

## Impact of Alternative Fuels Physical Properties on Combustor Performance

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### Abstract

This article describes a modeling procedure for calculating real fuel mixture thermophysical properties. First a GC-MS analysis gives the detailed composition of the fuel mixture. This enables to derive a multicomponent surrogate mixture, which encompasses all major fuel families and species. A property computation scheme is then described, which is based on pure species property semi-theoretical models and adequate mixing rules. Quantitative results are provided for the liquid mass density, viscosity and surface tension of crude-based kerosene and Diesel fuels and their alternatives. These properties are finally used to compute the Sauter mean diameter of two types of atomizers in order to compare the alternative fuels composition effect on combustor performance with respect to their respective crude-based fuel. The larger departures in physical properties between Diesel fuel and Canola methyl ester when compared to kerosene-type fuels yield larger differences in Sauter mean diameters. Concerning the atomizers, pressure swirl type atomizers display a stronger dependency upon fuel physical properties when compared to airblast atomizers.

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### Introduction

The “challenges of climate change, increasing import dependence and, higher energy prices are faced by all EU members” [1], and by most other industrialized countries. Solutions shall come from combined efforts, some directed toward improving the overall efficiency of energy conversion processes and some directed toward finding alternative energies and alternatives to crude-oil based fuels. As a result, different targeted initiatives were launched and among them those with the goal of introducing alternative fuels in civil aviation, for example the EU FP7 funded project “Alternative Fuels and Biofuels for Aircraft Development” (Alfa-Bird) or the US “Commercial Aviation Alternative Fuels Initiative” (CAAFI). Meanwhile, aero-engine manufacturers have invested more than a decade and a lot of resources in developing lean-burn low-NO<sub>x</sub> combustors. Their effort was and is mainly driven by emission legislations, in particular those concerning NO<sub>x</sub> level requirements. For example, in 2004 the sixth meeting of the Committee on Aviation Environmental Protection (CAEP), which was established by the International Civil Aviation Organization (ICAO), had released emission level targets that came into effect in January 2008.

A general consequence of such long term investment is that concerning the introduction of alternative fuels the different stakeholders are going to look initially at so-called “fit-for-purpose” or “drop-in” alternative fuels in order to avoid additional design modifications of modern low-NO<sub>x</sub> combustors. Criteria to define fit-for-purpose go beyond a simple match with Jet A-1 specifications (DefStan 91-91 for example). Actually, the Jet A-1 fuel specifications are quite broad, and a large variety of hydrocarbon mixtures can meet the specification requirements. Consequently, a fuel mixture complying with the Jet A-1 specifications might have a specific combination of physical properties that would substantially affect elementary processes occurring in a gas-turbine combustor. This could lead to a detrimental modification in the performances of those modern combustors. For instance, recent experimental investigations concerning the combustion of Fischer-Tropsch synthetic jet fuels [2] or biodiesels [3] in gas turbines have shown very similar NO<sub>x</sub> and CO emissions when compared to their crude-based counter-part. However, when it comes to soot formation there seemed to be larger differences depending on the nature of the fuel.

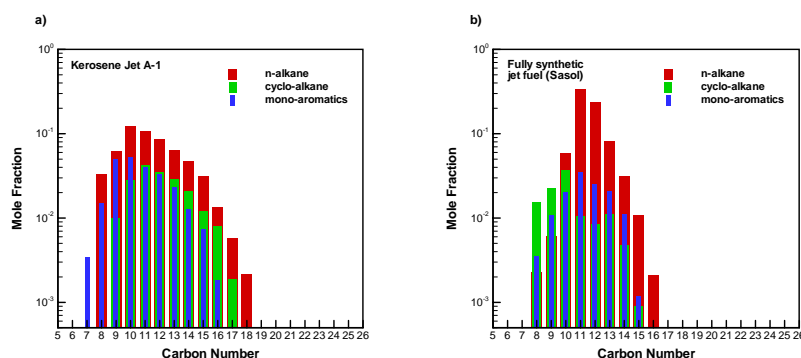
Although the carbon chain length of vegetable oils and biodiesels favors mainly their use for vehicles, these alternative fuels could serve in the power generation industry where dual - natural gas and Diesel fuel flexible - gas turbines are now standard technology. Thus, the purpose of the present article is to investigate the impact of crude-based kerosene/Diesel fuels and their alternatives’ physical properties on the outcome of an elementary process controlling combustor performance: atomization. Actually, according to Lefebvre [4] the liquid mass density, the liquid viscosity and, the surface tension are the three main physical properties defining pressure swirl and air-blast atomizer performance in terms of average droplet size and penetration length.

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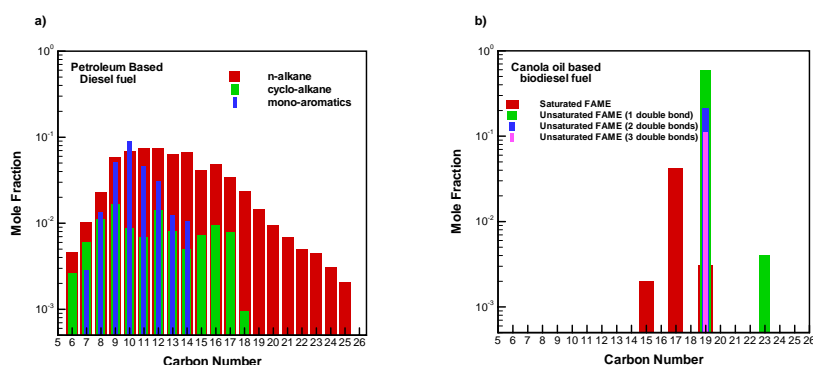
### Fuel composition

Figure 1 a) displays the composition of the kerosene Jet A-1 that was investigated by Southwestern Research Center for Sasol [5]. A gas chromatography analysis coupled to mass spectroscopy (GC-MS) enables identifying 85% to 100% of the species present in a crude-based refined liquid fuel depending on the origin of the batch and the experimental protocol. Then, based on such detailed composition we are able to define a multicomponent surrogate mixture of pure species covering the main families identified in the fuel under study. Instead of many hundreds of single species the surrogate mixture for Jet A-1 is composed of 32 pure species from the n-alkane, the cyclo-alkane and the mono-aromatic families. In the same fashion, one can see in Figure 1 b) the detailed composition of Sasol's CtL blend 3, which is the first fully synthetic jet fuel (FSJF) approved (in April 2008) for unrestricted use in aero-engines [5].



**Figure 1.** Composition in terms of mole fraction probability distribution function (log scale) and the carbon number as the distribution variable, of multicomponent-fuel (MC) surrogate a) Sasol petroleum-based Jet A-1 kerosene [5] and b) Sasol fully synthetic jet fuel blend 3 [5].

Similarly, Figure 2 a) displays the composition of the crude-based Diesel fuel initially analyzed by Dagaut [6] and here further simplified to form a surrogate multicomponent-diesel fuel mixture, which encompasses 54 pure components covering the same three families as the kerosene Jet A-1 above. Following the same procedure as the one above for the kerosene fuels we also show the composition of an alternative to the petroleum-based Diesel fuel. In Figure 2 b) one can see the composition of Canola oil based methyl ester according to Allen [7]. This biodiesel is composed of 7 species. Although it covers one big family, namely the fatty acids methyl esters (FAME), we introduced sub-families to differentiate between the different types of molecular structure: saturated, one double bond (22:1 for example), two double bonds (18:2 for example), and finally three double bonds (18:3 for example).

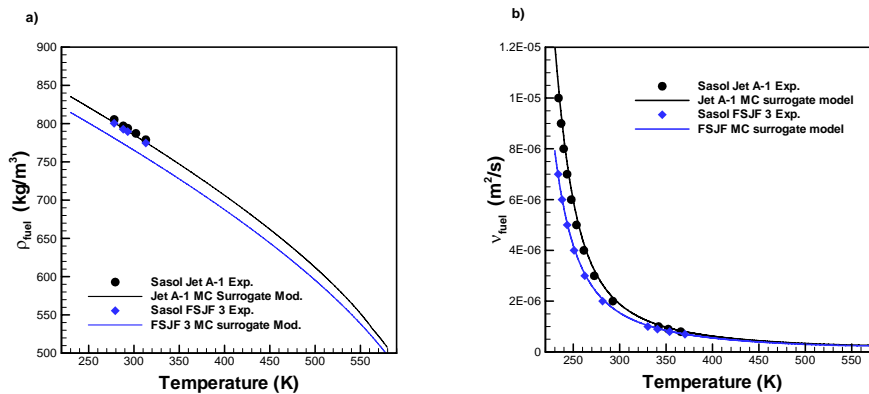


**Figure 2.** Composition in terms of mole fraction probability distribution function (log scale) and the carbon number as the distribution variable, of multicomponent-fuel (MC) surrogate a) petroleum-based Diesel fuel [6] and b) Canola oil based biodiesel [7].

### Pure species properties and mixing rules

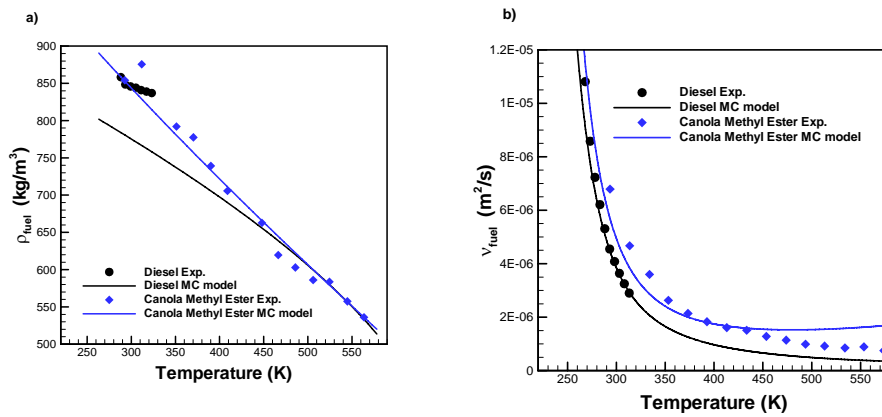
The model to compute the liquid mass density of pure species is the one of Yamada and Gunn described in Poling *et al* [8]. The mixing rule of Chueh and Prausnitz [8] is then used for crude-based fuel mixture while the mixing rule of Hankinson and Thomson [8] is used to determine the mixture critical temperature of Canola methyl ester fuel. For sake of generality the models we have chosen to compute the thermophysical properties need solely pure component physical constants: critical volume, critical pressure, critical temperature, and acentric factor as input variables rather than experimental curve-fitted coefficients. All such properties are available in the literature or in database for all common species (from C1 to C20) belonging to the crude-based families. However, aside from the mean molar mass and the normal boiling point all other FAME physical constants are seldom. Therefore, we have used the values of the normal boiling point given by Grabosky and McCormick [9] to compute the critical temperature, critical pressure, and critical volume according to the group contribution method of Joback [10]. In addition, we have used the group contribution method of Constantinou and Gani [11] to compute the acentric factor of all pure FAME. The method of Theja and Rice as explained in Poling *et al* [8] was used to determine the liquid viscosity. For all fuel mixtures except for the biodiesel, normal dodecane and toluene were chosen as the two reference fluids needed in this modeling approach. For the Canola methyl ester we decided to use Capric acid methyl ester and Oleic acid methyl ester as reference fluids because they display a large difference in their viscosity due to their different molecular structure (saturated and unsaturated with one double bond, respectively). The surface tension of pure components within both kerosene fuels and the Diesel fuel were modeled using the approach of Sastri and Rao [8] and a mass fraction averaged mixing rule was used for the fuel mixtures. The experimental measurement at 353 K found in Ejim *et al* [12] was used as reference value for the surface tension of Canola methyl ester. Then, the temperature dependency introduced by Sastri and Rao [8] was used to derive the surface tension for other temperatures. This is the only physical property which was not computed using the multicomponent approach because of a lack of data. Actually, the goal was not to derive or find in the literature the most accurate correlation for only one specific batch of fuel but rather to derive a versatile fuel mixture physical property computation procedure. However, when data are missing for single species it is better to rely on a measurement for the mixture.

These fuel mixture property models were tested using the multicomponent surrogate model compositions aforementioned. Figure 3 below shows for both Sasol's kerosene fuels, Jet A-1 and the fully synthetic jet fuel blend 3 the comparison results between measurements and computations based on the models listed above for the mass density and the kinematic viscosity. For both fuels and both properties there is an excellent agreement between measurements and computations with a maximum relative error of 2% for the FSJF mass density prediction. Such level of accuracy can be expected from semi-theoretical property models that were derived and optimized for hydrocarbon mixtures [8] as the one under consideration here. Noteworthy the fact that the detailed fuel composition and the property measurement results for different temperatures were available in the same reference document [5]. Although they can be approved for use in commercial aircrafts, fuel composition and properties can vary from one Jet A-1 fuel supplier to the other. This explains why a generic Jet A-1 fuel composition derived from one source might not lead to a perfect match in mixture properties with experimental measurements provided by another source.



**Figure 3.** Comparison between experimental measurements (symbols) and computations (lines) based on the multicomponent surrogate (MC surrogate model) for a) the liquid fuel mass density and b) the liquid kinematic viscosity. Petroleum-based kerosene in black and Sasol fully synthetic jet fuel [5] in blue.

Similarly, Figure 4 shows the comparison results for the Diesel-type of fuels of which the detailed composition is displayed above; one petroleum-based Diesel fuel and one biodiesel based on Canola oil methyl ester. As opposed to the kerosene fuels, here the compositions of the crude-based fuel [6] and its alternative [7] are taken from different sources as well as the properties measurement results [13] [14]. Again, Diesel fuel composition and properties can display large departures from one refiner to the other. This explains why the Diesel mass density evolution as a function of temperature, which is plotted in Figure 4 a) displays a higher maximum relative error (8%) with respect to the kerosene results. In the case of the biodiesel, there is less variation in the composition from one batch to the other because there are far less families and components; 57 pure species for the Diesel fuel and only 7 fatty acid methyl esters for the Canola methyl ester. As observed in other studies [3] the viscosity of biodiesel is substantially higher compared to that of Diesel. The discrepancy (>50%) in the kinematic viscosity computations with respect to the experimental measurements for the biodiesel is due to inaccuracies in the property modeling. While the property models for the kerosene and Diesel fuel mixtures could all rely on measurements for the critical properties and the acentric factor there was no such data that could be found in the literature for all single fatty acid methyl esters forming the present biodiesel. Moreover, pure component property models and mixing rules were all recommended [8] for mixtures of species found in the petroleum industry. There is a need for experimental data and model development and optimization for complex mixtures relevant in bio/synthetic fuels. Therefore, the biodiesel mass density and kinematic viscosity model predictions display a higher systematic error.



**Figure 4.** Comparison between experimental measurements (symbols) and computations (lines) based on the multicomponent surrogate (MC surrogate model) for a) the liquid fuel mass density and b) the liquid kinematic viscosity. Petroleum-based Diesel in black and Canola methyl ester (biodiesel) in blue.

Table 1 below shows that kerosene fuel mixture surface tension computed with the model described above is very well predicted (<4% relative difference with measurements) for 298 K temperature conditions but only fairly well ( $\approx 14\%$ ) in the low temperature region (233 K).

	Measurement [5] (N/m)		Computation (N/m)	
	@ 298.15 K	@ 233.15 K	@ 298.15	@ 233.15
Sasol Jet A-1	$27.1 \times 10^{-3}$	$29.5 \times 10^{-3}$	$26.4 \times 10^{-3}$	$32.5 \times 10^{-3}$
Sasol FSJF 3	$25.0 \times 10^{-3}$	$27.4 \times 10^{-3}$	$26.0 \times 10^{-3}$	$32.0 \times 10^{-3}$

**Table 1.** Comparison of surface tension for two temperatures between Jet A-1 and Sasol FSJF blend 3 [5].

Concerning the Diesel-type of fuels there was no difference in the surface tension values. For example, the computed surface tension of crude-based Diesel fuel and Canola methyl ester at 298 K is equal to  $31.60 \times 10^{-3}$  N/m.

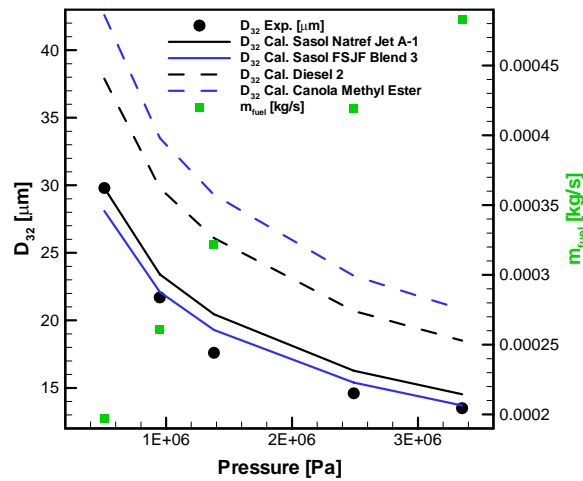
### Combustor performance in terms of atomization

“The fuel-injection process plays a major role in many aspects of combustion performance” [4]. Obviously combustor performances are not solely related to atomization. It is certainly one of the most important and there is experimental evidence [3] [16] that  $\text{NO}_x$  and CO emissions are determined mainly by the fuel atomization process. Two types of fuels, kerosene considered of low viscosity type and Diesel fuel, which is considered of higher viscosity were utilized here to investigate fuel-dependent atomization performance. In Figure 5, correlation results are displayed for atomization models compared with experimental results for pressure swirl atomizers. Although, pre-filming airblast atomizers were introduced by Lefebvre [4] in the mid 1960's to overcome the problem of improper fuel placement within the primary zone at higher combustion pressure, pressure swirl atomizers are still in use in aero-engines as pilot burners to ensure reliable start up and altitude relight performance. Pressure swirl atomizers are also of common use in stationary gas turbines.

The droplet size measurements performed by Schlieper [15] downstream a pressure swirl atomizer (simplex injector) were expressed in terms of the Sauter mean diameter  $D_{32}$ . This ensemble-averaged quantity is well correlated (see Figure 5) by the equation derived by Jasuja [16] for such atomizers:

$$D_{32} = 2.25\sigma^{0.25}\mu_l^{0.25}\dot{m}_l^{0.25}(\Delta P_l)^{-0.25}\rho_a^{-0.25} \quad (1)$$

where  $\sigma$  is the surface tension,  $\mu_l$  is the liquid dynamic viscosity,  $\rho_a$  is the ambient air mass density,  $\Delta P_l$  is the injection pressure difference and  $\dot{m}_l$  is the liquid mass flow rate. Figure 5 shows the experimental conditions in terms of injection pressure difference and the corresponding liquid mass flow rate for the measurement results presented here. For the temperature range under consideration, an average relative difference of 10% in the Sauter mean diameter of a spray generated by a pressure atomizer fed with crude-based Diesel and biodiesel yields a difference of about 20% in the characteristic droplet surface area. An average relative difference of 6% in the Sauter mean diameter (11% in the surface area) is observed when atomizing kerosene-type fuels. The departure observed in the Sauter mean diameter between a crude-based fuel and its alternative envisaged here will lead to differences in the characteristics of the primary zone, mainly its position, size and, local equivalence ratio, which in turn affects the overall combustor performance and engine emissions.



**Figure 5.** Comparison between experimental measurements (symbols) performed by Schlieper [15] on a simplex atomizer and computations (lines) based on the correlation of Jasuja [16] for different fuels.

Jasuja [16] also derived a correlation for pre-filming airblast atomizers:

$$D_{32} = 10^{-3} \frac{(\sigma \rho_l)^{0.5}}{\rho_a U_a} (1 - \dot{m}_l / \dot{m}_a)^{0.5} + 0.6 \times 10^{-4} \left( \frac{\mu_l^2}{\sigma \rho_a} \right)^{0.425} (1 - \dot{m}_l / \dot{m}_a)^{0.5} \quad (2)$$

Such correlations (Eq. 1 and 2) are limited to specific geometries and give an estimate of only one spray overall property. In addition to the average mean diameter the width of the size distribution (standard deviation), the spray penetration length, or the cone angle are parameters defining the spray characteristics with similar impact on combustor performance. However, those are less dependent upon liquid physical properties.

Under atmospheric conditions, with an ambient temperature of 295 K, an air velocity equal to 135 m/s and an air to liquid mass ratio of 8 the Sauter mean diameter found with Diesel fuel properties is equal to 42.8  $\mu\text{m}$  while it is equal to 44.2  $\mu\text{m}$  for Canola methyl ester. This corroborates the findings of Panchasara *et al* [4] who experimentally compared the combustion performance of an air-assisted injector when fueled with biodiesel and vegetable oil blends. Their atomizer had a similar phenomenology as the pre-filming airblast atomizer studied by Jasuja [16]. Panchasara *et al* [4] found that CO and NO<sub>x</sub> emissions are determined mainly by fuel atomization and fuel/air mixing and that the fuel composition effects are of secondary importance. In the present study we also argue that the combustor performance are highly dependent upon the outcome of the atomization process but we introduce the difference between two types of atomization phenomenology. As shown by the results of Equation (2) the different fuel compositions yield only a relative difference of 3% in the Sauter mean diameter (6% in droplet surface area) for combustors equipped with a pre-filming airblast atomizer while the relative difference is 10% for a pressure swirl type atomizer (Eq. 1). Similar figures are found for kerosene fuels. Thus, there is a stronger dependency upon fuel composition and thermophysical properties for pressure atomizers. Consequently, one should expect modifications in the combustor performance of an aero-engine gas turbine or a stationary dual gas turbine equipped with pressure atomizers.

## Conclusion

We described the different steps of a fuel mixture physical property modeling procedure. Based on the chemical composition, each species physical constants and, semi-theoretical single species property models and mixing rules we computed the liquid mass density, viscosity and surface tension of crude-based kerosene and Diesel fuels as well as their alternatives, CtL synthetic kerosene and Canola methyl ester, respectively. These physical properties were substituted into empirical atomization models. It was found that for pre-filming airblast atomizers as the ones found in the injection system of the main burners in aero-engine gas turbine, since aerodynamics is the dominant phenomenon in the atomization process the liquid properties had less effect on the atomization's outcome. However, the performance of combustors equipped with pressure atomizers for their piloting systems could reveal a substantial dependency upon the fuel physical properties.

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