selected as a third test liquid to also evaluate the viscosity effects in combination with a higher density and surface tension. Although surface tensions of pyrolysis oils are not as high as that of glycerin, they can exceed the typical values for fossil fuel oils depending on the temperature and water content.

The results showed that viscous damping strongly affected the spray quality by causing ligaments to travel further downstream. The delay in breakup of the fuel

sheet became measurable at the fixed sample location for viscosities above 7 cP. A further increase in viscosity resulted in more and besides larger ligaments, until the fuel sheet itself started to appear in the images at a viscosity of 17–18 cP. Regarding the mean droplet size in the sprays in terms of the Sauter mean diameter (SMD), the effect of viscosity was found to be insignificant. Over the tested pressure range of 10–30 bar, the SMDs were typically between 55 and 80 μm for biodiesel and vegetable oil. SMDs for the glycerin sprays were 10–30 μm higher depending on the pressure, which most likely should be attributed to the high surface tension. The decrease in SMD towards higher pressures was consistent for all three liquids.

The pressure-swirl atomizer used for producing the investigated sprays was also employed for combustion tests in a micro gas turbine. Experiments have been performed with diesel, biodiesel and vegetable oil at different temperatures to relate viscosity effects on the spray to combustion efficiencies. The results for idle mode showed that the CO emissions at 15% O_2 were similar for the three fuels when injected at the same viscosity. This result confirmed the assumption that the modest differences in molecular structure of these fuels have little influence on the evaporation or burning behavior. The engine performance proved to be sensitive to changes in fuel viscosity. The results for biodiesel as well as vegetable oil showed that the CO emissions increased linearly with viscosity. Once the viscosity exceeded 9 cP, however, a visible increase in opacity of the exhaust gas indicated that the atomization quality was clearly unacceptable. Since the mean droplet size was found to be rather constant in this viscosity range, the increase in primary breakup length was identified as the main problem. Based on the detected ligaments in the spray at similar injection conditions, it follows that the liquid must be fully atomized roughly within the first 20 mm of the spray.

The viscosity of pyrolysis oil is not strictly defined due to variations in composition and age, but may well exceed the allowable viscosity limit identified for the investigated configuration, even when preheated to 80 °C. Higher temperatures should be avoided due to the oil's limited stability. Taking into account also the slower evaporation and burning process compared to hydrocarbon oils, it is evident that the application of pyrolysis oil in the unmodified micro gas turbine is technically not feasible.

6.3 Guidelines for burning pyrolysis oil in gas turbines

The simulations and experiments performed in this research have led to a number of guidelines regarding the design of a gas turbine combustor suitable for pyrolysis oil. Firstly, it is found that the flame tube of such a combustor must be considerably wider than that of a diesel combustor to accommodate the increased spray length. From both simulations and experiments, it is concluded that the diameter should be increased by at least 70%. A larger primary zone is also required in view of the slower combustion kinetics because of the significantly lower combustion tempera-

tures. Gas turbines with externally mounted combustors offer relatively high flexibility for design changes, and are therefore more suitable for burning pyrolysis oil than configurations with internal burners. The pyrolysis oil flame is characterized by a lower stability due to the limited heat release close to the atomizer. Therefore, especially at part load, the addition of a miscible, volatile fuel such as ethanol can be necessary to improve the ignition properties. A pilot flame can also be used to provide sufficient heat to the ignition region, but adds complexity to the system.

Good atomization is essential to limit the spray length and minimize char formation inside the droplets. The use of pressure-swirl atomizers is not advised due to the strong influence of fuel viscosity on the breakup length and the relatively large droplets produced at reasonable injection pressures. Twin-fluid atomizers should be able to provide superior spray quality, especially for viscous fuels. Still, to prevent the buildup of sediments in case a minor part of the pyrolysis oil spray impacts on the liner, it is important to maximize the inner surface temperature of the flame tube.

6.4 Recommendations for future research

Based on the insights obtained in this research, the following suggestions are made for future work:

- The CFD results should be validated in more detail, for example by measuring the temperature field inside the combustor using thermocouples. For an extensive validation of the model, however, it is recommended to make a comparative study using a laboratory test rig with improved optical and physical access to the primary combustion zone. Characterization of the spray produced by OPRA's airblast atomizer would be useful to verify the estimated droplet size distributions used in the simulations.
- It is suggested to examine the influence of radiative heat transfer by including a radiation model. Also, it could be interesting to add a small char fraction to the initial droplet composition. This would allow to estimate the evaporation time of the liquid phase as well as the burnout time of the solid particle that is potentially formed during the evaporation process.
- The literature on the evaporation or burning of small pyrolysis oil droplets ($D < 100\text{ }\mu\text{m}$) at high heating rates is very limited. More empirical knowledge is required to determine how the droplet modeling should be improved. Firstly, it is important to validate the rapid mixing assumption for such conditions. In case substantial droplet swelling occurs or if microexplosions frequently disrupt the entire droplet, it might be necessary to account for these phenomena in the model. Further information is also needed regarding the release of matter after evaporation of the water. Evaporation, cracking and char formation occur at the same time in this stage. Useful insights may be obtained by studying free droplets evaporating or burning in a hot coflow using high-speed imaging.

- The micro gas turbine setup was also prepared for mixtures of diesel and alcohol, or mixtures containing a minor amount of pyrolysis oil. A test campaign with these (preheated) mixtures can be interesting to measure the sensitivity of the engine to changes in fuel composition while the viscosity remains constant. A stainless steel atomizer is available to replace the original carbon steel atomizer for such experiments. This alternative atomizer showed similar performance during preliminary test runs in the lab. However, it should be noted that the high-pressure gear pump is not suitable for mixtures with high acidity.
- There is surely potential for improvement of the standard spray quality in the micro gas turbine. Especially twin-fluid atomizers are known for their good atomization performance for viscous liquids, and may provide SMDs down to 30 μm using less atomization energy. The measurements in this research indicated that the pressure-swirl atomizer could not produce SMDs below 50 μm , not even under the test conditions most favorable for fast atomization (high pressure, low viscosity, low surface tension). Therefore, an internally mixed air-assist atomizer producing a similar cone angle has been modified to replace the pressure-swirl atomizer in the micro gas turbine. It remains to be investigated whether this atomizer delivers a finer spray in the near field and maintains its performance when the fuel viscosity increases.

Appendix A

Properties of the surrogate fuel components

The properties of the components included in the fuel model for pyrolysis oil have largely been found in the Fluent built-in database, in other property databases [38, 64, 65, 93] or in the literature [36, 41, 66, 92, 140, 148]. Property data that were not directly available have been estimated using the specified methods.

The symbols used in this appendix are defined as follows:

M	Molecular weight (g/mol)
ρ_l	Density in liquid state (kg/m ³)
$C_{p,l}$	Specific heat capacity in liquid state (J/kgK)
T_b	Boiling point at atmospheric pressure (K)
T_c	Critical temperature (K)
L	Latent heat of vaporization (kJ/kg)
$\Delta_f H_{\text{gas}}^\circ$	Standard enthalpy of formation in gaseous state (kJ/mol)
$\Delta_f S_{\text{gas}}$	Standard entropy of formation in gaseous state (J/molK)

Vapor pressure data were implemented as piecewise linear functions of temperature based on the data shown in Fig. A.1.

Table A.1: Constant properties of the components.

Name	Formula	M	ρ_l	$C_{p,l}^a$	T_b	T_c	L	$\Delta_f H_{\text{gas}}^\circ$	$\Delta_f S_{\text{gas}}^\circ$
Methanol	CH_3OH	32.04	785	2546	338	513	1100	-201.1	239.6
Water	H_2O	18.02	998	4181	373	647	2263	-241.8	188.7
Acetic acid	CH_3COOH	60.05	1045	2147	391	593	395	-432.2	283.5
Acetol	$\text{C}_3\text{H}_6\text{O}_2$	74.08	1081	2314 ^b	419	596 ^c	624 ^d	-358.1	339.6
Phenol	$\text{C}_6\text{H}_5\text{OH}$	94.11	1055	2185	455	694	486	-104.6	321.9
Eugenol	$\text{C}_{10}\text{H}_{12}\text{O}_2$	164.20	1065	2090	526	700	404	-250.4 ^e	486.8 ^e
Levoglucozan	$\text{C}_6\text{H}_{10}\text{O}_5$	162.14	1317 ^f	2081 ^b	623 ^g	791 ^c	593 ^d	-789.5	401.9

^a At room temperature. Liquid heat capacities of methanol, water, acetic acid and phenol have been implemented as function of temperature.
^b Estimated using the Acree and Chickos method [123].
^c Estimated using the Joback method [123].
^d Estimated using the Vetere method [66].
^e Estimated using the Donalski and Hearing method [66].
^f Estimated using the Girolami method [9].
^g Derived from vapor pressure data measured by Sæberg and Oja [140].

Table A.2: Polynomials in CHEMKIN-format describing the gas phase heat capacity as function of temperature.

Name	$T_{\min}$	$T_{\max}$	a_1	a_2	a_3	a_4	a_5	a_6	a_7
Methanol	300	1000	.266011500E+01	.734150800E-02	.717005000E-05	-.879319400E-08	.239057000E-11	-.253534800E+05	.112326310E+02
	1000	5000	.402906100E+01	.937659300E-02	-.305025400E-05	.435879300E-09	-.222472300E-13	-.261579100E+05	.237819500E+01
Water	300	1000	.338684200E+01	.347498200E-02	-.635469600E-05	.696858100E-08	-.250658800E-11	-.302081100E+05	.259023200E+01
	1000	5000	.267214500E+01	.305629300E-02	-.873026000E-06	.120099640E-09	-.639161800E-14	-.298992100E+05	.686281700E+01
Acetic acid	300	1000	.846928500E+00	.292145000E-01	-.186455200E-04	.464098720E-08	.000000000E+00	-.536761800E+05	.211901500E+02
	1000	5000	.691666936E+01	.128920800E-01	-.420990320E-05	.458049540E-09	.000000000E+00	-.553508487E+05	-.102392103E+02
Acetol	300	1000	.189301000E+01	.388019000E-01	-.200598000E-04	-.139069000E-08	.361041000E-11	-.451778000E+05	.193862000E+02
	1000	5000	.102647000E+02	.186637000E-01	-.721806000E-05	.128787000E-08	-.867014000E-13	-.476911000E+05	-.246944000E+02
Phenol	300	1000	.139145560E+01	.393195700E-01	.177709600E-05	-.227767300E-07	.830965900E-11	-.147218090E+05	.191781300E+02
	1000	5000	.182163200E+02	.114242690E-01	-.109668430E-05	-.642744200E-09	.119889300E-12	-.205366400E+05	-.730423300E+02
Eugenol ^a	300	1000	-.251909000E+01	.110539000E+00	-.893351000E-04	.404424000E-07	-.827807000E-11	-.335674000E+05	.435739000E+02
	1000	3000	.105912000E+02	.683704000E-01	-.362874000E-04	.907629000E-08	-.876861000E-12	-.369147000E+05	-.227390000E+02
Levogluconan	300	1000	-.448795000E+01	.951530000E-01	-.487680000E-04	-.959272000E-08	.124112000E-10	-.974046000E+05	.477686000E+02
	1000	6000	.234811000E+02	.305600000E-01	-.105693000E-04	.165503000E-08	-.966273000E-13	-.106120000E+06	-.100563000E+03

^a Estimated using the Rihani and Doraiswamy method [124].

Name	a_1	a_2	a_3
Methanol	-3.91957E-06	3.66172E-08	1.02962E-10
Water	-6.52045E-06	6.09149E-08	1.71284E-10
Acetic acid	-2.83482E-06	2.64832E-08	7.44670E-11
Acetol	-2.41319E-06	2.25443E-08	6.33913E-11
Phenol	-1.94192E-06	1.81416E-08	5.10116E-11
Eugenol	-1.44754E-06	1.35231E-08	3.80250E-11
Levogluconan	-1.64935E-06	1.54085E-08	4.33264E-11

Table A.3: Coefficients of the polynomials describing the binary diffusivity of the components in air as function temperature. The diffusivity data were estimated using the Fuller et al. method [123].

Figure A.1: Vapor pressure of the components as function of temperature.

Appendix B

Evaporation and combustion models for pyrolysis oil

Given the complexity of pyrolysis oil, the evaporation and combustion behavior of this biofuel have been investigated mostly by using experimental methods. Thanks to these efforts, there is a basic understanding of the phenomena taking place when pyrolysis oil is exposed to a high temperature environment. Although still many questions remain to be answered for the time and length scales relevant in practical combustion applications, this empirical knowledge has served as a basis for the first numerical models. The few models that have been reported in the literature to date are shortly discussed here as background information.

Lederlin [83] proposed a model for the evaporation of pyrolysis oil droplets using a discrete component approach. The model is largely based on the Spalding formulations explained in Sec. 3.2, with the assumption that the droplet temperature remained at its initial value except on the evaporating surface. Heat conduction in the liquid is therefore not taken into account, and the energy required to heat the droplet is distributed over the droplet lifetime. The multicomponent character of the pyrolysis oil droplet is represented by non-mixing shells of individual components that evaporate strictly one after the other based on their boiling points. The evaporation curve is thus constructed from linear segments corresponding to each of the chemical compounds. Solid content and vapor formation inside the droplet (i.e. char and microexplosions) are not considered. Nine compounds are included to cover the boiling range of pyrolysis oil observed in distillation curves. However, it must be noted that 89 wt.% of the fuel model has a boiling point below 150 °C. Considering that the weight loss of pyrolysis oil in this temperature range is typically 50% or lower (see Sec. 3.3), the proposed surrogate fuel contains an unrealistically high fraction of volatiles. The model indicated that the evaporation of a pyrolysis oil droplet proceeds with a strongly varying rate at low ambient temperatures ($T_\infty \leq 600$ K), but behaves according to the D^2 -law at high temperatures ($T_\infty \geq 1200$ K).

An advanced model was developed by Hallett and Clark [69] based on the principles of continuous thermodynamics. In this approach, the multicomponent nature of pyrolysis oil is modeled using probability density functions that represent the main chemical groups. Four gamma distribution functions were included to describe the properties of the selected groups: acids, aldehydes/ketones, water and pyrolytic lignin. In the base case, the respective mass fractions of these groups are chosen to be 10, 20, 25 and 45%. The pyrolytic lignin is modeled as a heavy fraction that barely evaporates and converts into either char or gas at high temperatures via a one-step first order pyrolysis reaction. The gas phase equations derived in this work are very similar to those in the Spalding model (see Sec. 3.2) and to formulations for mixtures of pure components. The liquid phase is assumed to be well-mixed, an assumption that was justified by the bubbling behavior that is often observed in an evaporating pyrolysis oil droplet. Polymerization reactions in the liquid phase and char burnout are not included. The model was validated against suspended droplet evaporation experiments in an inert environment, performed with droplet diameters of 1400 to 1700 μm . The comparison showed that the predictions of the release of volatiles and the droplet temperature agreed fairly well with the experimental observations. Results of the calculations also indicate that the evaporation behavior is not very sensitive to the fuel composition, except for the water and pyrolytic lignin fractions. It was therefore assumed that the model will give reasonable predictions even if the pyrolysis oil composition is not known in detail.

Brett et al. [21] presented an evaporation model that includes diffusion in the liquid phase. To evaluate the effect of diffusive transport in the droplet on the evaporation process, the aim was to reproduce the results obtained by Hallett and Clark [69], who assumed the droplets to be well-mixed. A discrete formulation was chosen over a continuous description to allow for the implementation of chemical reactions in a later stage. The fuel composition represented by Hallett and Clark's distribution functions was approximated using eleven compounds. The pyrolytic lignin fraction was not modeled, however, but replaced by a fully evaporating compound with a high boiling point instead. Simulations showed that the limited rate of diffusion within the pyrolysis oil droplet slows down the evaporation. The mass loss characteristics were similar to those predicted by Hallett and Clark in qualitative sense, though evaporation rates were lower. This was mainly attributed to the effect of diffusive transport within the droplet, but it should be noted that the results did not change very much after multiplying the diffusion rates with a factor 5. The authors conclude that enhanced internal mixing will reduce the occurrence of explosive boiling in engine applications. Nevertheless, it is not clearly explained why this boiling phenomena would negatively influence the combustion performance.

The discrete approach was also employed by McGrath [100], who simulated both the evaporation and combustion of pyrolysis oil in an experimental burner using ANSYS Fluent. In this work, pyrolysis oil was divided into a distillable phase, represented by seven volatile compounds, and a non-distillable phase that accounts for primary and secondary char. The surrogate fuel was then designed to match four cri-

teria: the lower heating value, atomic balance, water content and distillation residue. Based on TGA data, the amount of char was set to 20% in the base case. However, since the char residue of a droplet will reduce under influence of the high heating rates in a combustor, a ‘low char’ case with a residue content of 5% was considered as well. Devolatilization of the distillable phase was described by a single kinetic rate model. The pre-exponential factor and activation energy expressing the rate of mass loss was derived from scaled TGA curves. This method implies that the different components in the fuel are released in the ratio that was defined by the initial fraction, regardless of their individual vapor pressures (no internal mass transport). The droplet temperature was assumed to be uniform. Gas phase reactions were modeled using equilibrium chemistry, while the char phase was treated as a coal particle in the combustion process. Burnout of the char was modeled using a diffusion-limited model, for which the diffusion coefficient was fitted to scaled experimental data. Results from the evaporation model alone are not discussed in this work.

Another evaporation model using a discrete pyrolysis oil composition was suggested by Zhang and Kong [153]. The 10 selected components and their initial fractions were determined from a list of pyrolysis oil constituents reported by Branca et al. [19]. The water content was fixed at the measured value, while the fractions of the remaining 9 components were scaled up to account for the other compounds. Here, it is important to note that the chemical characterization performed by Branca et al. covered 62–65% of the total sample mass. The remainder of the oil, presumably consisting of non-volatile compounds and pyrolytic lignin, is therefore not modeled. Simulation results were presented for a stagnant, perfectly mixed droplet with a diameter of 100 μm in an environment at 800 K and 1 atm. It is shown that the composition of the released vapors strongly varies over the droplet lifetime, and that the D^2 -curve deviates from the typical linear trend seen for single-component fuels. The model was not validated with experimental data.

Appendix C

The non-adiabatic flamelet model

In the flamelet concept, the turbulent flame is assumed to consist of thin, laminar flame sheets embedded in the turbulent flow field. Temperature and species mass fractions in such laminar flamelets are uniquely defined in terms of the mixture fraction, Z , and the scalar dissipation rate, χ . These two parameters respectively describe the fuel-to-air ratio and the departure from equilibrium due to aerodynamic strain. The flamelet profiles in mixture fraction space at different strain rates can be obtained by solving the one-dimensional flamelet equations for a range of χ -values up to extinction:

$$\rho \frac{\partial Y_i}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} + S_i \quad (\text{C.1})$$

$$\rho \frac{\partial T}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial Z^2} - \frac{1}{C_p} \sum_i H_i S_i + \frac{1}{2C_p} \rho \chi \left[\frac{\partial C_p}{\partial Z} + \sum_i C_{p,i} \frac{\partial Y_i}{\partial Z} \right] \frac{\partial T}{\partial Z} \quad (\text{C.2})$$

where Y_i , S_i and H_i are respectively the mass fraction, reaction rate and specific enthalpy of species i . The flamelet chemistry is described by a reaction mechanism that must be provided for the fuel under investigation.

To account for the random fluctuations in the turbulent flow field, Favre-averaged values of the temperature, density and species mass fractions are computed as follows:

$$\tilde{\phi} = \int \int \phi(Z, \chi_{\text{st}}) p(Z, \chi_{\text{st}}) dZ d\chi_{\text{st}} \quad (\text{C.3})$$

where ϕ represents T , ρ or Y_i , and χ_{st} is the stoichiometric scalar dissipation rate. By assuming that Z and χ_{st} are statistically independent, the joint probability density function (PDF) $p(Z, \chi_{\text{st}})$ can be simplified to:

$$p(Z, \chi_{st}) = p(Z)p(\chi_{st}) \quad (C.4)$$

For the mixture fraction, the turbulent fluctuations are modeled by using a beta PDF. The shape of this PDF is defined by the mean mixture fraction, $\tilde{Z}$, and the mixture fraction variance, $\widetilde{Z''^2}$. The influence of turbulence on the stoichiometric scalar dissipation rate is ignored. A delta PDF is therefore employed for $\tilde{\chi}_{st}$, of which the shape is defined only by the average value modeled as:

$$\tilde{\chi}_{st} = \frac{C_\chi \epsilon \widetilde{Z''^2}}{k} \quad (C.5)$$

where C_χ is a constant with a default value of 2.

The average temperature, density and species mass fractions in the turbulent flame are computed beforehand to minimize the computational effort during the simulations. After solving transport equations for $\tilde{Z}$ and $\widetilde{Z''^2}$, the corresponding thermochemical state of the gas is then easily found in multidimensional look-up tables of the form:

$$\tilde{\phi} = \tilde{\phi}(\tilde{Z}, \widetilde{Z''^2}, \tilde{\chi}_{st}, \tilde{H}) \quad (C.6)$$

where $\tilde{\phi}$ is the quantity of interest. The mean enthalpy level, $\tilde{H}$, is an additional dimension in the tables to account for heat losses, which requires adjustment of the adiabatic quantities. However, it must be noted that this correction is not applied for the species mass fractions under non-equilibrium conditions (i.e. $\tilde{\chi}_{st} \neq 0$), since modeling the flamelets over a range of enthalpies is prohibitive.

Appendix D

Notes on the validity of the rapid mixing assumption

Neglecting any gradients within the droplet greatly simplifies the calculations, but is not self-evident even for single-component fuels. Experimental studies with pure liquids have shown that the temperature field in an evaporating drop seems to be dependent on the diameter [49]. The temperatures in large droplets ($D > 1000 \mu\text{m}$) were observed to be relatively uniform due to internal circulations, while considerable temperature gradients were measured in small drops because the circulations stabilized. Despite this difference in behavior of the liquid phase, however, it was shown by Sirignano and Law [136] that lifetime predictions for single-component droplets are not very sensitive to the internal transport modeling. Hence, the rapid mixing assumption seems adequate for the ethanol cases considered in this study.

For multicomponent fuels such as pyrolysis oil, the validity of this approach is more arguable. Next to temperature gradients, also concentration gradients may appear due to limited internal mass transfer rates. Since the evaporation behavior of multicomponent fuels can be fundamentally different depending on the mixing state, simulation results are highly sensitive to the internal transport model used. The occurrence of gradients inside the drop can be predicted by evaluating the liquid-phase Lewis number and Péclet number defined in Eq. D.1, where k is the thermal conductivity and D_{AB} the diffusion coefficient [98, 130, 152]. In a high temperature environment, the diffusive mass transfer in liquids is generally slower than both the surface regression rate and the rate of heat conduction. The evaporation process is hence characterized by high Le and Pe numbers. The more volatile species in the fuel mixture are unable to reach the surface fast enough ($Pe \gg 1$) and the total evaporation rate will level off. This situation is described more accurately by the diffusion-limited model whereby the diffusion equation is solved [135]. As the temperature keeps increasing during the process ($Le \gg 1$), the species trapped in the droplet interior are superheated so that bubbling or explosive boiling may occur.

$$\text{Le} = \frac{k}{\rho C_p D_{AB}} \quad \text{Pe} = \frac{K(t)}{D_{AB}} \quad (\text{D.1})$$

Internal boiling phenomena have been observed for several multicomponent fuels, for instance during the combustion of heavy fuel oil droplets, and of fuel oil droplets emulsified with water or methanol [136]. In a more recent study, microexplosions were observed in freely-falling, burning droplets of ethanol, diesel, (castor oil) biodiesel, and their mixtures [14]. Detailed observations of evaporating or burning pyrolysis oil droplets have also illustrated the occurrence of swelling, bubbling and microexplosions during the process, and therefore the existence of concentration gradients in the liquid phase [23, 40, 54, 130, 152]. The experiments indicate that the outer layer of the droplet becomes rich in nonvolatile species due to polymerization reactions and fast evaporation of the light components at the surface. As a result, the remaining volatiles become trapped within a viscous layer with low permeability and eventually reach their boiling point as the drop temperature continues to rise. The presence of char particles at the same time favors the formation of nucleates and enhances the probability of microexplosions [130]. Due to experimental difficulties, however, these studies only considered relatively large drops (typically $D > 300 \mu\text{m}$) in a static or low-speed atmosphere. It is hence unclear whether the evaporation characteristics described above are representative for much smaller drops ($D < 100 \mu\text{m}$) subjected to high temperatures in a convective flow. It has been reported that smaller drops show a reduced tendency for explosive boiling compared to larger ones, but that the formation of vapor bubbles is promoted by high heating rates [54]. The water and char contents are also found to influence the probability and intensity of microexplosions [131].

In accordance with single-component fuels, the influence of convective transport on the mixing state of the droplet should not be neglected. Sirignano and Law [136] refer to a number of studies on two-component nonviscous droplets which all indicate that the liquid phase is well-mixed, presumably due to internal circulations induced by forced or natural convection. A theoretical analysis by Sirignano [135] confirms that these circulations enhance the transport rates in the liquid. However, it was shown that this effect cannot justify the rapid mixing assumption since the mixing time remains a controlling factor even at high velocities relative to the gas. Hence, it remains unclear to what extent the rapid mixing assumption violates the real mixing state of multicomponent droplets in spray combustion applications, especially for pyrolysis oil.

Appendix E

Additional results from the spray imaging setup

E.1 Depth of field analysis

Figure E.1: GI as function of the distance from the focal plane.

Figure E.2: VC as function of the distance from the focal plane.

Figure E.3: Relative measurement error as function of the distance from the focal plane.

E.2 Convergence of the mean droplet size

(a) Convergence for a pressure of 10 bar.

(b) Convergence for a pressure of 30 bar.

Figure E.4: SMD as function of the number of images in the data set for sprays at 60 °C.

E.3 Droplet size distributions

Figure E.5: Number distributions of the biodiesel, vegetable oil and glycerin sprays for an injection pressure of 10 bar (left) and 30 bar (right). In all cases, the viscosity of the liquid is 6.3 cP. The droplet count has been corrected for differences in the depth of field.

Appendix F

Biodiesel combustion in the micro gas turbine setup

In addition to the tests with diesel and vegetable oil (VO), combustion experiments with biodiesel (BD) have been performed. In these tests, the fuel injection temperature was varied between 17 and 61 °C while running without a load. The results are presented after a short discussion of the biodiesel properties.

The biodiesel used for the present experiments is produced by Sunoil in Emmen (The Netherlands). Sunoil produces fatty acid methyl esters (FAME) via transesterification of primarily used fats originating from plants and animals [139]. The Sunoil biodiesel is commercially sold as B100 and complies to the EN 14214 norm. The properties of this biodiesel are summarized in Table F.1 and can be compared with the properties of the other fuels tested in the MMGT, which are reported in Table 5.3.

Table F.1: Properties of the tested biodiesel. Data obtained from the EN 14214 norm and from literature [53, 67]. Reported viscosities were measured (see Fig. F.1).

Property	Unit	Biodiesel
Lower heating value	MJ/kg	39–41
Density ^a	kg/L	0.86–0.90
Surface tension ^b	mN/m	26–32
Flash point	°C	> 101
Viscosity	cP	
at 20 °C		6.3
at 40 °C		3.6
at 80 °C		1.6

^a Density at 20 °C.

^b Surface tension at 25 °C.

Figure F.1: Dynamic viscosity of No.2 diesel, biodiesel, vegetable oil and pyrolysis oil as function of temperature. Pyrolysis oil data is taken from literature [16, 56, 95, 104, 150].

In Fig. F.1, results from biodiesel viscosity measurements are compared to the viscosity data for the other fuels as presented in Fig. 5.3. The graph shows that biodiesel is slightly more viscous than diesel.

The normalized CO emissions measured as function of the fuel injection temperature are shown in Figure F.2. Emissions are reduced by increasing the temperature, as was seen in case of diesel and vegetable oil combustion (see Figs. 5.8 and 5.11). However, the effect diminishes until no further reduction in CO level can be observed around a temperature of 60 °C. At this temperature, the viscosity of biodiesel is approximately 2 cP. The result confirms the trend for diesel shown in Fig. 5.8 above 40 °C. In that temperature region, corresponding to viscosities below 2 cP, the effect of injection temperature is negligible as well.

Figure F.3 presents the normalized CO emissions as function of the fuel viscosity. The results from the biodiesel tests have been added to the data shown in Fig. 5.12. The trends are linear in both cases and the slopes are in good agreement. In absolute sense, CO concentrations are lower in case of biodiesel combustion.

Figure F2: Normalized CO emissions as function of injection temperature for BD combustion without load.

Figure F3: Normalized CO emissions as function of fuel viscosity for diesel, VO and BD combustion without load.

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Publications

J.L.H.P. Sallevelt, A.K. Pozarlik, and G. Brem. "Modeling of the combustion of fast pyrolysis oil in an industrial gas turbine". *Submitted for journal publication*.

J.L.H.P. Sallevelt, A.K. Pozarlik, and G. Brem. "Characterization of viscous biofuel sprays using digital imaging in the near field region". In: *Applied Energy* 147 (2015), pp. 161–175.

J.L.H.P. Sallevelt, J.E.P. Gudde, A.K. Pozarlik, and G. Brem. "The impact of spray quality on the combustion of a viscous biofuel in a micro gas turbine". In: *Applied Energy* 132 (2014), pp. 575–585.

J.L.H.P. Sallevelt, A.K. Pozarlik, M. Beran, L.-U. Axelsson, and G. Brem. "Bioethanol Combustion in an Industrial Gas Turbine Combustor: Simulations and Experiments". In: *J Eng Gas Turb Power* 136.7 (2014).

J.L.H.P. Sallevelt, A.K. Pozarlik, M. Beran, L.-U. Axelsson, and G. Brem. "Numerical and Experimental Study of Ethanol Combustion in an Industrial Gas Turbine". In: *ASME Turbo Expo 2013*. San Antonio, TX, USA: ASME, 2013, pp. V002T03A006.

J.A.M. Withag, J.L.H.P. Sallevelt, E.A. Bramer, D.W.F. Brilman, and G. Brem. "Heat transfer characteristics of supercritical water in a tube: Application for 2D and an experimental validation". In: *The Journal of Supercritical Fluids* 70 (2012), pp. 156–170.

J.L.H.P. Sallevelt, J.A.M. Withag, E.A. Bramer, D.W.F. Brilman, and G. Brem. "One-dimensional model for heat transfer to a supercritical water flow in a tube". In: *The Journal of Supercritical Fluids* 68 (2012), pp. 1–12.

Stellingen behorende bij het proefschrift

ON THE ATOMIZATION AND COMBUSTION OF LIQUID BIOFUELS IN GAS TURBINES

Towards the application of biomass-derived pyrolysis oil

door Joost Salleveld

1. Er is een bredere experimentele basis nodig om modellen voor de verbranding van pyrolyseolie verder te kunnen verfijnen.
2. Uiteindelijk zal de toepassing van bio-energie niet worden belemmerd door technologie, maar door de beperkte beschikbaarheid van duurzame biomassa.
3. Bij veranderende omstandigheden bepaalt het aanpassingsvermogen de overlevingskans.
(*Charles Darwin / Herbert Spencer*)
4. De milieudiscussie gaat in feite niet over het redden van de Aarde, maar over het verlengen van onze eigen verblijfsvergunning.
5. Een democratie veronderstelt veel kennis bij haar kiezers.
6. De grote diversiteit tussen landen in de EU maakt verdere politieke en economische centralisatie voorlopig onhaalbaar en onwenselijk.
7. Economische groei staat in Nederland niet meer gelijk aan maatschappelijke vooruitgang.
8. Het publicatieproces wordt hoog viskeus als een reviewer achttien keer over het woord 'gasturbine' heen leest en daarom aanneemt dat het manuscript over zuigermotoren gaat.
9. De sterke daling van de olieprijs gedurende dit project (van \$115 naar \$66 per vat) maskeert de urgentie van het energievraagstuk.

Propositions accompanying the dissertation

ON THE ATOMIZATION AND COMBUSTION OF LIQUID BIOFUELS IN GAS TURBINES

Towards the application of biomass-derived pyrolysis oil

by Joost Sallevelt

1. Further refinement of models for pyrolysis oil combustion requires a broader experimental basis.
2. The application of bioenergy will eventually not be hindered by technology, but by the limited availability of sustainable biomass.
3. When conditions are changing, the ability to adapt determines the chance to survive.
(*Charles Darwin / Herbert Spencer*)
4. The environmental debate is actually not about saving the Earth, but about extending our own residence permit.
5. A democracy presumes that its voters have much knowledge.
6. For the present, the large diversity between countries within the EU makes further political and economic centralization infeasible and undesirable.
7. In the Netherlands, economic growth is not equivalent to social progress anymore.
8. The publication process becomes highly viscous when a reviewer misses the words 'gas turbine' eighteen times and hence assumes that the manuscript is about piston engines.
9. The sharp decrease in oil price during this project (from \$115 to \$66 per barrel) conceals the urgency of the energy issue.