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Numerical study of pyrolysis oil combustion in an industrial gas turbine

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ABSTRACT

The growing demand for the use of biofuels for decentralized power generation initiates new research in gas turbine technology. However, development of new combustors for low calorific fuels is costly in terms of time and money. To give momentum to biofuels application for power generation robust numerical models for multicomponent biofuels must be developed. This paper 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. Comparative simulations have been performed to examine the influence of the initial droplet size and to evaluate different combustion models. The results were compared to available experimental data for pyrolysis oil and ethanol combustion. A qualitatively good agreement was achieved.

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1. Introduction

Fast pyrolysis oil is a renewable biofuel produced from biomass waste materials that can potentially be used as a fuel for industrial applications $[1-10]$. 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 $[11-13]$. 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 $[4,14-16]$. 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. Only a few models have been proposed to approximate the behavior of pyrolysis oil droplets in a high temperature environment [\[17–24\]](#page--1-0). 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 paper 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-caloric fuel combustor that was recently developed by OPRA for the application of biofuels in their OP16 gas turbine $[22]$. The aim is to capture the main burning characteristics of pyrolysis oil. The results have been compared to simulations with ethanol, a single-component biofuel. Additional computations have been performed to verify the sensitivity of the results to the initial droplet size and to the combustion model. Although the detailed experimental data regarding flow and temperature field at various locations inside the combustor, as well as droplet size and distribution were not available for validation purpose, the model outcome was compared to experimental exhaust gas temperature and $CO₂$ emissions. Comparison with outlet measurements is frequently performed in case the detailed data regarding specific flow profiles is out of reach current experimental techniques, see [\[25–28\].](#page--1-0)

2. Pyrolysis oil fuel model

Considering the large number of compounds present in pyrolysis oil, the composition was simplified using a discrete component

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0196-8904/© 2016 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license ([http://creativecommons.org/licenses/by/4.0/\)](http://creativecommons.org/licenses/by/4.0/). 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. [\[23\]](#page--1-0) 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 37 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 curve due to its high latent heat of vaporization. This approach resulted in the fuel model specified in Table 1. The surrogate fuel has an elemental composition of C 40% H 8.5% O 51% by weight and a lower heating value (LHV) of 15.6 MJ/kg, both of which are typical for fast pyrolysis oils [\[24,29–31\]](#page--1-0).

The initial mass fractions of the surrogate fuel components have been estimated by evaluating TGA data reported in the literature. Branca et al. [\[23\]](#page--1-0) determined devolatilization curves for the abovementioned pyrolysis oils using a heating rate of 5 K/min up to a final temperature of 600 K. The measured weight loss in each of the six temperature zones was compared to their prediction for the mass loss in the zones. These predictions were based on the mass fractions of the oil constituents that were allocated to the zone based on their boiling points.

For the Dynamotive and BTG oils, the TGA data obtained from these experiments are listed alongside the predictions in Table 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 2 also shows the TGA results reported by Van Rossum et al. [\[30\]](#page--1-0). These experiments were performed with pyrolysis oil produced from forest residue by VTT using a heating rate of 50 K/min up to an oil temperature of 823 K. The latter two columns in the table show TGA data for the same VTT oil, but the reported temperatures are of the sample cup in those cases.

The weight loss of the Dynamotive and BTG oils measured by Branca et al. deviates 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 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.% and a heating rate of 50 K/min is generally similar to that of the BTG oil. A large difference is seen in the highest temperature zone, however, presumably because the VTT sample was heated to a higher final temperature.

Table 1

Specification of the discrete fuel model used as a surrogate for pyrolysis oil. The temperature zones have been adopted from Branca et al. [\[23\].](#page--1-0) T_b and Y_{init} denote respectively the boiling point and the initial mass fraction.

Zone	Oil temperature (K)	Component	Formula	T_{b} (K)	Y_{init} (%)
	< 360	Methanol	CH ₃ OH	338	10
	360-400	Water	H ₂ O	373	25
		Acetic acid	CH ₃ COOH	391	10
	400-450	Acetol	$C_3H_6O_2$	419	10
	450-500	Phenol	C_6H_5OH	455	10
	500-550	Eugenol	$C_{10}H_{12}O_2$	527	
	>550	Levoglucosan	$C_6H_{10}O_5$	623	20

Table 2

Weight loss (WL) in wt.% for the different temperature zones as measured using TGA. Predictions are based on oil composition and boiling points. Data reproduced from Branca et al. [\[23\]](#page--1-0) and from Van Rossum et al. [\[30\]](#page--1-0).

Zone	Temp. zone (K)	WL vs T_{oil}					WL vs T_{cup}	
		Dynamotive ^a		BTG^b		VTT ^c	VTT ^d	VTT^e
		TGA	Pred.	TGA	Pred.	TGA	TGA	TGA
	360	16.7	7.8	27.6	7.9	28.0	28	
	360-400	13.3	33.2	16.6	44.4	18.4	15	17
	400-450	13.7	8.4	13.1	6.5	9.6	11	16
	450-500	9.7	2.9	8.3	1.6	7.0	8	10
	500-550	8.9	4.7	5.7	3.1	5.0	4	9
6	>550	6.0	7.2	4.2	4.9	16.0	16	26
$1 - 2$	$<$ 400	30	41	44	52	46	43	24
$1 - 3$	$<$ 450	44	49	57	59	56	54	40
1-6	Full range	68	64	76	68	84	82	85

Dynamotive oil, 21% water, heating rate 5 K/min up to 600 K based on oil temperature.

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

VTT oil, 24% water, heating rate 50 K/min up to 823 K based on oil temperature. Predictions are not available

^d VTT oil, 24% water, heating rate 1 K/min up to 1073 K based on sample cup temperature.

^e VTT oil, 24% water, heating rate 100 K/min up to 1073 K based on sample cup temperature.

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