Theoretical Assessment of Different Aviation Fuel Blends based on their Physical-Chemical Properties

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ABSTRACT

The current study focuses on the theoretical assessment of Sustainable Aviation Fuels (SAFs) obtained by blending traditional jet fuel (Jet A) and different liquids (biodiesel and alcohols) from an analytical point of view. Aeroshell 500 oil was added (5% vol.) to ensure the lubrication of the turbo engine. An in-depth analysis of the physical-chemical properties of Jet A fuel blended with different biodiesels and alcohols was performed. The considered blends consisted of Jet A fuel and biodiesel from palm oil, pork fat, and sunflower and methanol, ethanol, and butanol. All six liquids were mixed with Jet A by 10, 20 and 30%. Flash point, kinematic viscosity, density, freezing point, elemental analysis, and FTIR analysis were conducted for all the blends. The acquired results show the influence of each component on the physical-chemical properties of the blends. Based on the physical-chemical analysis of the blends, conclusions on the latter's behavior during burning were drawn and the gaseous pollutants resulting from the burning process were examined.

Keywords-Jet A; sustainable aviation fuel; kerosene; fuel blends; chemical-physical analysis; FTIR

I. INTRODUCTION

The aviation industry is increasingly exploring alternative fuels and fuel blends as a means of reducing its environmental impact and dependence on conventional fossil fuels. Recent scientific investigations have focused on assessing the feasibility and performance of aviation fuel mixtures containing biodiesel and alcohols. These studies have shed light on the physical-chemical properties, combustion characteristics, and environmental implications of these alternative fuel formulations. Sustainable Aviation Fuels (SAFs) have emerged as a critical solution to reduce greenhouse gas emissions in the aviation industry. From a physical-chemical properties perspective, SAFs differ from conventional jet fuels primarily in terms of feedstock sources and production processes. The current paper explores the key physical-chemical properties of SAFs and their relevance in aviation, drawing upon recent research and developments.

Even though it was published in 1983, the handbook [1] provides a historical perspective on aviation fuel properties, reflecting the state of knowledge and industry standards at that time. While some details may have evolved since then, it remains a valuable reference for understanding the fundamentals of aviation fuels. It serves as a valuable reference document offering a comprehensive source of information on the latter's properties. It also provides easy access to data pertaining to aviation fuel properties, including information on fuel composition, physical properties, combustion characteristics, and other relevant factors.

Recent research has evaluated the physical-chemical properties of aviation fuel blends with biodiesel and alcohols. For instance, authors in [2] examined the density, viscosity, and thermal stability of such mixtures. These properties are essential for ensuring compatibility with existing aviation infrastructure and safe engine operation. SAFs can be derived from a variety of feedstock, including biomass, waste oils, and synthetic processes like Fischer-Tropsch (FT) synthesis and hydro treatment of triglycerides. These diverse feedstocks result in a wide range of chemical compositions for SAFs [3]. The chemical composition impacts properties such as density, viscosity, and combustion characteristics, influencing engine performance [4]. The hydrocarbon structure of SAFs affects their energy density and combustion behavior. Hydro processed SAFs typically contain paraffinic hydrocarbons, which contribute to improved energy content and reduced emissions compared to conventional kerosene-based jet fuels. The absence of sulphur in most SAFs leads to lower sulphur dioxide emissions [5, 6].

Density, viscosity, freezing point, and thermal stability are critical physical properties affecting fuel handling and combustion. SAFs generally exhibit higher densities and viscosities and have higher freezing points than conventional fuels. This fact may necessitate the use of additives or blending with conventional jet fuel to ensure low-temperature operability and thermal stability, which may vary according to feedstock and production processes [7-10]. As research continues, understanding and optimizing these properties will be vital in integrating SAFs into the aviation sector.

Many studies regarding the assessment of the combustion characteristics of such fuel blends have been published. Parameters like ignition delay, flame stability, and emission profiles during combustion were investigated in [11]. Understanding the combustion behavior is crucial for optimizing engine performance and reducing emissions. Also, the environmental impact of aviation fuel mixtures involving biodiesel and alcohols has been thoroughly studied. Emissions of particulate matter, nitrogen oxides (NO_x), and carbon dioxide (CO_2) have been quantified [12]. These assessments promote our understanding of the prospective reductions in greenhouse gas emissions and particulate matter, which are critical for air quality and climate change mitigation.

Authors in [13] explored the latest developments in SAFs with a focus on their impact on CO_2 and NO_x emissions. Additionally, they evaluated the potential of hydrogen as an alternative to SAFs in the aviation industry. They discuss recent advancements in SAFs, highlighting their ability to reduce greenhouse gas emissions in the aviation sector. These fuels have gained attention as a promising solution for mitigating the environmental impact of aviation. Authors in [14] studied the combustion characteristics of a blend consisting of SAF and hydrogen. This composition is analyzed in terms of its combustion behavior with the purpose of assessing its potentiality as a sustainable alternative for aviation. The evaluation included parameters, such as combustion efficiency, emissions, and combustion stability, providing valuable data on the fuel's feasibility for use in aviation applications. There are several studies investigating the use of bio fuels in piston engines, such as biodiesel utilization [15], and bio ethanol [16]. Additionally, biofuels have been also used in turbine engines [17-19].

The current paper aims to analyze how the most utilized jet fuel Jet A and different types of biodiesels and alcohols in different concentrations influence the burning process and gaseous pollution. The obtained results exhibit the influence of each of the blend's components on the physical-chemical properties of the blends. Based on the physical-chemical analysis of the blends, conclusions on the latter's behavior during burning and on the gaseous pollutants resulting from the burning process were drawn, thus making the current study one of the most comprehensive ones in terms of parallel analysis for different fuels considered as sustainable aviation fuels.

II. MATERIALS AND METHODS

A. Blend Preparation

The blends were prepared in the laboratory and consisted of: Jet A fuel, 3 types of biodiesels (obtained from: used sunflower oil, pork fat, and used palm oil) and 3 types of alcohol (methanol, ethanol, and butanol). Also, Aeroshell 500 oil was added into the blends (5% vol.). Jet A aviation fuel, in accordance with STANAG 3747, was acquired from OMV Petrom, Romania. Aeroshell 500 oil was provided by Shell Romania and is in accordance with MIL-PRF-23699G Grade SDT, British DEF STAN 91-101 Grade OX-27, and NATO code O-156. The biodiesels were provided by Bunge 200, Romania, and were produced at Lehliu, Romania from domestic raw materials. The following alcohols were provided by VWR Chemicals, Romania: Methanol 98.5% purity, Ethanol 99.8% purity, and n-Butanol 99.8% purity. All the considered liquids had good miscibility, therefore, in general, all the blends displayed homogeny except for the blends with methanol that demonstrated separation due to the latter's highly polar nature if the blend was not stirred constantly, as observed in Figure 1.

The blends were made as volume percentages so, all the liquids were separately measured by using a 1000 ml cylinder and after that they were mixed into a larger vessel by a mechanical stirrer. After stirring, the lends were left alone for 24 h and then were assessed with regard to the homogeneity of the resulting blend.

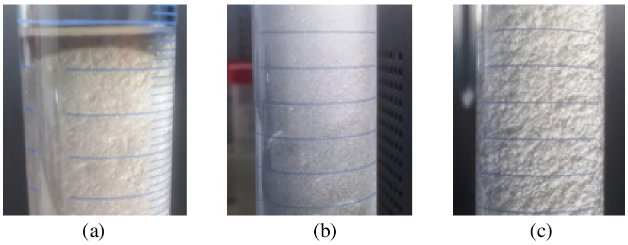
(a) (b) (c)

Fig. 1. Separation of methanol blends (a) 10%, (b) 20%, (c) 30%.

B. Freezing Point Determination

The freezing point of a liquid is a very important parameter that needs to be determined in order to assess the compatibility of the liquid to work as aviation fuel. The instrument employed to determine the freezing point was provided by Ducom Instruments (Europe) B.V., Netherlands and has the following characteristics: temperature range +80 to -90 °C, resolution: 0.01 °C, accuracy: ±0.1°C, temperature measurement: PT100, class A.

C. Elemental Analysis Determination

Elemental analysis determination is a method for assessing the percentages of different atoms within a substance according to their molecular mass. Elemental analysis provides the elemental composition of minerals, chemical compounds, soil, and waste. Elemental analysis can be qualitative and quantitative and applied to bulk and surface analysis. Elemental analysis can be:

- Qualitative: Describes what elements are present or the presence of a particular element.
- Quantitative: Describes how much of each element is present.

The elemental analyzer was provided by Horiba GmbH Tulln, Romania branch, and it is an EMIA-Pro device having the following characteristics: sample amount: 1 g ± 0.1 g, carrier gas: oxygen 99.5% purity, operation gas: nitrogen 99.5% purity, measurement range: carbon: 1.6 ppm, sulphur: 2.0 ppm.

D. Flash Point Determination

Flash point is the lowest temperature where the vapors ignite. The used instrument is an opened cup flash/fire point measurement apparatus provided by Scavini, Italy and it is deployed to determine the flash and/or fire temperature of a liquid. Its main characteristics are: working temperature: 400 °C, number of cups: 1, working gas: propane for domestic use, a sensor to correct the obtained results with the ambient temperature and relative humidity.

E. Cinematic Viscosity at 40°C

Kinematic viscosity is experimentally determined, according to SR EN ISO 3104/2002, by utilizing a capillary viscometer kept in a bath provided with a mechanical stirrer and thermostatic control. This method focuses on the identification of the necessary time for a known volume of a sample to flow through a standardized capillary tube. The kinematic viscosity is calculated by multiplying the measured time with the capillary constant (that differs from one capillary to another), resulting in the measurement unit of mm^2/s ($1\ mm^2/s = 1$ cSt). The main features of the apparatus are: working temperature: room to 100 °C, number of simultaneous measurements: 6, thermostat precision: ±0.1 °C.

F. FTIR Spectrometry

Fourier-transform infrared (FTIR) spectrometry is a very versatile method for establishing the chemical transformations within a substance. The instrument implemented is a Spectrum Oil Express 100, from Perkin Elmer, USA. The FTIR apparatus determines the spectrum of a liquid and compares it with an already existing one (in its database) showing the main differences between the two spectra. Its main traits are: working wavenumber: 7800 - 370 cm^{-1}, DTGS (deuterated tri-glycerin sulphate) detector, electronic signal processing system, CO_2 laser, auto sampler, borosilicate based working cell, used solvent: n-heptane 99.5% purity.

G. Density at 22 °C

Thermo-density was used to define the density of the liquids. One litre of every liquid was kept at constant temperature of 22 °C and was measured with a thermo-densimeter provided by Thermodensirom, Romania, able to show density from 0.6 and to 1.2 g/cm^3. Six of them were utilized, each one being able to show the density with an accuracy of ± 0.01 g/cm^3.

III. RESULTS AND DISCUSSION

The results obtained are portrayed in Table I, where: Ke is Jet A fuel +5% Aeroshell 500, A1 – methanol, A2 – ethanol, A3 - n-butanol, B1 - biodiesel acquired from used sunflower oil, B2 - biodiesel from pork fat, B3 - biodiesel from used palm oil.

TABLE I. RESULT SUMMARY

Sample	Flash point [°C]	Viscosity [cSt]	Density [g/cm^3]	Calorific power [MJ/kg]	Elemental analysis [%]			
					C	H	N	O
Jet A	40.1	1.27	0.808	45.59	84.71	15.29	0.00	0.00
Aeroshell 500	188.6	25.11	0.999	35.26	94.50	3.5	0	2
Ke	42.3	1.39	0.817	45.29	85.17	13.31	0.07	1.45
A_1	11.8	0.55	0.792	19.07	37.45	12.48	0	49.94
A_2	13	1.20	0.789	29.45	52.09	13.02	0	34.73
A_3	35	2.57	0.810	35.77	64.76	13.49	0	21.59
Ke+10A_1	23.7	1.31	0.815	42.67	80.40	13.23	0.06	6.30
Ke+20A_1	23.4	1.22	0.812	40.05	75.63	13.14	0.06	11.15
Ke+30A_1	23.3	1.14	0.810	37.42	70.85	13.06	0.05	16.00
Ke+10A_2	23.7	1.37	0.814	43.71	81.86	13.28	0.06	4.78
Ke+20A_2	23.6	1.35	0.811	42.12	78.55	13.25	0.06	8.11
Ke+30A_2	23.3	1.33	0.809	40.54	75.25	13.22	0.05	11.43
Ke+10A_3	33.9	1.51	0.816	44.34	83.13	13.33	0.06	3.46
Ke+20A_3	33.7	1.63	0.816	43.39	81.09	13.35	0.06	5.48
Ke+30A_3	33.1	1.74	0.815	42.43	79.05	13.36	0.05	7.49
B_1	86	5	0.884	39.42	77.28	12	0.07	10.65
B_2	164	9.47	0.882	40.89	78.65	12.61	0.07	8.67
B_3	161	5.08	0.875	39.32	77.43	12.38	0.06	10.13
Ke+10B_1	42.9	1.55	0.824	44.15	84.38	13.18	0.07	2.37
Ke+20B_1	46.2	1.73	0.832	43.93	83.59	13.05	0.07	3.29
Ke+30B_1	49.7	1.98	0.839	43.05	82.8	12.92	0.07	4.21
Ke+10B_2	45.6	1.75	0.832	44.69	84.52	13.24	0.07	2.17
Ke+20B_2	49.44	2.15	0.843	44.23	83.87	13.17	0.07	2.89
Ke+30B_2	53.5	2.54	0.854	43.68	83.21	13.1	0.07	3.62
Ke+10B_3	44.2	1.51	0.823	44.4	84.4	13.22	0.07	2.32
Ke+20B_3	50.2	1.82	0.83	43.3	83.62	13.12	0.07	3.19
Ke+30B_3	54.7	2.06	0.836	41.98	82.85	13.03	0.07	4.05

The variation of the flash point of the blends made from Jet A and alcohols is observed in Figure 2.

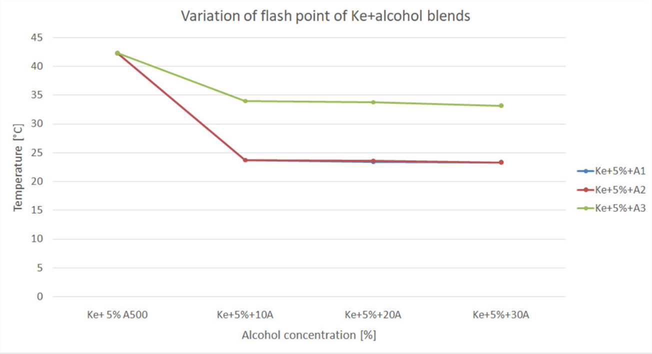

Fig. 2. Variation of flash point of Ke + alcohol blends.

As it can be noticed in Figure 2 and assessed from Table I, A1 and A2 have similar flash points, therefore the graphs are overlapping, whereas A3 is well represented having a flash point higher that the other two. As expected, the flash point decreases as alcohol concentration within the blend increases, but the decrease is rather insignificant. Nevertheless, a lower flash point means that the combustion of the blends starts at temperatures lower than regular aviation fuel.

The variation of the flash points of kerosene and biodiesels blends is illustrated in Figure 3.

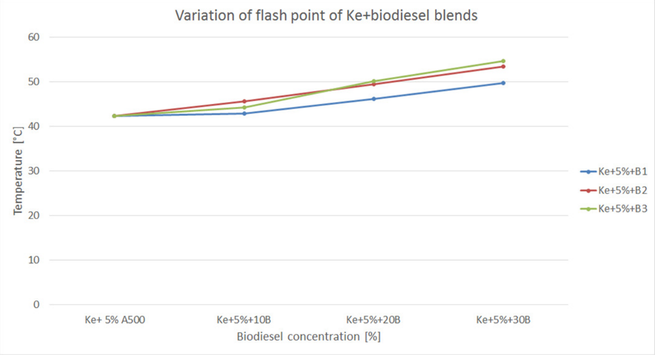

Fig. 3. Variation of flash point of Ke + biodiesel blends.

All biodiesels used within the blends have flash points higher than regular aviation fuel, therefore, the flash point of the blends is higher than that of Jet A. As expected, the flash point value increases as the biodiesel concentration increases. If blends consisting of regular aviation fuel and biodiesel are to be utilized as sustainable aviation fuels, these increased values of the flash point must be taken into account.

Calorific power of the blends differs from the calorific power of the regular aviation fuel. The variation of the calorific power of the blends made from kerosene and alcohols is spotted in Figure 4. As it can be assessed from Figure 4, all the blends' calorific power decreases as the concentration of the alcohols increases, in accordance with the alcohols' own calorific power. Thus, the blends made out of kerosene and A1 show the lowest calorific power and the blends made with A3 show the highest. This aspect can be observed also in Table I, since A3's calorific power is the highest. Nevertheless, all blends manifest an important decrease in calorific power. This aspect may influence the fuel consumption of an aviation engine while trying to maintain a specific power output. Low calorific power means poorer combustion.

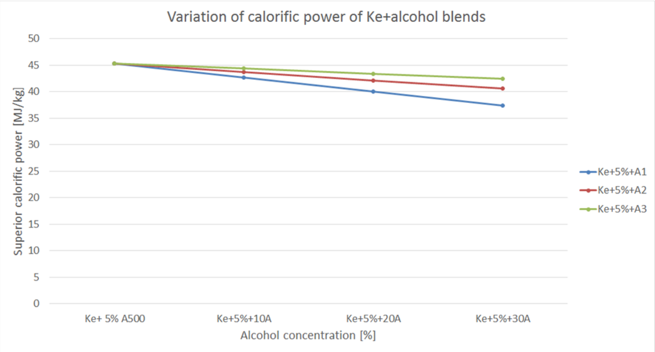

Fig. 4. Variation of calorific power of Ke + alcohol blends.

Figure 5 represents the variation of calorific power of the blends made out of kerosene and biodiesel. As it can be assessed from both Figure 5 and Table I, the calorific power of the blends also decreases but not as drastically as in the case of kerosene/alcohols blends due to the fact that Jet A is basically a diesel-like liquid. Therefore, the calorific power of the biodiesel is close to the one of the kerosene. Accordingly, the calorific power decreases as the biodiesel concentration increases but the decrease is rather small, thus resulting in similar fuel consumption as regular aviation fuel. As compared to kerosene/alcohols blends, the kerosene/biodiesel blends seem more suitable to be used as aviation fuel.

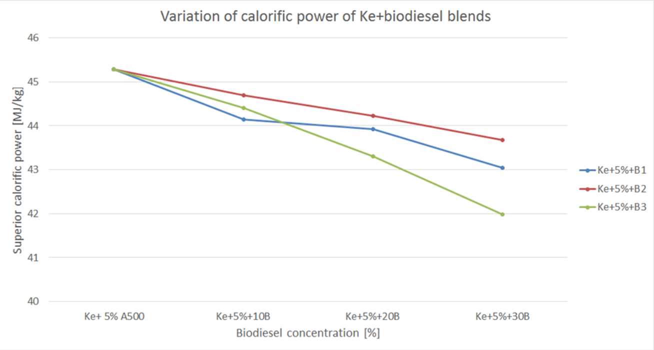

Fig. 5. Variation of calorific power of Ke + biodiesel blends.

The percentage of the carbon atoms within the blends gives an idea of the way the combustion process unfolds. It is widely known that in an ideal combustion process, the end products will be H_2O and CO_2. Nevertheless, the combustion process in an aviation turbo engine is far from ideal, therefore secondary products such as NO_x and CO, will form. Figure 6 demonstrates the variation of carbon content within the blends made out of kerosene and alcohol.

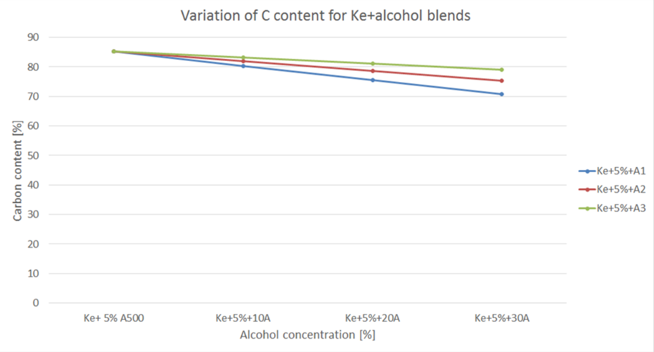

Fig. 6. Variation of C content in Ke + alcohol blends.

As it can be observed in Figure 6, the carbon content of the blends decreases due to the fact that alcohols have lower carbon percentage than biodiesel. Also, carbon content decreases, as expected, as the alcohol concentration increases. Lower carbon content means lower CO_2 formation as the end product. However, correlated with the variation of calorific power, therefore with increased fuel consumption, the actual CO_2 production of an aviation turbo engine might be higher than that of the regular fuels. Also, alcohols having small structure (C1 – C3) are burning more efficiently than structures, such as jet A (having C9 – C11), consequently, intermediate products such as CO and NO_x are likely to be lower.

The variation of carbon content in the blends made out of kerosene and biodiesel is shown in Figure 7.

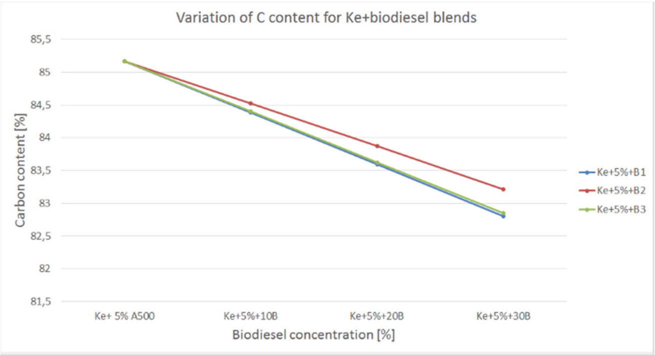

Fig. 7. Variation of C content of Ke + biodiesel blends.

All biodiesels used to form the blends exhibit similar carbon concentration to that of the regular aviation fuel, but only slightly lower. Therefore, even though the carbon concentration decreases as compared to kerosene, the values are still high. This means that higher concentrations of CO_2 are likely to be produced as combustion end-product but given the fact that the calorific power of the blends is higher, fuel consumption should be lower. Also, given that biodiesel as well as regular aviation fuel have long structure (C9 – C11), the combustion process might not be as efficient as in the case of alcohols, therefore intermediate products, such as CO and $NO_{x,}$ are likely to be higher.

The oxygen content of a fuel is also an important aspect to be taken into consideration since higher O_2 content means lower air intake for the combustion process. Figure 8 discloses the variation of O_2 content within the blends made of kerosene and alcohols.

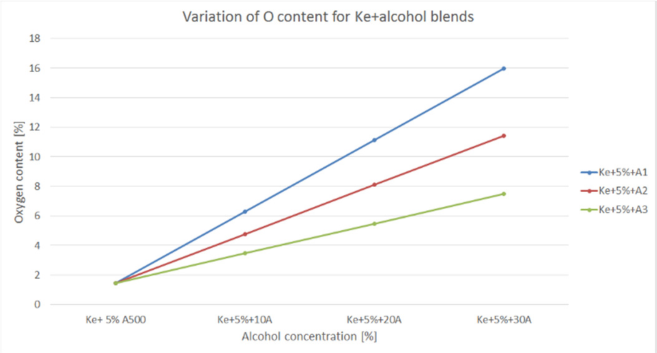

Fig. 8. Variation of O_2 content of Ke + alcohol blends.

In Figure 8, it can be noticed that the oxygen content increases as the alcohol concentration increases and the oxygen content of the alcohol is higher. Therefore, A1 reveals the highest O_2 concentration, thus it is likely for the blend consisting of kerosene and A1 to have the highest efficiency in terms of combustion. Nevertheless, one can take into consideration the fact that A1 has the lowest calorific power as detected in Figure 1. In theory, those blends should improve the combustion behavior. However, alcohols bring a huge amount of oxygen within the structure of the newly formed blends, theoretically resulting in a more efficient combustion process. This can be translated into lower CO, NO_x, and CO_2 concentrations. The variation of the oxygen content of the blends made of kerosene and biodiesel is illustrated in Figure 9.

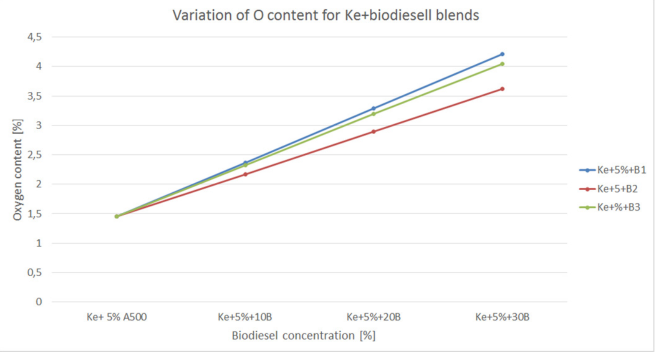

Fig. 9. Variation of O_2 content of Ke + biodiesel blends.

As in the case of alcohols, biodiesel brings more oxygen into the fuel, therefore the combustion process should be more efficient. It should be noted that the amount of oxygen is significantly lower than in the case of alcohols, thus the combustion might be less effective leading to increased amounts of CO, NO_x, and CO_2. Nevertheless, those concentrations should be, theoretically, lower that in the case of regular aviation fuel combustion.

The FT-IR spectroscopy is a very useful tool in assessing the chemical modifications within a substance. By adding alcohols or biodiesel in the regular aviation fuel, its chemical composition is modified. Figures 10-12 demonstrate how the alcohols are modifying the structure of the regular aviation fuel, where green: Ke; black: Ke+10% alcohol; purple: Ke+20% alcohol; red: Ke+30% alcohol.

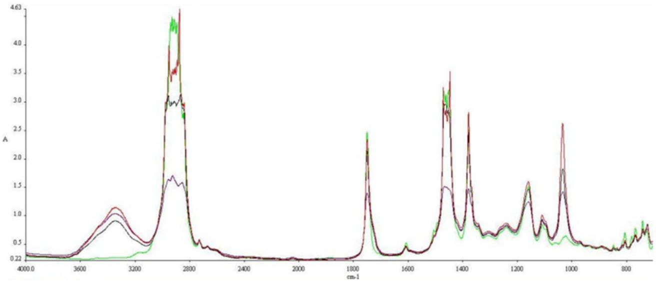

Fig. 10. FT-IR spectra of Ke+A1.

As can be seen in Figures 10-12, the main differences between the spectra of the regular aviation fuel (Ke) and the blends are at 3200-3600 cm^{-1}, meaning that hydroxyl (-O-H) has been brought into the structure. As expected, the higher the alcohol concentration is, the higher the peak is. Another important modification appears at 1750 cm^{-1} representing the presence of oxygen bonded by a C atom (C-O). At 1450 cm^{-1}, the presence of methylene groups ($-CH_2$) shows a slight decrease compared to Ke. The radiation absorbed at 1350 cm^{-1} displays an increase of methyl groups ($-CH_3$). Another large difference is noticed at 1000 cm^{-1}, representing the C-OH bond. As in the case of –OH, as the concentration of the alcohol increases, C-OH increases.

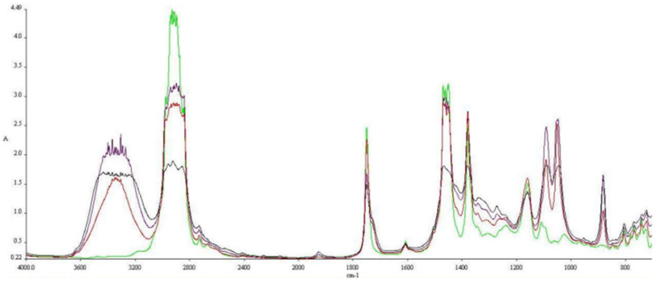

Fig. 11. FT-IR spectra of Ke+A2.

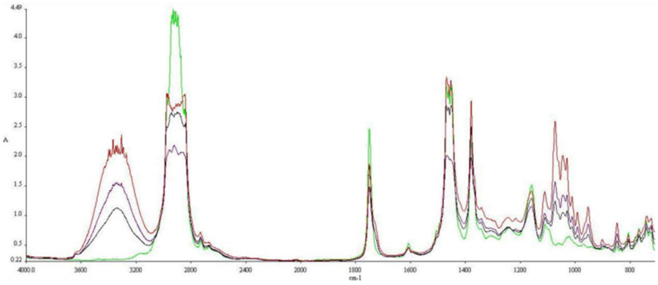

Fig. 12. FT-IR spectra of Ke+A3.

The FT-IR spectra representing the blends consisting of kerosene and biodiesel are shown in Figures 13-15, where green: Ke; black: Ke+10% biodiesel; purple: Ke+20% biodiesel; red: Ke+30% biodiesel.

As it can be observed in Figures 13-15, the main differences between the spectra of the regular aviation fuel (Ke) and the blends are spotted at 1280 cm^{-1}, representing the presence of ethers (C-O-C) and esters (C=O). Obtaining biodiesel is a succession of etherification followed by esterification reactions, therefore ether and ester groups are present within the structure. Those groups bring oxygen into the structure, resulting in a more efficient combustion process. Also, large differences can be observed at 2850 cm^{-1} representing asymmetric and symmetric stretching vibrations of ($-CH_2$) groups.

By analyzing the physical-chemical properties of the alcohol-based and biodiesel-based blends, it can be stated that from the group of alcohol-based blends, the blend most likely to perform satisfactorily is the Ke+A2 (ethanol) blend, since it shows the most consistent values of flash point, calorific power, and C and O content. Similarly, the best performing biodiesel-based blend should be Ke+B1 (biodiesel from sunflower), since it exhibits the best values for calorific power, O content, and flash point.

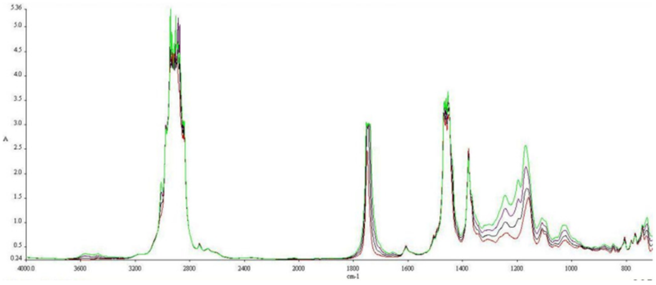

Fig. 13. FT-IR spectra of Ke+B1.

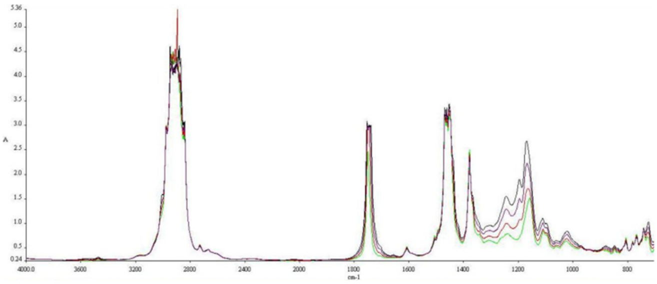

Fig. 14. FT-IR spectra of Ke+B2.

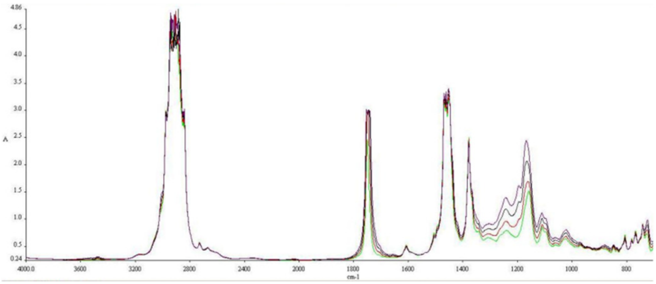

Fig. 15. FT-IR spectra of Ke+B3.

IV. CONCLUSIONS

- Biodiesel and alcohols are two suitable substances to be used in blends with regular aviation fuel with the aim of decreasing the gaseous pollutants resulting from the combustion in an aviation turbo engine.
- The engine's performance and fuel consumption must be taken into consideration when fuel blends are formed.
- Alcohols bring more oxygen into the structure, but have lower calorific power, therefore fuel consumption would increase.
- Biodiesel also brings oxygen into the structure, but in a lower amount. However, biodiesel has calorific power similar to that of the regular aviation fuel, so it is more likely to keep the fuel consumption constant.
- The carbon content is decreasing for both alcohol and biodiesel, meaning that CO and CO_2 emissions should, in theory, decrease.
- The flash point is lower for blends with alcohol and higher for blends with biodiesel.

- Ke+A2 and Ke+B1 demonstrated the most consistent values of the considered physical-chemical properties, therefore these two are the most likely to behave better in combustion experiments regarding both the engine's performance and the gaseous pollutants emissions.

Combustion tests must be carried out on an aviation turbo engine in order to assess the fuel consumption, gaseous pollution, and engine's performance and so experimentally assess the most suitable blend for the transition towards sustainable aviation fuels.

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