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THEORETICAL INVESTIGATION OF THE PERFORMANCE OF ALTERNATIVE AVIATION FUELS IN AN AERO-ENGINE COMBUSTION CHAMBER

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Abstract

When considering alternative fuels for aviation, factors such as the overall efficiency of the combustion process and the levels of emissions emitted to the atmosphere, need to be critically evaluated. The physical and chemical properties of a fuel influence the combustion efficiency and emissions and therefore need to be considered. The energy content of a biofuel, which is influenced negatively by the presence of oxygen in the molecular structure (i.e. oxygenated chemical compounds), is relatively low when compared with that of conventional jet fuel. This means that the overall efficiency of the process will be different. In this paper two possible scenarios have been investigated in order to assess the potential to directly replace conventional jet fuel with Methyl Buthanoate - MB (a short chain FAME representing biofuel) and a synthetic jet fuel (FT fuel) using Computational Fluid Dynamics (CFD) modelling in a typical Modern Air-Spray Combustor (MAC). In addition the impact of fuel blending on the combustion performance has been investigated.

Computational Fluid Dynamics (CFD) has been verified and validated over past decades to be a powerful design tool in industries where experimental work can be costly, hazardous and time consuming, to support the design and development process. With recent developments in processor speeds and solver improvements, CFD has been successfully validated and used as a tool for optimizing combustor technology. Combustion of each fuel is calculated using a mixture fraction/pdf approach and the turbulence-chemistry interaction has been modelled using the Laminar Flamelet approach. Detailed chemical reaction mechanisms, developed and validated recently by the authors for aviation fuel including kerosene, synthetic fuel and bio-aviation fuel have been employed in the CFD modelling. A detailed comparison of kerosene with alternative fuel performance has been made.

1   Introduction

Petroleum products have always been considered as supreme fuels for the transportation sector due to their beneficial combination of high energy content, performance, availability and ease of handling at a low cost. However, the continuing increases in oil price, concern over energy security and the reducing availability of petroleum have focused the industry into investigating alternative fuel solutions. In the aviation industry there is a strong focus on developing bio-aviation and other alternative fuels that can be used with current engine technology [1]. Although commercial aircraft are only responsible for around 3% of total emissions compared with other sectors, the impact of emissions being directly into the upper atmosphere means they potentially have a more pronounced effect on changes in the climate [2,3]. As discussed, utilizing alternative fuels in aviation is a challenge, but there is the potential to reduce the quantities of engine emissions released into the atmosphere from aircraft. One of the most important issues is the challenge to find an ideal candidate to supplement or even replace conventional kerosene. A number of possible directions are considered and presented in this paper.

The main objective of this work has been to investigate the effect of using alternative aviation fuel, specifically biofuel and synthetic fuel (n-heptane), on the combustion characteristics within a typical aircraft engine. The combustion of conventional jet fuel (kerosene), MB and FT fuel has been investigated theoretically using CFD. For this fundamental study of the combustion process, the Modern Air-Spray Combustor (MAC) has been utilized. The CFD approach has previously been

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validated against the experimental measurements in the MAC combustor for kerosene fuel [4,5]. Detailed oxidation mechanisms for kerosene and biofuel, recently developed by the authors [6], have been employed using the 3D CFD solver. Since fundamental information about the reaction kinetics is essential for a combustion model, these new reaction mechanisms facilitate the modelling of chemistry aspects required for an accurate combustion simulation. The synthetic fuel combustion scheme was represented by n-heptane mechanism proposed by Seiser [7]. For modelling purposes a reduced mechanism has been adopted.

2 Alternative aviation fuels - new challenges

Since their conception, aircraft gas turbines have utilized kerosene as a basic fuel because of its availability on a large scale and its robust stability properties combined with high energy content. Typical petroleum based jet fuels such as Jet A and Jet A-1 (used in civil aviation) as well as JP-5 and JP-8 (utilized in military aircraft), have been developed extensively over a number of years. The composition of jet fuel, primarily based on wide ranging sizes of hydrocarbons (different molecular weight and carbon number), offers a relatively high volumetric and gravimetric energy [8,9].

The problems associated with using alternative fuels in aviation have attracted considerable attention recently and have become an internationally important topic for discussion. A number of studies have been published in which the performance of these alternative fuels has been examined [4,6, 10,11,12,13].

The bio- jet fuels which are derived from sustainable sources can produce significant savings in carbon dioxide emissions, making them attractive for consideration. However, given that the aviation fuel specification requirements are very stringent, using a pure bio-jet fuel in aviation requires investigation, with direct replacement potentially requiring significant modifications to the engine design. The most common biodiesel developed and employed recently are the fatty acid methyl esters (FAMEs). Produced via a process of trans-estirification of oils and fats with methanol (Fig.1), these esters have similar chemical and physical properties compared with conventional diesel fuel [14].
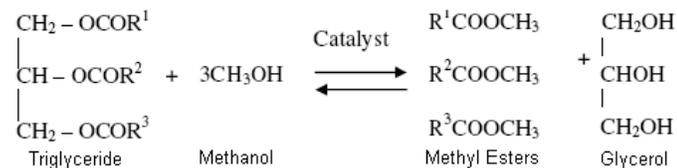

Fig. 1 Production of FAMEs - transesterification of triglycerides with alcohol.

The estirification process brings changes in the structure of the vegetable oil molecules such as: viscosity and saturation, thus the properties of the final product (methyl ester) are different in comparison to jet fuel. A number of studies have shown that FAMEs can be used for aircraft transportation, in particular as a blended component. However, there are some properties (including freezing point and thermal stability etc.) of biodiesels which are very poor compared to conventional jet fuel. Furthermore, the oxygen present in the biofuel molecule has an impact on the overall energy content. Consequently the energy is lower (typical LHVbiofuel=36-39MJ/kg) when compared with conventional jet fuel (typical LHVjet fuel=42MJ/kg). This is one of the major problems related to biofuels, since it results in the engine power profile being modified [14,15]. As such with the current state of knowledge, it is still a technical challenge to use pure biofuel in a jet aircraft.

The synthetic fuel produced via the high temperature Fisher-Tropsch (FT) method (1) from coal, gas or biomass is a further alternative which has been studied for aviation purposes. The nature of the process is expressed by the exothermic reaction (1) listed below [14]:

$$(2n+1)H_2 + nCO \rightarrow C_nH_{(2n+2)} + nH_2O \qquad (1)$$
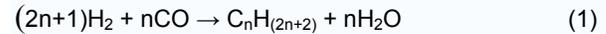
FT fuel has been implemented successfully in Johannesburg as a 50:50 blend (SASOL) and recently 100% SASOL has been approved for use in commercial aircraft. FT fuel is comparable in performance to conventional jet fuel and exhibits superior thermal stability. Experimental studies have shown that the FT product is almost entirely free of heteroatoms and aromatics making it very attractive for use in both biodiesel and in jet applications. The major advantage of aromatic free fuels are that they are cleaner burning with, generally, lower particulates remaining after combustion (no sulphur dioxide (SO_2) and sulphuric acid (H_2SO_4)) compared with those from the conventional jet fuel. However, this lack of aromatics results in FT fuel not meeting density requirements and also can cause problems due to issues relating to engine material compatibility [14]. This is a distinct disadvantage of synthetic fuels. Experiments show that the drawbacks can be reduced significantly when FT fuels are blended with jet fuel [13,14].

3 Combustion system

A detailed description of the MAC engine has been provided in previous publications [1, 2]. Combustion simulations were carried out using the Modern Air-Spray Combustor (MAC) shown in Fig.2. For CFD simulation purposes a single burner port (1/22 of the combustion chamber) has been considered assuming the rotational symmetry of the MAC. The structured mesh created for the MAC consists of 198000 hexahedral and 3600 prismatic wedge elements. Fuel was injected as droplets (with an initial temperature of 340K) through a thin annulus (5.6mm radius) located at the centre of the injector (see figures 2(a) and 2(b)). For the purposes of comparing CFD results a line perpendicular to the injector, running along z-axis through the centre of the combustor, is marked in the Fig. 2(c). Additional air was provided via the primary and dilution holes in order to complete the combustion process and cool the hot products leaving the combustor. The boundary conditions for both air and fuel inlets, as well as drop size and spray angles of the fuel for the model, have been taken from experimental data. Due to the differences in energy content of the alternative fuels compared with kerosene (Fig. 3), the mass flow has been recalculated to make the input energy per second equivalent for all fuels. This has been achieved by normalising based on the mechanism for each fuel (taking the enthalpies into account). This approach is considered a more realistic approach for obtaining comparative engine performance. Initial results with the lower energy input case is considered for biofuel, i.e. the mass flow of the biofuel was kept constant with respect to the kerosene, are presented in a previous publication [4].
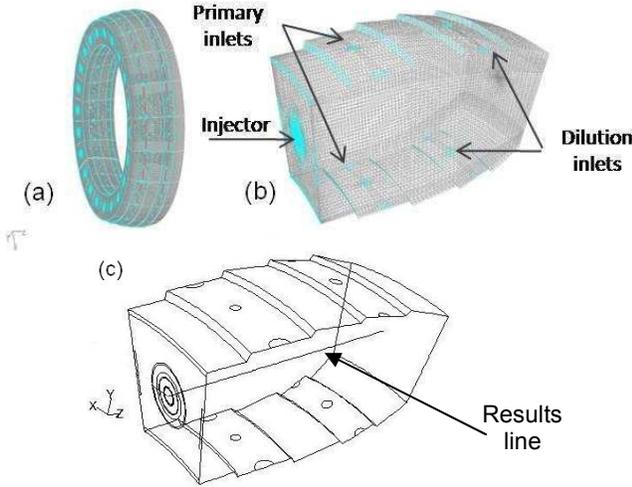
Fig. 2 The geometry of the combustor a) full annular geometry of the MAC with 22 burner ports and b) meshed computational domain c) geometry of the combustor section showing central line where the results can be compared.
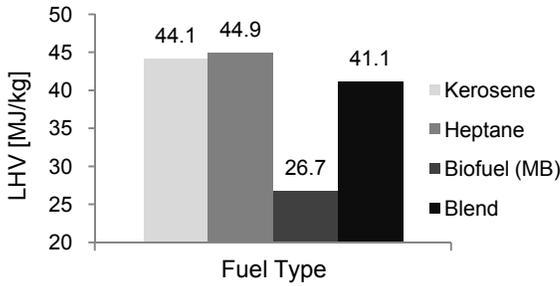

Fig. 3 Lower heating values are taken into account through normalising input energy to the combustor by adjusting fuel mass flow rates accordingly.

4   CFD modelling approach
4.1   Turbulent combustion simulation

A range of different models have been applied during this investigation in order to solve the considered problem both efficiently and with high accuracy. Based on steady state Reynolds-averaged Navier Stokes equations the Reynolds Stress Model (RSM) model has been applied to solve turbulent flow within the combustor. The RSM approach has been extensively examined for gas turbine combustion problems and is considered an accurate choice in the case of highly swirling flows. Consequently, using RSM is an efficient way to improve the simulation accuracy [16,17].

Non-premixed flames can be used to describe general liquid combustion processes in gas turbines. The problem is simplified to the mixing and reaction of two opposing streams of fuel and oxidizer. The flamelet model employed in this case is based on the assumption that a turbulent diffusion flame appears as a steady, one-dimensional laminar strained flame. This assumptions holds in many applications for turbulent gas diffusion flames [18, 19, 20, 23]. A flamelet model gives a compromise between accuracy of results and simulation time for

reacting flows and simultaneously incorporates the detailed chemical kinetics for the turbulent combustion simulations. In order to couple the impact of the flow field on the flame structure and shape, the flamelet library is created for two input parameters, the mixture fraction f and the so-called scalar dissipation rate χ. The relation between them is expressed by equation (2). Within the model the scalar dissipation rate is considered as a parameter that incorporates the convection-diffusion effect in the mixture fraction space. The information enclosed in the flamelet library, in the form of look-up tables, incorporates species, density and temperature profiles in the mixture fraction space required for further evaluation of the combustion characteristics and formation of pollutants. A statistical distribution of the mixture fraction and the scalar dissipation in the turbulent flow field is specified by a beta PDF function which provides the information for the mean values of the temperature, density and species mass fractions [19,20].

$$\chi = 2D|\nabla f|^2 \qquad (2)$$

Where :
D- diffusion coefficient,
f - mixture fraction.

The principle of the flamelet generation is expressed by the set of the following partial differential equations (3) and (4) listed below for the species mass fraction Y_i and temperature T for a given scalar dissipation rates [19]:

$$\rho \frac{\partial Y_i}{\partial t} = \frac{1}{2}\rho\chi\frac{\partial^2 Y_i}{\partial f^2} + S_i \qquad (3)$$

$$\rho \frac{\partial T}{\partial t} = \frac{1}{2}\rho\chi\frac{\partial^2 T}{\partial f^2} - \frac{1}{c_p}\sum_i H_i S_i + \frac{1}{2c_p}\rho\chi\left[\frac{\partial c_p}{\partial f} + \sum_i c_{p,i}\frac{\partial Y_i}{\partial f}\right]\frac{\partial T}{\partial f} \quad (4)$$

For the multiple flamelet library generation the scalar dissipation rates of between 0.01 and 36.0 have been implemented.

NOx formation in turbulent reacting flows is a complex process that involves fluid dynamics, chemical kinetics, mixing processes and requires hundreds of elementary reactions to be considered. In this paper the NOx is computed as a post-processor task given that solving the pollutant species equations jointly with the combustion model is more complex and time consuming [25]. This is an efficient and reliable approach that involves solving additional transport equation for nitric oxide (NO) based on a calculated flow field. The thermal and prompt NO which have been employed in the computation are expressed in the reactions proposed by Zeldovich and Fenimore, respectively [21, 22].

5   Theoretical study on alternative aviation fuel reaction mechanism

Simulation of the combustion in a gas turbine requires a conceptual understanding of the process chemistry, as such an accurate reaction mechanism is essential. In this case we require mechanisms for both the biofuel and heptane. In the present study a detailed chemical reaction mechanism AFRMv.2.0, recently developed and validated by Catalanotti et al. [6]; which incorporates a number of different aviation fuels including both a conventional aviation fuel (kerosene) and biofuel, has been implemented in the CFD simulations. The mechanism has previously been tested in several relevant areas including CHEMIKIN[TM] - PSR and Premix simulations in which

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robust results over a wide range of operating conditions were obtained (covering combustion temperature, pressure and different equivalence ratios). The oxidation of n-heptane, represented by mechanism from Seiser et al. [7] has been applied to the calculations for predictions for the synthetic fuel.

In this section the performance of the mechanisms has been examined to predict the combustion chemistry within the aircraft engine with special concentration on the flame structure. Accordingly, the mechanism has been applied to the one-dimensional laminar flamelet model to calculate the flame (i.e. temperature and concentration of the species within the flame) required for further simulations. The detailed kinetics of the following fuels indicated in the table 1 have been incorporated into the calculations. This section provides the initial data related to the flame structure (prior to considering the specific geometry of the MAC), results of which are employed to the later CFD calculations within the model.

Case	Component	Fuel composition (%)
Kerosene	n-decane $C_{10}H_{22}$	89%
	toluene -$C_6H_5CH_3$	11%
FT fuel	n-Heptane - C_7H_{16}	100%
MB (Biofuel)	Methyl Butanoate - $C_5H_{10}O_2$	100%
Blend	Kerosene	80%
	Methyl Butanoate	20%

Table 1 Overview of the different fuel composition used for the flamelet calculations.

5.1 Comparison of chemical kinetics for alternative aviation fuels - OPPDIF calculations

When undertaking this modelling approach the first stage is to undertake Opposed Flow Diffusion Flame (OPPDIF) calculations using the appropriate reaction mechanisms for each fuel. Fig. 4 and 5 (a)-(d) outline the predictions for the temperature and mass fractions of CO_2, CO, O and OH obtained from the OPPDIF calculations. In both Fig. 4 and 5 the temperature and species mass fractions for each fuel are plotted against the mixture fraction, based on the two streams of fuel and oxidiser. An examination of the results of these calculations provides information on each fuel's combustion characteristics prior to solving the full CFD flow field for a particular combustor geometry. The dashed lines (f_{1-2}, f_3, f_4) denote the position of the stoichiometric mixture fraction for each fuel. It can be observed in Fig. 4 that the maximum flame temperature is comparable for pure kerosene and heptane which occurs at mixture fraction f_{1-2}~0.07. With regards to the blended fuel temperature profile, only a minor difference can be observed (f_3) compared to the kerosene. Consequently, it can be concluded that the oxygen from the methyl ester molecule has an effect on the overall temperature characteristic in the MB and blended fuel. The same trend can be observed for the mass fractions of major and minor species such as O and OH (Fig. 5 (a)-(b)). There is good agreement between the kerosene and the blended case. This reinforces the conclusion that the combustion chemistry is not significantly impacted when using 20% MB blended with 80% kerosene fuel. With regards to MB, a considerable decrease in concentration of O and OH can be

noticed. Additionally, the trend in figures 5(a)-(d) for O, OH, CO, CO_2 respectively is similar to that in Fig.4 where we see the maximum values predicted at richer mixture fractions. Again, this can be attributed to the additional oxygen in the MB molecule. As such, a significant variation in the combustion chemistry is observed when kerosene is compared with 100% MB. The peak of the flame temperature for MB (Fig. 4) is reached at a mixture fraction f_4~0.12 with a slightly lower peak temperature. From the combustion chemistry point of view the deviations can be attributed to differences in the properties of the biofuel compared with conventional aviation fuel. Oxygen present in the methyl ester molecules indicates that there will be typically 10% or greater oxygen content by mass in the biofuel. This will impact on the combustion chemistry in terms of the air to fuel ratio and emission levels. Additional oxygen included in the MB molecule takes part in combustion and appears to promote more complete combustion which partially explains variations in CO-CO_2 conversion.

The combustion kinetics of both kerosene and alternative fuels are determined by the molecular structure of the particular fuel components. The strength of the molecular bonds in the different fuels are fundamentally responsible for all the differences between them and the path of the oxidation process. This is demonstrated clearly in the case of biofuel where the energy for C-O bond fission (pyrolysis mechanism) is lower than for the C-H and C-C bonds (found in the all three fuels). Consequently, the C-O bonds break more rapidly and propagate the pyrolysis at relatively low temperatures. The consequences of this is a variation in ignition delay between the fuels with a shorter ignition delay occurring in the case of MB where the major processes begin at much lower ignition temperature (Fig.4). This is seem to have a significant effect on the CO-CO_2 conversion process.

In the case of heptane it should be noted that unlike kerosene this fuel does not include aromatics and therefore there is the expected difference in the performance. The overall effect of aromatics is not fully clear in the combustion but this subject demands further investigation.

Finally, it has been identified that MB has a low combustion enthalpy: lower than that of kerosene fuel due to the oxygen content of the molecules which necessitates a larger fuel flow to the combustor in order to deliver the same amount of energy to that provided by kerosene. Further analysis of the combustion chemistry of the biofuel and synthetic fuel has been discussed by authors elsewhere [17], [18], [19].
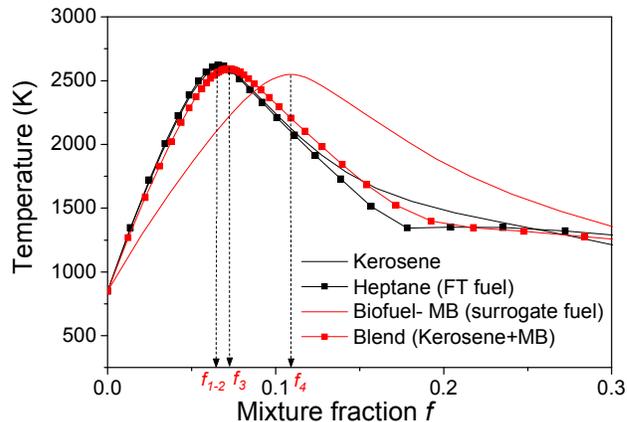

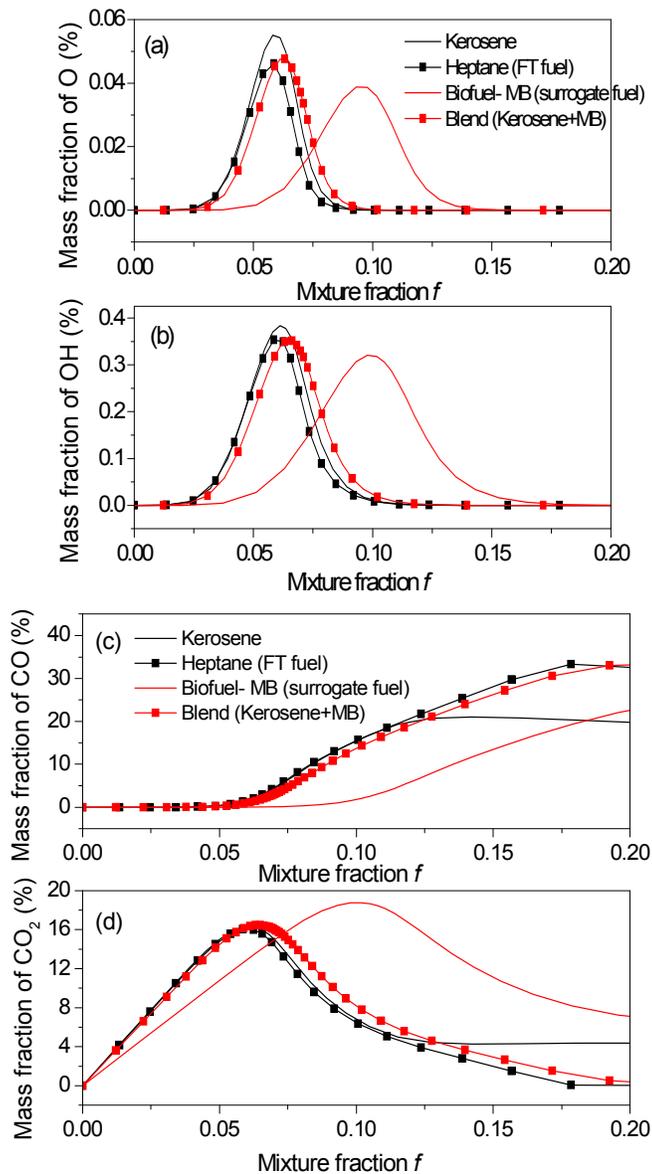**Fig. 4 OPPDIF calculations for the temperature.**

Fig. 5 OPPDIF calculations for (a) - mass fraction of O ; (b) mass fraction of OH; (c) mass fraction of CO; (d) mass fraction of CO_2 respectively.

6 Discussion of CFD predictions
6.1 The performance of alternative fuels in the aero-engine combustion chamber

In this section the predictions obtained from the full CFD simulation for each fuels performance in the MAC are outlined. During this research it has been observed that when modelling the turbulence, the accuracy of simulation performed using Reynolds stress model (RSM) was significantly improved when compared with the Standard k-ε model. As such the results outlined in this paper will focus on those produced using the RSM approach.

The results of numerical simulations are presented for the four fuels indicated in table 1. Predictions for all fuels are based on equivalent mass flow and equivalent energy content. In the first instance, models have been verified by reproducing the conditions and predictions for the combustion of kerosene in the MAC [4]. Following previous successful validation of the modelling approach, predictions for the alternative fuel cases, where no current empirical data is exists, are performed.

In Fig. 6 (a)-(d) simulation result data is displayed on planes parallel to the injector at the following positions relative to the burner: Z=0.038m, Z=0.068m, Z=0.106m, Z=0.14m, Z=0.17m (where Z=0 describes a plane that passes through the injector nozzle) are presented. These planes make useful comparison positions for validating the model predictions and observing the behaviour of the alternative fuels.

In the predicted temperature contour plots for kerosene, n-heptane, MB and blend given in Fig. 6(a)-(d) an important observation is that the overall temperature distribution in the combustion chamber is comparable for all the considered fuels. When taking into account the blend and n-heptane temperature profiles (Fig. 6(b) and Fig. 6(d), respectively) it can be observed that combustion chemistry is not significantly affected by the alternative fuel and there is no noticeable influence on the performance. However, it has been found that temperature for MB is slightly lower than that of the reference kerosene fuel (Fig. 6(a) and Fig. 6(c)). This discrepancy can be attributed to the oxygen in the methyl ester molecule impacting on the combustion characteristics. Obviously the physical properties of the alternative fuel (lower heating value, density etc.) can influence not only the efficiency of the overall system, but also the size of the tank and the weight of the aircraft. However, in the case when the fuel flow rate is increased to take account of the reduced combustion enthalpy the result for MB and blend can be observed to be much closer in character to that of kerosene, but with marginally reduced temperatures. The differences in predictions can be seen more clearly on the plots in Fig. 7(a)-(f) where the results of temperature and species mole fractions (O_2, CO, CO_2, H_2O, UHc), respectively, have been plotted for the range of fuels mixtures described in the table 1 on the horizontal result line passing through the centre of the combustor (shown in Fig. 2 (c)). As discussed earlier the results outlined for kerosene have been validated against the experiential data therefore we consider them as a base for the assessment of the alternative fuels performance.

Figure 7(a) refers to the temperature obtained within the combustion chamber. The results demonstrate that there is a good agreement between all the tested fuels. In figures 7(c)-(e) the predictions for CO, CO_2 and UHc mole fractions, respectively, have been plotted against the axial distance from the injector. It can be observed that for the intermediate temperature regions, where the concentration of OH appears to be lower, the level of CO and UHc is higher as a consequence of reduced conversion of CO to CO_2. Figure 7(e) illustrates a comparison of the water concentration for the indicated fuels. It can be observed that in the case of heptane, there is a low water concentration close to the injector. This is attributed to a deficit of oxygen in this region. It is also worth to mention that the H/C ratio in C_7H_{16} is very high, which partially explains the reduction in the water mole fraction which provides the peak in H_2 concentration.

Figure 8, shows the temperature data averaged at radial positions on the outlet. This is meaningful data since it

represents the predicted temperature that a turbine blade situated at the exit of combustor would experience. Any significant differences in temperature could have detrimental consequences on the operating lifetime of the turbine blades which have been designed to be used with fuels that provide a distinctive temperature profile under typical operating conditions. These results do not indicate that this would be a significant problem in the case of the fuels investigated. However, the temperature profile for the MB is slightly lower in part due to the physical properties of the methyl ester.
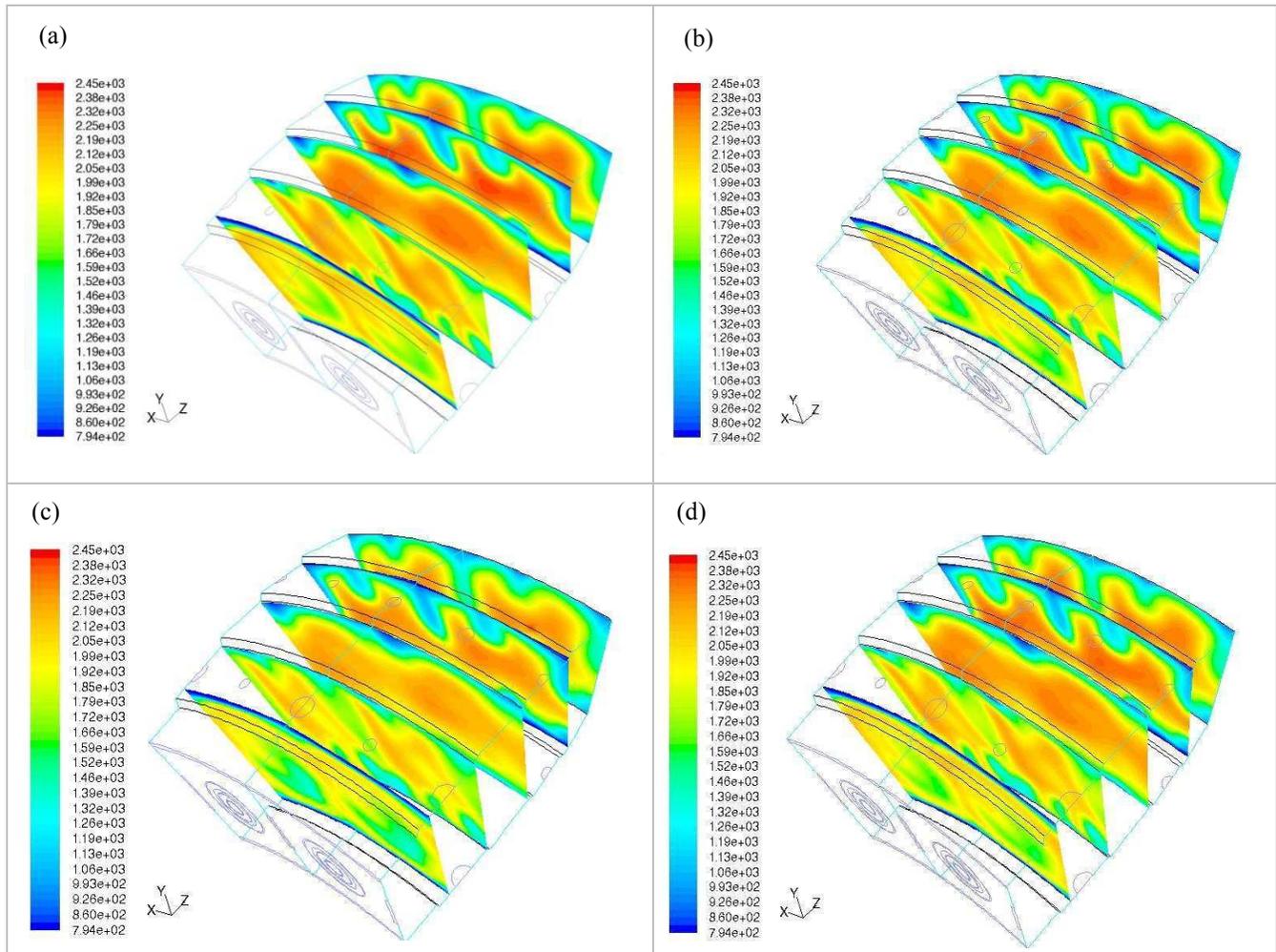

Fig. 6 Comparison of temperature contour plots for considered fuels. From left pictures (a)-(d) represent respectively: kerosene, n-Heptane, MB and blend.

6.2   Predictions for NOx emissions

Investigating the impact on NOx emissions and formation when using the alternative fuels was of prime importance in this study. For the purposes of this research the NOx production characteristics within the MAC combustor were computed with a partial equilibrium approach using the calculated temperature and species mixture fractions. The turbulence-chemistry interaction was modelled using a joint pdf approach.

The kinetics of thermal NOx formation are governed by the Zeldovich mechanism where according to this theory NOx can be formed from the atmospheric nitrogen at sufficiently high temperatures. The oxidation occurs mainly in the post flame area where the concentration of major radicals O and OH is sufficient for the process to occurs. Thermal is the leading process for NOx production at high temperatures (above 1800K) in the gas turbine [18]. In contrast, prompt NOx is supported by fuel rich conditions since C_2H_2 as a precursor of the radical CH, is formed and accumulated under rich fuel combustion it therefore supplies only 10% of total NOx formed in the engine [18, 24, 25].

The predicted thermal and prompt NOx profiles along the centre of the combustor are shown on Fig. 9 and 10. In Fig. 9 the mole fraction of NOx is given for each fuel in parts per million whereas in Fig. 10 the NOx emission index is shown. For all cases, the predicted values indicate the correct trend of increasing NOx concentration towards the combustor outlet. The

NOx concentration for MB, blend and heptane were found to be lower than for conventional kerosene fuel. The differences in the predicted NOx concentration between kerosene (base-line) and the alternative fuels can be attributed to disparity in the flame location and the O and OH concentrations which are important in NOx formation processes. Reduced temperatures in the case of MB and blend results in decreases in NOx . It should be noted that the NOx emissions are a strongly temperature dependent phenomenon and therefore the lower level of NOx emissions may be primarily due to the lower temperature on the outlet of the combustor.
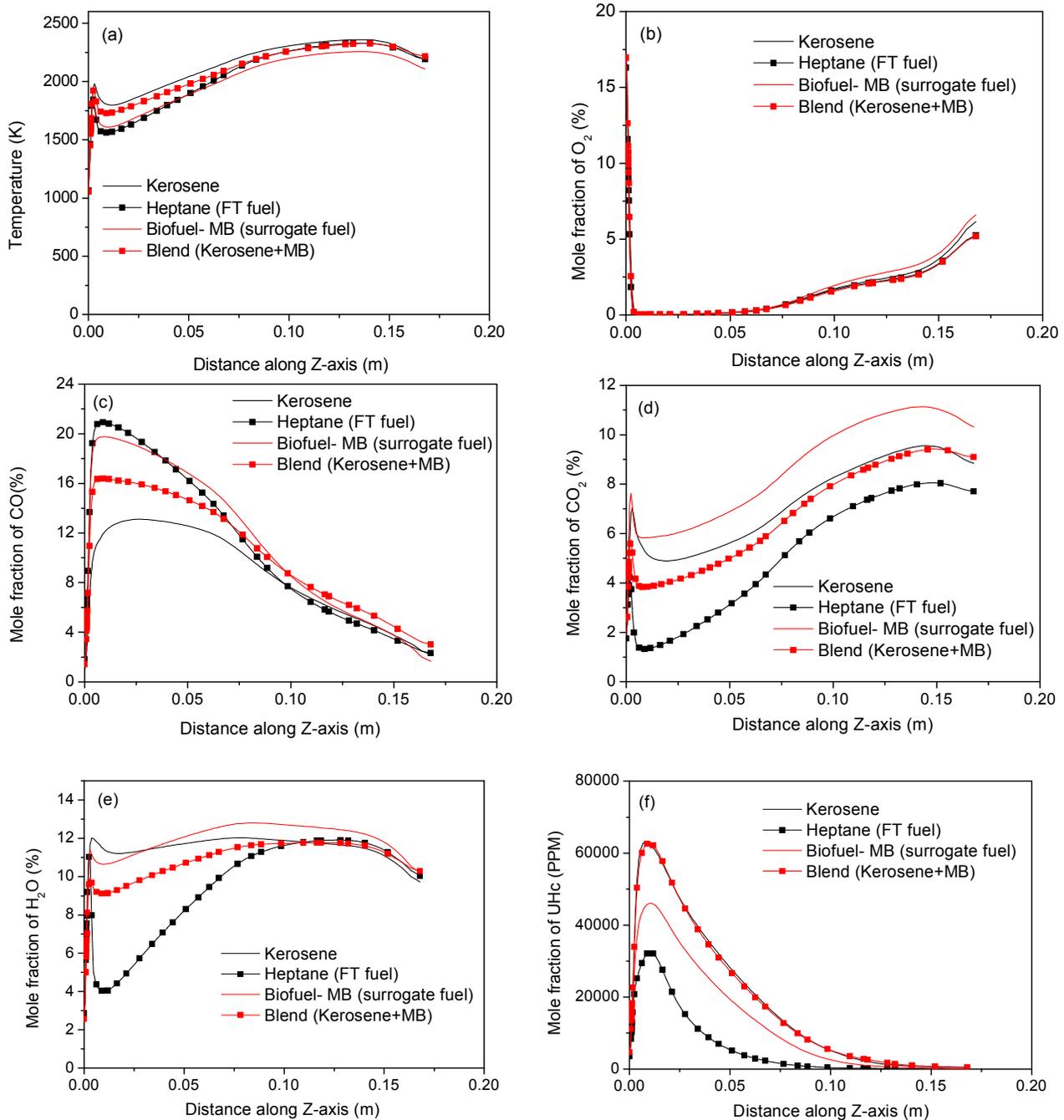

Fig. 7 Comparison of the CFD predictions for species mole fraction (a) - temperature; (b) - O_2; (c)- CO (d) - CO_2; (e) - H_2O; (f) - UHc.
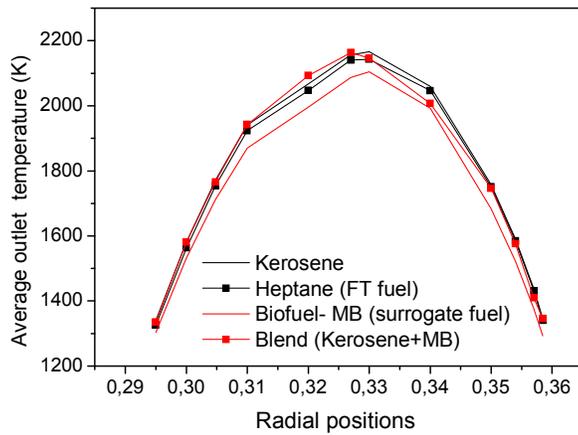
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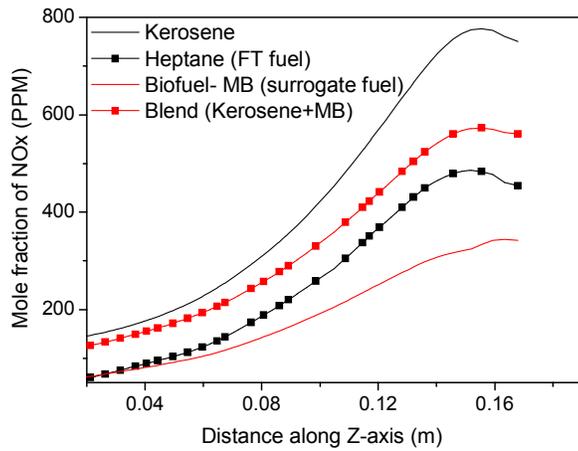**Fig. 8 CFD results for the average outlet temperature.**

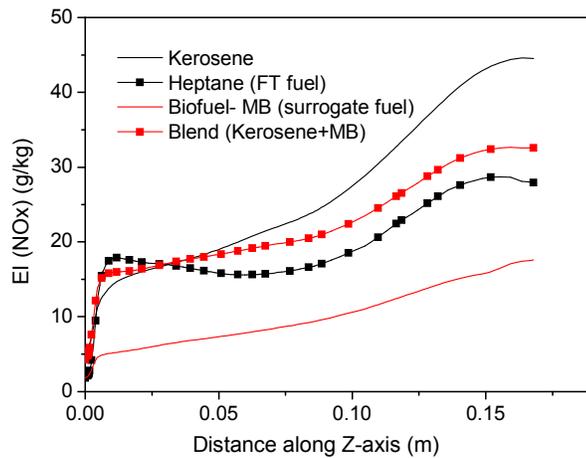**Fig. 9 Comparison of theoretical CFD profiles of NOx.**

Fig. 10 Comparison of theoretical CFD profiles of NOx.

7   Concluding remarks

In this paper the properties of two alternative aviation fuels, synthetic kerosene (n-heptane) and bio-aviation fuel (MB), have been compared against kerosene for their combustion performance in a modern air-spray combustor (MAC). This has been achieved using the recently developed detailed reaction mechanisms, AFRMv2.0 and n-heptane, coupled to a CFD simulation approach. The CFD predictions for kerosene were previously validated against experimental data from QinetiQ. The objective of this study was to evaluate the effect of using alternative fuel on the combustion characteristics. The following conclusions can be drawn from the present study:

- The impact of using the blended fuel has been shown to be very similar in combustion performance to that of the 100% kerosene. A combustor can perform satisfactorily using blended fuel (MB and kerosene). It has been recognised that 20 percent methyl butanoate blend is an optimum concentration for biofuel blend where the predicted performance results are acceptable.
- The use of heptane (synthetic fuel) appears to provide comparable results to that of kerosene when considering overall performance. There is also a significant predicted drop in emissions of NO$_x$. However, further research is required to understand the consequences of using synthetic fuels with respect to a range of issues including that of their low aromatics content.
- The differences in properties between biofuel and jet fuel (viscosity, density, energy content) are responsible for a variety of undesirable combustion properties. Based on the theoretical investigations in this paper it can be concluded that biofuel cannot be directly adopted as an alternative fuel for existing engines without modifications being required to the system. When using the 100% MB with increased fuel flow rates to equalize the energy contents, the combustion characteristics are much closer aligned to those of kerosene. This aspect of the work requires further experimental study in order to provide a detailed understanding of the issues and as a means to confirm the accuracy of the predicted results.

8   Nomenclature

c_p	Mixture - averaged specific heat (J kg^{-1} K^{-1})
$C_{p,i}$	Specific heat of species i (J kg^{-1} K^{-1})
Δ	change in variable
D	Diffusion coefficient (m^2 s^{-1})
f	Mixture fraction (dimensionless)
EI_{NO_x}	Emission index of NO_x (g kg^{-1})
H_i	Specific enthalpy of species i (J kg^{-1})
LHV	Lower calorific value (MJ kg^{-1})
S_i	Reaction rate of species i (units vary)
T	Temperature (K)
t	Time (s)
Y_i	Mass fraction of species i (dimensionless)
ρ	Density (kg m^{-3})
χ	Scalar dissipation rate (s^{-1})

9   Acknowledgments

10   References

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