

**SAMPLEIV [EASA.2020.FC05]**

**[DELIVERABLE 7: REPORT]**

# Report on fuel specifications and corrections – nvPM emissions



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## EXECUTIVE SUMMARY

This report details the activities performed in the delivery of the SAMPLE IV Deliverable 7, 'Development of recommendations on updates to ICAO certification of fuel specifications' of the SAMPLEIV project (Assessment of environmental impacts framework contract – Research on characteristics of aircraft engine emissions, EASA Contract Number – EASA.2020.FC05).

Specifically, the work reported here assesses the tasks associated with 'Effects of different blending ratios of Jet A-1 with SBC on emission levels' and 'Assessment of current fuel correction methods and potential limitations or improvements' in addition to reporting new data concerning the impact of fuel composition on regulated nvPM collected by the SAMPLEIV consortium whilst undertaking Deliverable 5 'non-regulated emission tests.

- The fuel composition parameter that correlates most strongly with emission indices is the fuel hydrogen content but, at present, it is difficult to reach a high degree of confidence between variation observed in fuel hydrogen content methods and variation in measured nvPM emission indices.
- The ICAO fuel composition correction was observed to perform relatively well for engine sizes ranging from 17 to 249 kN, with predicted nvPM EI reductions agreeing within  $\pm 20\%$  of measured ones  $>7\%$  thrust, and within  $\pm 40\% \leq 7\%$  thrust and overall averaging around the 1:1 line. This analysis included fuels of up to 14.5% hydrogen content.
- The main uncertainties in the ICAO fuel composition correction are the fuel hydrogen content measurement, and the repeatability of engine power condition at low thrust.

Recommendations are to:

- 1) Assess whether the bounds of fuel hydrogen content, currently permitted in ICAO Annex 16 Volume II, should be changed to better align and narrowed with current and future conventional fuels and blended SAF hydrogen content, to reduce the average uncertainty in correction and for practical supply of certification fuel (since it will become more and more difficult to obtain commercially available low hydrogen content fuel as aviation fuel hydrogen content increases).
- 2) Improve fuel nvPM correction methods, further work is required towards reducing the uncertainty associated with fuel hydrogen content determination. If the hydrogen content is only required for nvPM fuel correction, then potentially specifying only one highly reproducible test method. This method should then be used to develop correction correlations over a very broad range of fuel hydrogen concentrations (inclusive of 100% SBC) and different engine technologies, including lean burn. There may be uncertainty benefit to use a combustion correlatory metric instead of thrust, and nvPM size (at engine exit) should also be assessed as a partial correlatory parameter.

One fuel analysis method which may offer this high reproducibility is GCxGC, but in order to adopt this approach, first an internationally accepted standardised method should be developed, in order there is confidence that there is not potential significant laboratory bias. Another potential method is high resolution NMR which also needs an internationally accepted standardised method.

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## LIST OF ABBREVIATIONS

Term	Definition
ASTM	American Society for Testing and Materials
ATJ	Alcohol to Jet
BC	Black Carbon
CHJ	Catalytic Hydrothermolysis Jet
EASA	European Union Aviation Safety Agency
EI	Emission Index
FT	Fischer-Tropsch
GCxGC	Comprehensive two-dimensional gas chromatography
HEFA	Hydroprocessed Esters and Fatty Acids
HC	HydroCarbons
ICAO	International Civil Aviation Organization
LOD	Limit of Detection
LTO	Landing Take Off cycle
MSEP	Materials Science and Engineering Program
NDIR	Non-Dispersive Infrared Detector
nvPM	non-volatile Particulate Matter
PAH	Polycyclic Aromatic Hydrocarbons
PM	Particulate Matter
RQL	Rich-Quick Quench Lean-burn combustor
SAF	Sustainable Aviation Fuel
SBC	Synthetic Blending Component used in SAF
SIP	Synthesized Iso-Paraffins
SPK	Synthetic Paraffinic Kerosene
SPKA	Synthetic Paraffinic Kerosene with aromatics
U.K. DEF	United Kingdom Defence Department
vPM	volatile Particulate Matter

## 1. Introduction

Aviation's impact on climate change includes not just CO<sub>2</sub> emissions, but also the creation of contrails and particulate matter (PM). These effects result from the intricate interplay between jet fuel composition, combustion processes, and atmospheric conditions. Understanding and improving fuel composition is a vital step towards reducing aviation's environmental footprint, especially as the industry moves towards sustainable aviation fuels (SAFs) and sophisticated engine technology. Jet exhaust comprises water vapour and carbon dioxide from fuel burning, as well as trace particles such as soot and condensable gases, which act as nuclei for ice crystal formation [1]. The formation of ice crystals in the upper stratosphere and lower troposphere results in contrails, which modifies the global radiation balance. As a result, the development of contrails is a key source of concern regarding global warming. Soot, a carbonaceous material produced as a result of incomplete combustion, is a primary contributor to ice formation. Since the 1980's soot has been regulated by the Smoke Number standard, which was introduced to reduce the visibility of the plume of an aircraft to the naked eye. However, since January 2020 carbonaceous particles have been regulated in a more quantifiable manner with the introduction of the ICAO non-volatile particulate matter (nvPM) mass standard, which was further strengthened in January 2023, with the addition of an nvPM number standard. nvPM is defined as 'emitted particles that exit at a gas turbine engine exhaust nozzle exit plane that do not volatilise when heated to a temperature of 350 °C' [2].

Recent studies have indicated that the quantity of nvPM generated and emitted is directly related to the fuel composition and the combustion technology used in the aircraft [3], [4]. The physicochemical properties of nvPM and secondary organic aerosols strongly influence the ice nucleation process, and these properties are significantly impacted by the fuel composition and combustion conditions [5]. Particulate Matter (PM) porosity and oxygen surface functional groups control the ice nucleation process, and these properties can be influenced by the combustion process. The extent of nvPM formation is strongly correlated to the presence of aromatic compounds within the fuel, and new sustainable aviation fuels aim to reduce aircraft emissions by carefully controlling the fuel composition and eliminating compounds such as naphthalene. This report explores the current properties of 'fossil' based conventional Jet fuels and considers how these will change as SAFs are introduced. The ICAO fuel specifications as defined for emissions certification testing, in Annex 16 Volume II, Appendix 4, are then appraised in view of the ASTM fuel specifications and fuel properties typically available on the commercial marketplace at present, to understand if they are still optimal for ensuring consistency of reported emissions given the introduction of the new nvPM standards.

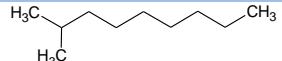
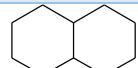
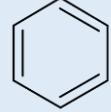
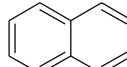
An empirical assessment of uncertainties associated with different fuel analysis techniques, used to determine fuel hydrogen content, is then presented towards understanding the current level of confidence that should be placed in the new ICAO fuel composition correction for nvPM emissions reporting. This assessment is finally supported using new nvPM data sets created as part of SAMPLE IV Deliverable 5 using SBC blends, and from data available to the SAMPLE IV consortium from contemporary research projects that have been undertaken in the past few years.

## 2. Jet Fuel Specification and Properties

### 2.1. Conventional Jet Fuel Composition

Conventional ‘fossil’ based jet fuel is a complex mixture of organic molecules and has a composition that is difficult to quantify precisely. The two primary jet fuels utilised worldwide are Jet A and Jet A-1. While Jet A-1 is utilised internationally, Jet A is mostly employed in the United States. The main difference between the fuels is their respective freezing points, which is  $-40^{\circ}\text{C}$  for Jet A and  $-47^{\circ}\text{C}$  for Jet A-1. Jet A-1 also contains an antistatic additive, which is not present in Jet A. In this report, fossil-based Jet fuels are referred to as Jet A-1. The major organic component groups of Jet A-1 fuels are listed and described in Table 1 below. Rather than characterise the composition explicitly, jet fuel is assessed based on performance specifications, with safe operational performance evaluated either on: (1) the lower and upper limits of selected chemical and thermophysical properties, or (2) the composition limits of several selected chemical species.

Table 1: Jet fuel composition and key chemical components [6]

Hydrocarbon	Definition	Examples	Formula	Chemical Structure Example
<b>n-Alkanes (straight chain alkanes)</b>	Saturated hydrocarbons with a straight carbon chain structure	n-decane ( $\text{C}_{10}\text{H}_{22}$ ) n-dodecane ( $\text{C}_{12}\text{H}_{26}$ )	$\text{C}_n\text{H}_{2n+2}$	
<b>Iso-Alkanes (branched alkanes)</b>	Saturated hydrocarbons with one or more branches in the carbon chain	Iso-Octane ( $\text{C}_8\text{H}_{18}$ ) Iso-Decane ( $\text{C}_{10}\text{H}_{22}$ )	$\text{C}_n\text{H}_{2n+2}$	
<b>Mono-cyclo-alkanes</b>	Saturated hydrocarbons containing a single cyclic ring	Cyclohexane ( $\text{C}_6\text{H}_{12}$ ) Methylcyclohexane ( $\text{C}_7\text{H}_{14}$ )	$\text{C}_n\text{H}_{2n}$	
<b>Bi-cyclo-alkanes</b>	Saturated hydrocarbons with two fused or separate cyclic rings	Decalin ( $\text{C}_{10}\text{H}_{18}$ ) Bicyclohexane ( $\text{C}_{12}\text{H}_{22}$ )	$\text{C}_n\text{H}_{2n-2}$	
<b>Mono-cyclic-aromatics</b>	Unsaturated hydrocarbons with one aromatic ring	Benzene ( $\text{C}_6\text{H}_6$ )	$\text{C}_{4r+2}\text{H}_{2r+4}$ r = number of rings	
<b>Bi-cyclic-aromatics</b>	Unsaturated hydrocarbons with two aromatic rings	Naphthalenes ( $\text{C}_{10}\text{H}_8$ )	$\text{C}_{4r+2}\text{H}_{2r+4}$ r = number of rings	

## 2.2. ASTM & ICAO Fuel Specifications

Table 2 [7] lists the main specification features of Jet A-1, as listed in ASTM D1655 [8] and the UK DEF STAN 91-091 [9], which are used to ensure the safe operability of Jet fuels. Other elements in the list, like 10% Distillation, Distillation loss, Copper Strip Corrosion, Thermal stability, MSEP rating or Electrical conductivity, have been omitted as they are not directly relevant for the purpose of this work, which is concerned with emissions regulation. As can be seen in right hand column, the ICAO Annex 16 volume II emissions regulations define even tighter specifications for the fuel, in an attempt to standardise the reported emissions from different engine manufacturers across different times.

Table 2: Jet A-1 main specification features

Feature (Unit)	ASTM/DEF STAN Specification	ICAO Specification
Acidity (mg KOH/g)	<b>0.10</b> Max.	Not specified
Aromatics (Vol. %)	<b>25.0</b> Max	<b>15 to 23</b>
Sulphur, total (Wt. %)	<b>0.30</b> Max	<b>0.30</b> Max
10 per cent Boiling Point (°C)	Not specified	<b>155 to 201</b>
Final Boiling Point (°C)	<b>300.0</b> Max	<b>235 to 285</b>
Distillation Residue (%)	<b>1.5</b> Max	Not specified
Flash Point (°C)	<b>38.0</b> Min	Not specified
Density@15°C (kg/m <sup>3</sup> )	<b>775.0 to 840.0</b>	<b>780 to 820</b>
Freezing Point (°C)	-47.0 Max	Not specified
Max	<b>8.000</b> Max	Not specified
Hydrogen (mass %)	Not specified	<b>13.4 to 14.3</b>
Kinematic Viscosity at -20 °C (mm <sup>2</sup> /s)	Not specified	<b>2.5 to 6.5</b>
Neat Heat of Combustion (MJ/kg)	<b>42.80</b> Min	<b>42.86 to 43.50</b>
Smoke Point (mm)	<b>25.0</b> Min	<b>20 to 28</b>
Naphthalenes (Vol. %)	<b>3.00</b> Max	<b>0 to 3.0</b>
Existent Gum (mg/100mL)	<b>7</b> Max	Not specified

As can be seen, most of the ASTM fuel specification requirements are expressed in the format of either a maximum or minimum permissible quantity/concentration, except for density, which must be within the range of 775-840 kg/m<sup>3</sup> to meet specification. However, ICAO certification requirements also bound other fuel properties which are sensitive to emissions such as aromatic content, final boiling point, etc. Currently, policies specifying SAF usage pathways are based on the development of drop-in fuels, complying with ASTM D7566 [10], with strict limited SBC blend ratios (up to a maximum of 50% currently permitted) with Jet A-1, to comply with airworthiness

requirements. As such, it is perceived that small changes in properties, permitted as a consequence of the defined fuel specifications and blending of standard-fossil and the synthetic/ sustainable blending component (SBC), should not alter substantially the safety and operability of the fuel in-flight, but such changes have been observed to result in significant changes in witnessed nvPM emissions as discussed further in sections.

### 2.3. Conventional Jet Fuel Vs. Sustainable Aviation Fuel

Fuel composition, particularly aromatic and sulphur content, directly influences nvPM emissions, and the composition of conventional jet fuel can vary markedly. The distribution of aromatics follows a Gaussian function and can vary between 5 to 25 % on a v/v basis at the extremes, with the majority of fuels ranging between 15 to 20 % v/v. Aromatic compounds serve as soot precursors, with naphthalene causing the highest soot emissions; therefore, reducing the aromatic content in fuels reduces nvPM particle formation [11]. The sulphur atoms in sulphur-containing fuels oxidise to SO<sub>x</sub> during combustion and this promotes the nucleation of secondary particles. Reducing the sulphur content reduces both SO<sub>x</sub> emissions and the size of nucleated particles, thereby impacting contrail ice formation.

SBC blends have demonstrated a reduction in particle emissions by up to an order of magnitude compared to traditional fuels. This emission reduction has been negatively correlated with an increased hydrogen content in SBC blends, which affects the chemical kinetics of soot production. Due to their higher hydrogen-to-carbon ratio, paraffinic SBCs generate far fewer nvPM particles. Higher hydrogen content in fuels, such as synthetic paraffinic kerosene (SPKs), reduces nvPM emissions, potentially resulting in fewer ice crystals in contrails and decreased radiative forcing. However, these fuels may increase water vapour emissions, thus creating a difficult trade-off scenario in emissions optimisation. Two fuel refining technologies are commonly used to lower aromatic and sulphur content in jet fuels: (1) Hydrotreating is a catalytic process that removes sulphur, nitrogen, and aromatics, which increases the hydrogen content of the fuel and reduces soot emissions. (2) Extractive distillation is a process that separates and selectively removes aromatic compounds, allowing for precise control and tailoring of the final aromatic content of the fuel [11]. Paraffinic SBCs have a higher n-alkane and iso-alkane content compared to conventional crude-oil based fuels, while Jet A-1 has a higher total number of components such as n-alkanes, iso-alkanes, mono-cycloalkanes, bi-cyclo-alkanes, and single or multiring aromatic compounds. As previously mentioned, fuels from the same production pathway can differ significantly. Today SBC's are typically produced via the following industrial chemical processing routes:

- **HEFA Synthesis (Hydroprocessed Esters and Fatty Acids):** Produces paraffinic hydrocarbons like n- and iso-alkanes.
- **Fischer-Tropsch (FT) Synthesis:** Produces a range of hydrocarbons, predominantly paraffinic, with limited cyclo- and aromatic components.
- **Alcohol-to-Jet (ATJ):** Converts alcohols into paraffinic hydrocarbons, contributing iso- and n-alkanes.

The approved sustainable aviation fuels are listed in the Table 3 below [10]. Only A4, A6, and A8 contain aromatic compounds.

Table 3 Approved SAF listed in the annexes of ASTM D7566<sup>8</sup> and D1655

ASTM Reference	Processing Route	Name	Approved SBC Blending Ratio (vol%)
<b>D7566 Annex A1</b>	Fischer-Tropsch hydroprocessed synthesised paraffinic kerosine using coal, natural gas and biomass sources	FT-SPK	≤ 50%
<b>D7566 Annex A2</b>	Synthesised paraffinic kerosine from hydroprocessed esters and fatty acids using vegetable oil, animal fats, and used cooking oil	HEFA-SPK	≤ 50%
<b>D7566 Annex A3</b>	Synthesised Iso-Paraffins from hydroprocessed fermented sugars using biomass from sugar production	SIP	≤ 10%
<b>D7566 Annex A4</b>	Synthesised kerosine with aromatics derived by alkylation of light aromatics from nonpetroleum sources, such as coal biomass, and natural gas	FT-SPK/A	≤ 50%
<b>D7566 Annex A5</b>	Alcohol-to-Jet synthetic paraffinic kerosene using ethanol, isobutanol and isobutene from biomass	ATJ-SPK	≤ 50%
<b>D7566 Annex A6</b>	Synthesised kerosine from catalytic hydrothermal conversion of fatty acid esters and fatty acids using vegetable oils, animal fats, and used cooking oil	CHJ	≤ 50%
<b>D7566 Annex A7</b>	Synthesized paraffinic kerosine from hydroprocessed esters and fatty acids using algae	HC-HEFA-SPK	≤ 10%
<b>D7566 Annex A8</b>	Alcohol-to-Jet synthetic paraffinic kerosene with aromatics using C2-C5 alcohols from biomass	(ATJ-SKA)	
<b>D1655 Annex A1</b>	Fats, oils, and greases co-processing with petroleum intermediates using vegetable oils, animal fats, and used cooking oils	FOG	≤ 5%
<b>D1655 Annex A1</b>	Fischer-Tropsch hydrocarbons co-processed with petroleum crude oil	FT coprocessing	≤ 5%
<b>D1655 Annex A1</b>	Co-processing of HEFA (Hydroprocessed esters and fatty acids) from biomass	HEFA coprocessing	≤ 10%

The composition of four SAFs analysed by GC x GC, a two-dimensional gas chromatography method, is shown in Figure 1 below. Two-dimensional gas chromatography is a technique that can provide chemical group type separation and quantification in jet fuels. The carbon chain length (C5 to C20) is shown on the x-axis, and the y-axis shows the mass fraction of the fuel component (%).

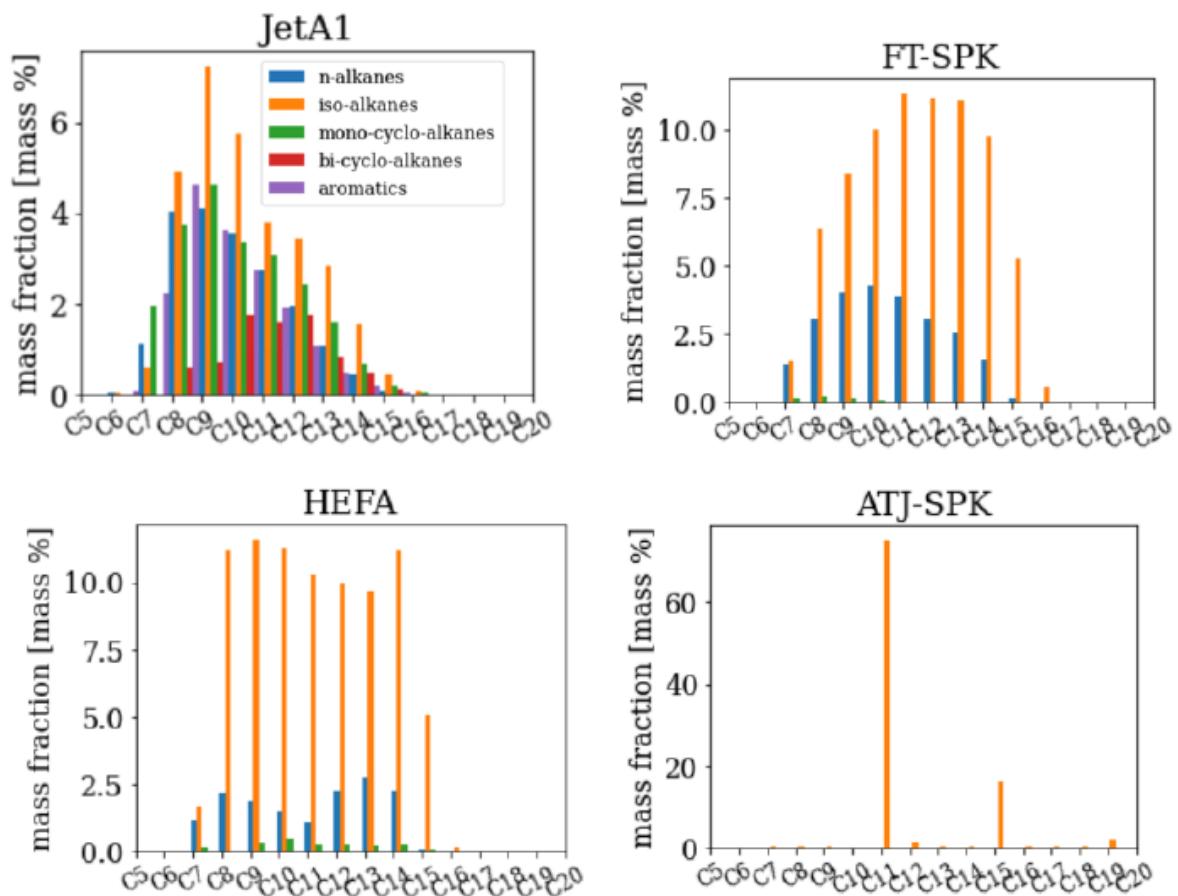


Figure 1: Fuel compositional GC x GC analysis of Jet A-1 and three SAF fuels: ATJ-SPK, HEFA, and ATJ-SPK (Gierens et al. [12])

It is evident that Jet A-1 is comprised of a complex mixture of organic molecules including n-alkanes, iso-alkanes, mono- and bi-cyclo-alkanes, as well as aromatic compounds. FT-SPK and HEFA fuels are similar and contain mainly iso-alkanes with a smaller fraction of n-alkanes and a residual number of mono-cyclo-alkanes. The ATJ-SPK fuel only contains iso-alkanes, with other compounds below detection limits. The key differences in conventional fuel vs. SBC chemical composition are shown in Table 4.

Table 4: Key compositional differences between SAF and Jet A-1 fuel

Property	Description
<b>Higher iso-alkane content</b>	SAFs have a larger fraction of iso-alkanes, improving cold flow properties and reducing particulate emissions compared to fuels containing polycyclic aromatic compounds.
<b>Lower Aromatic content</b>	SAFs generally have less than 8% aromatics by volume, significantly lower than conventional Jet A-1 fuels, which may have up to 25%.
<b>Absence of sulphur compounds</b>	SBCs are virtually sulphur-free, reducing SO <sub>2</sub> emissions and enabling cleaner combustion.
<b>High paraffin content</b>	Generally, SBCs are highly paraffinic, with a high fraction of n- and iso-alkanes leading to cleaner combustion.

## 2.4. Effect of Fuel Composition on Combustion and Emission Properties

Fuel combustion kinetics in the jet engine combustion chamber can all be impacted by changes in the composition of the jet fuel. Jet A-1 is a complex mixture of many molecules containing straight-chain (n-alkanes), branched-chain (iso-alkanes), mono and polycyclic alkanes, and mono and polycyclic aromatic species. The concentration ratio of these species influences the combustion characteristics of the fuel significantly. In general, when considering nvPM and soot formation, the following scheme describes how fuel components affect the tendency to form soot:

linear hydrocarbons < branched hydrocarbons << aromatics <<< polyaromatics

The problem is that fuel mixtures have complex combustion reactions, and the overall sooting tendency is not always the sum of the sooting tendencies of the component parts. The fundamental difficulty today is that sustainable aviation fuels, such as HEFA, contain very low concentrations of aromatic compounds but are predominantly composed of long-chained branched hydrocarbons. These branched hydrocarbon compounds have a modest sooting tendency but are a better option than aromatics or polyaromatics. Understanding the interaction between fuel components during the combustion process is crucial in predicting particulate matter emissions from any given engine burning any given fuel. Also, this understanding is required so that reported regulatory emissions concentrations, which may be derived using a range of fuel compositions (as shown in Table 2), can be corrected to allow consistent reporting of emissions across different aircraft engines and / or across different temporal testing programmes.

Jet exhaust gases consist primarily of CO<sub>2</sub> and H<sub>2</sub>O with trace amounts of CO, hydrocarbons (HC), particulate matter (PM), NO<sub>x</sub> and SO<sub>x</sub>, as well as atmospheric O<sub>2</sub> and N<sub>2</sub>. Given, modern gas turbine engines typically exhibit overall efficiencies of >99%, most of their gaseous emissions are nominally similar and directly correlate to the hydrogen to carbon ratio of the fuel they are burning. However, as a reference point, the exhaust gas composition for a V2527-A5M engine burning conventional Jet A-1 fuel is given in Table 5 below. As can be seen, CO<sub>2</sub> and H<sub>2</sub>O are the main products of the combustion process, with traces of CO and HC resulting from inefficiencies associated with incomplete combustion. SO<sub>x</sub> emissions are a direct result of sulphur present in the fuel; sulphur atoms are oxidised during combustion to produce SO<sub>x</sub> compounds. NO<sub>x</sub> is formed due to the Zeldovich mechanism, which describes the oxidation of nitrogen in air due to movement of atmospheric air through the engine compression, combustion, and turbine stages [13].

Table 5: Exhaust gas composition of V2527-A5M engine from the ICAO Aircraft Engine Emissions Databank

Component	g / kg fuel	%
CO <sub>2</sub>	3160.00	71.634
H <sub>2</sub> O	1230.00	27.883
NO <sub>x</sub>	19.40	0.440
SO <sub>x</sub>	1.08	0.024
CO	0.44	0.010
nvPM	0.33	0.008
HC	0.03	0.001

As discussed further in later sections, the hydrogen content of fuel, which inversely correlates with fuel aromatic content, has been shown to offer the best (negative) correlation with both nvPM number and mass emissions indices, with a relatively small variation in the fuel hydrogen content resulting in significant differences in witness nvPM emission indices. This is demonstrated by analysis of the combined emission data from the JETSCREEN project [14] and the work of Tucker et al. [12] on the effects of fuel desulphurisation. The emission data were measured at 50% thrust . Figure 2: Impact of hydrotreatment on aromatics and hydrogen content on the relative change of nvPM emissions at 50 % thrust (calculated by the method of Teoh et al. [4]). The fuels used are described in Tucker et al. [12] and the JETSCREEN Project [14].Figure 2 for fuel samples that were hydrotreated to remove aromatic and sulphur compounds. Figure 2A and B show that, as the aromatic content decreases, there is a corresponding increase in fuel hydrogen content resulting in a decrease in nvPM. Figure 2C shows a linear correlation between the hydrogen content and the nvPM emission index, demonstrating the sensitivity of fuel hydrogen content on particulate matter emissions.

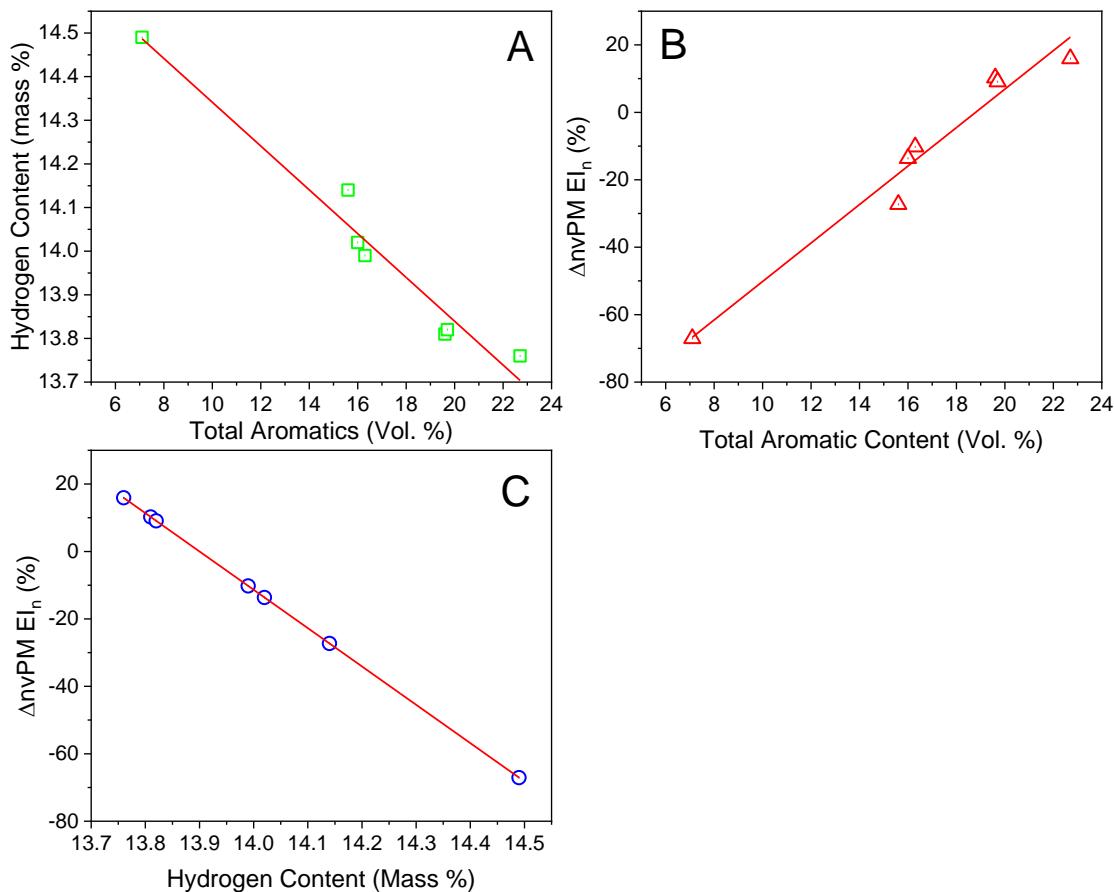


Figure 2: Impact of hydrotreatment on aromatics and hydrogen content on the relative change of nvPM emissions at 50 % thrust (calculated by the method of Teoh et al. [4]). The fuels used are described in Tucker et al. [12] and the JETSCREEN Project [14].

It is evident from Figure 2 that hydrogen/aromatic content directly impacts combustion efficiency and emissions and is a critical parameter for accurate emission prediction.

## 2.5. Typical Hydrogen Contents of Fuels

Figure 3 illustrates the hydrogen content (mass %) of different types of jet fuels tested in the ECLIF 1 and ECLIF 2/ND-MAX campaigns, alongside data from the DLR SimFuel database. It details typical fuel compositions of commercially available conventional fuels derived from fossil fuels, blends (mixtures) of conventional jet fuels with sustainable aviation fuel (SAFs), and pure hydro-processed esters and fatty acids (HEFA) feedstock SAF, which is a synthetic paraffinic kerosene (SPKs). As would be expected, the conventional fuels, which typically contain higher levels of aromatics, show a lower and narrower range of hydrogen content while the more paraffinic blends exhibit a wider distribution, reflecting variability in the blending ratio and the hydrogen content of individual components. HEFA fuels display the highest hydrogen content due to the large volume fraction of paraffinic components. Fuels with higher hydrogen content, such as HEFA, typically produce a lower concentration of and soot particles which contributes to a reduced environmental impact.

The large variability in blended fuel hydrogen content with individual fuel groups and across different fuel types emphasises the wide range of fuel properties available, which ultimately results in wide ranging witnessed emissions. The figure also emphasises that in the medium to long term future, there will likely be a trend of ever-increasing hydrogen concentrations in fuel stocks worldwide as the adoption of SAF becomes more prevalent.

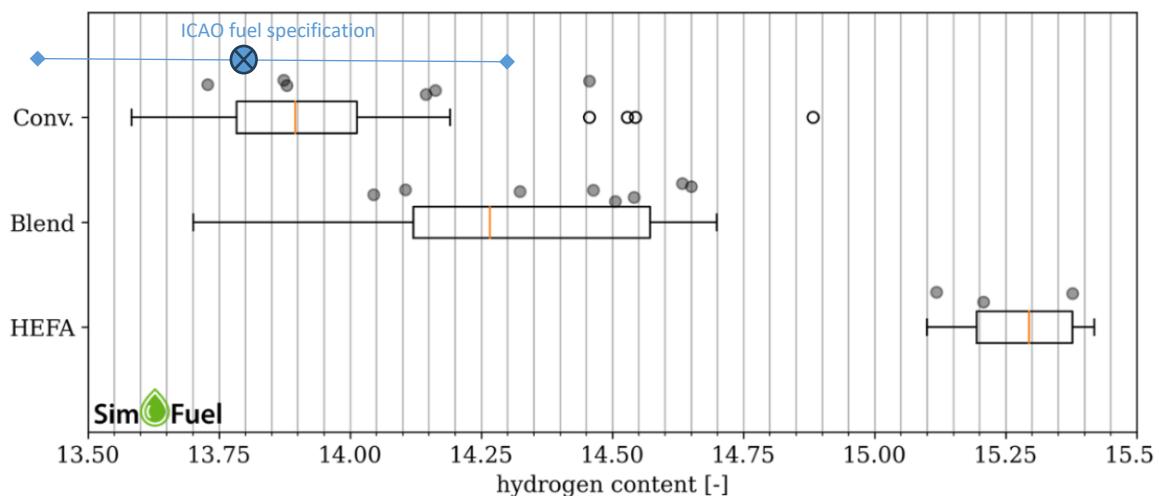


Figure 3: Box and whisker plot showing the variability in hydrogen content (mass %) for conventional jet fuel, Jet A-1+SBC blends, and neat HEFA [12]

When considering the ICAO Annex 16, Volume II Appendix 4 fuel specifications, as presented in Table 2, which defines a permissible hydrogen content range of 13.4-14.3% with the data presented in Figure 3, it is seen by the added blue band line that the permissible hydrogen content in ICAO is far wider than the range of conventional jet fuels that the DLR SimFuel database indicates are typically available. Given the trend towards SAF blends in the future, it could be argued that the upper limit permissible by ICAO is suitable as it encompasses the lower centiles blends that in theory could already be commercially available. However, in terms of the lower hydrogen limit, where it is perceived nvPM emissions will be highest, it is seen that this is well below what is typically being consumed by the commercial fleet. As such there is potentially an argument to support an increase in this lower bound to bring it in-line with fuels of today and in the future.

Similarly, as discussed further in section 3.3, the ICAO 'standard' fuel hydrogen content fuel (as shown by the blue cross) to which measured nvPM emissions are corrected is currently set at 13.8%

hydrogen content. Depending on whether ICAO wish reported EI's to be conservative, in that they are representing realistic worst case, or representative of typical real-world emissions again would open the debate as to whether this value should also be slightly increased in the future, towards average conventional fuels.

However, as is further discussed in Section 4, with any analysis technique, there are uncertainties in quoted fuel hydrogen contents. Therefore, accurate and precise, or at least reproducible, quantification of hydrogen content in jet fuel is paramount to be able to apply empirically derived fuel composition corrections in order to correct measured nvPM values to equivalent nvPM emission indices, that would have been witnessed if a fuel of a different hydrogen content was utilised.

## 2.6. Summary

In summary, it is seen that conventional 'fossil' jet fuels are composed of a wide range of organic compounds, which leads to variability in the fuels carbon to hydrogen ratio. It is also seen that these variations result in significant differences in witnessed nvPM, with lower concentrations of nvPM typically witnessed at lower fuel aromatic/ higher fuel hydrogen contents. The fuel composition parameter that correlates most strongly with emission indices is the fuel hydrogen content, which is further described in section **0Error! Reference source not found..**

Conventional jet fuels typically exhibit fuel hydrogen contents in the range of 13.55– 14.2%, with SAF blends expected to increase this range from 13.7-14.7%, however the current ICAO Annex 16 fuels specification or engine emissions certification testing defines a range of 13.4-14.3%, which it could be argued is too broad and should at least have its lower bound raised, to be more representative of conventional fuels. The fuel hydrogen content to which nvPM emissions are to be standardised is currently defined at 13.8%. This value falls within the range of current conventional jet fuels. However, if a decision is made to increase the minimum permitted hydrogen content in fuel, it is also worth considering raising this value to better align with average fuel properties. Doing so could help minimise the applied corrections across the allowable range of fuel hydrogen content. Note that since fuel Smoke Point, aromatics and density are linked to nvPM emissions and hydrogen content, these parameter ranges would also likely need to be updated. They could simply be brought in line with ASTM requirement, since the specific range of fuel hydrogen content would control the standardisation of nvPM emissions.

### 3. Fuel Composition Correction Methods for nvPM

As discussed in Section 2, depending on the feedstock and refining methods used, the global composition of standardised jet fuel, is subject to variation and is permitted via the ranges permitted in the relevant fuel specifications (e.g. ASTM 1655 and Table 2: Jet A-1 main specification features Table 2). Compared to European Jet A-1, Jet A which is mostly utilised in North America, has a higher percentage of aromatic compounds [15], [16]. Recent research has demonstrated that, in contrast to aromatic concentrations, fuel with increasing hydrogen mass content and hydrogen-to-carbon (H/C) ratios exhibits a negative correlation with sooting propensity [16].

In general, three models are available in the literature for the correction of nvPM mass and number concentration due to fuel compositional variation. These include:

1. The model developed by Brem et al. (2015)[3]
2. The Teoh et al. model (2022)[4], which is an extension of the Brem et al model
3. The International Civil Aviation Organisation (ICAO) model [2]

The metric used in these models is the emission index (EI), which measures the amount of nvPM produced per unit of fuel burned. The following equations show the EI calculations for nvPM mass (Eq.1) and number (Eq.2). The nvPM emission index was first defined in a SAE Aerospace Information Report (AIR6421) and is calculated using measured values of nvPM along with measured gaseous CO<sub>2</sub>, CO, and HC species to predict the fuel burned [17].

$$EI_{nvPM_{Mass}} = \frac{BC_{Mass} \times 10^6}{([CO_2] + [CO] - [CO_2]_{Background} + [HC] - [HC]_{Background})(M_C + \alpha M_H)} \frac{0.082T}{P} \quad (Eq.1)$$

$$EI_{nvPM_{Number}} = \frac{nvPM_{Number} \times 10^{12}}{([CO_2] + [CO] - [CO_2]_{Background} + [HC] - [HC]_{Background})(M_C + \alpha M_H)} \frac{0.082T}{P} \quad (Eq.2)$$

Where EI<sub>nvPM<sub>Mass</sub></sub> and EI<sub>nvPM<sub>Number</sub></sub> are the calculated emission indices for nvPM mass (g kg<sup>-1</sup>) and nvPM number (kg<sup>-1</sup>), respectively. BC<sub>Mass</sub> is the particle mass concentration (g m<sup>-3</sup>), typically measured using a traceably calibrated Photo Acoustic Soot Sensor (PSS) or Laser Induced Incandescence (LII) instrument. Particle number concentration (# cm<sup>-3</sup>), is defined as to be measured using a Condensate Particle Counter after a suitable dilution and volatile removal stage. T and P are the ambient temperature (K) and the pressure (atm) in the respective measurement cells. CO<sub>2</sub> represents the emitted CO<sub>2</sub> in units of ppm, measured using NDIR, and CO<sub>2</sub> background is the CO<sub>2</sub> concentration of the ambient atmosphere. CO is the emitted carbon monoxide, measured using NDIR, in units of ppm. HC and HC<sub>Background</sub> represent the methane equivalent hydrocarbon concentrations in the exhaust (ppm) and the ambient air (ppm), respectively as measured using a Flame Ionisation Detector (FID). The coefficient  $\alpha$  is the atomic hydrogen-to-carbon ratio (H/C) of the fuel, and M<sub>C</sub> and M<sub>H</sub> are the molecular weights of carbon (12.1 g mol<sup>-1</sup>) and hydrogen (1.01 g mol<sup>-1</sup>), respectively. The measured nvPM data (BC<sub>mass</sub> and nvPM<sub>number</sub>) are used to calculate the emission index (EI).

### 3.1. Brem at al. Fuel Correction Model (2015)

Prior to 2015, no research had comprehensively investigated the influence of fuel aromatic concentration on nvPM emissions, in the actual fuel range required for engine certification (15-23%). Brem et al. [3] conducted a seminal study to address these inadequacies, with the goal of accomplishing the following: (1) to investigate the impact of fuel aromatic content on nvPM emissions, in an emissions certification-like environment, utilising representative fuels with total aromatic content ranging from 17.8 to 23.5% (v/v), (2) to determine the effect of naphthalene versus monoaromatic content on emissions, and (3) Model and define parameters for the measured results so that they can be utilised to appropriately correct engine nvPM data for fuel composition differences.

Emissions measurements were conducted on a hi-bypass turbofan engine, with fuel composition varied using an aromatic injection system integrated into the test facilities fuel delivery line, at thrust levels ranging from 3% to 100%. Two different aromatic additives, consisting of a naphthalene-depleted solvent and a solvent with naphthalene at 6% (v/v) were investigated, facilitating a range of fuel aromatic contents ranging from circa 18-24% (v/v). Particle losses in the sampling lines were not measured, but particle loss correction factors were estimated. From these measurements, it was seen that nvPM number and nvPM mass reductions correlated well with increasing hydrogen content as seen in Figure 4.

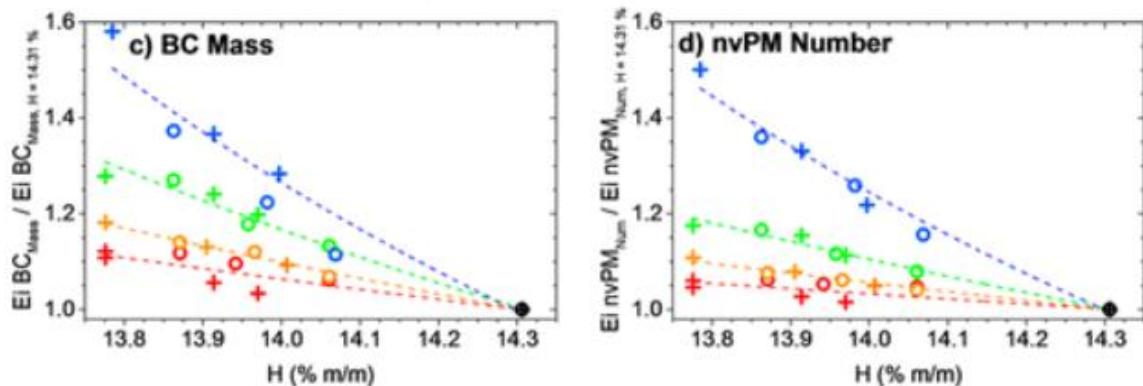


Figure 4: Correlation of nvPM number and mass reductions and increased hydrogen content

From this data a correction model was developed that predicted the nvPM EI's as a function of engine thrust and change in hydrogen mass content ( $\Delta H$ ), in relation to a reference fuel. Comparing the results from the 2 different solvents highlighted that nvPM emission indices exhibited a better correlation with hydrogen mass content compared to aromatic content. The correction model is shown in Equation 3. With Figure 5 showing a surface plot of the nvPM mass and number EI's and the fitted model.

$$\Delta EI_x = (\sigma_0 + \sigma_1 \times \hat{F}) \times \Delta H \quad (\text{Eq.3})$$

$\Delta EI_x$  is the percentage change in the emission index for either the nvPM mass or number concentration. Where  $\sigma_0$  and  $\sigma_1$  are the model coefficients estimated from regression analysis,  $\hat{F}$  is the thrust (%), and  $\Delta H$  is the change in fuel hydrogen mass content (%). The coefficients derived from regression analysis are shown in Table 7, for EI's describing nvPM mass and number, as well as the combined data, which can be used as a simplification.

Table 6: Coefficients for the correction of nvPM EI (%) due to variation in fuel H mass content (%, m/m) for the Brem et al. [3] model

Dependent Variable (%)	Coefficient $\sigma_0$	Coefficient $\sigma_1$	Adjusted R <sup>2</sup>
$\Delta EI$ nvPM <sub>Mass</sub>	<b>-124.05 ± 5.04</b>	<b>1.02 ± 0.06</b>	<b>0.94</b>
$\Delta EI$ nvPM <sub>Number</sub>	<b>-114.21 ± 3.63</b>	<b>1.06 ± 0.05</b>	<b>0.96</b>
$\Delta EI$ nvPM combined	<b>-119.31 ± 3.94</b>	<b>1.03 ± 0.05</b>	<b>0.92</b>

It is thought that the model is valid for engines that utilise similar rich-burn, quick-mix, lean-burn (RQL) combustor technology, which was developed to reduce NO<sub>x</sub>, and with fuels that are compliant with the Jet A-1 specification. The results show a decrease in both mass and number emission indices with increasing hydrogen mass content ( $\Delta H$ , %). The model's shortcomings include substantial inaccuracies for thrusts smaller than 30%. Hence, the fuel correction model is valid only above 30% thrust and when the arithmetic difference in hydrogen mass content ( $\Delta H$ , %) between the blend and standardised fuel is less than 0.6%. As a result, extrapolations beyond this have significant prediction uncertainty.

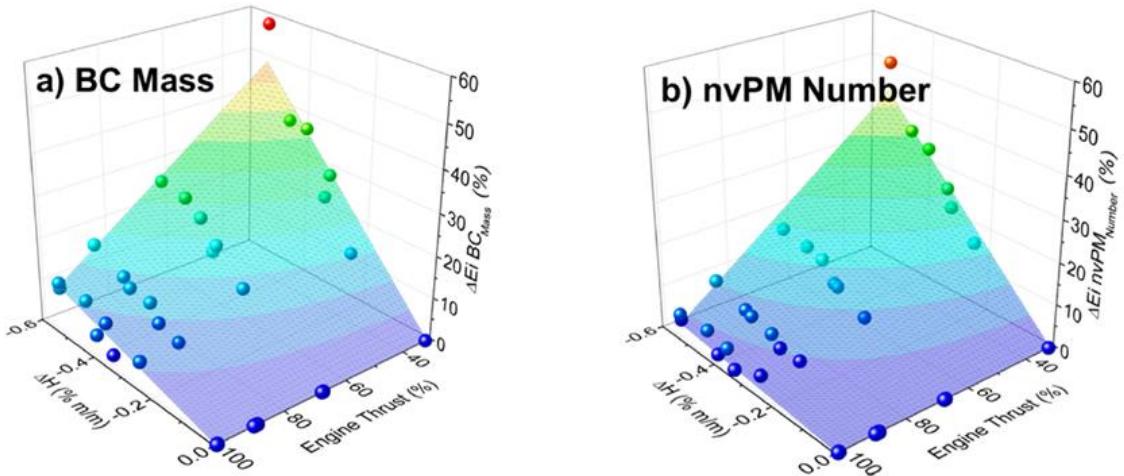


Figure 5: Surface fits to the emission indices for percentage change in nvPM (a) mass and (b) number concentration as a function of engine thrust (%) and change in hydrogen mass content (%) (adapted from Brem et al. [3])

### 3.2. Teoh et al. Fuel Correction Model (2022)

The fuel correction model proposed by Teoh et al. [4] expands on Brem et al., covering a wider thrust range (10 – 100%) and a higher change in hydrogen mass content ( $\Delta H$ ) up to 1.1%, which corresponds to H of 14.7%. The piecewise model is shown in Equations 4 and 5.

For  $\Delta H \leq 0.5\%$

$$\Delta nvPM EI_n = (\sigma_0 + \sigma_1 \times \hat{F}) \times \Delta H \quad (\text{Eq.4})$$

For  $\Delta H > 0.5\%$

$$\Delta nvPM EI_n = (\sigma_0 + \sigma_1 \times \hat{F}) \times \Delta H \times e^{(0.5 - \Delta H)} \quad (\text{Eq.5})$$

Where  $\Delta nvPM EI_n$  is the change in the nvPM number emission index (%),  $\sigma_0$  and  $\sigma_1$  are the original coefficients from Brem et al. (see Table 7),  $\hat{F}$  is the thrust (%), and  $\Delta H$  is the change in hydrogen mass content (%) relative to standard jet fuel.

### 3.3. ICAO Fuel Correction Model

In light of the recommendations of Brem et al. [3], which highlighted the benefits of hydrogen correlated corrections, the ICAO Committee on Aviation Environmental Protection (CAEP) developed a hydrogen based, standardised fuel composition correction model to account for variation in the properties of standard jet fuel. The calculation, detailed in ICAO Annex 16 [2], corrects the measured nvPM  $EI_n$  and  $EI_m$  to a fixed H value of 13.8%. The correction factors calculations are shown in equations 6 & 7 below:

$$k_{fuel\_M} = \exp \left\{ \left( 1.08 \frac{F}{F_{00}} - 1.31 \right) \times (13.8 - H) \right\} \quad [\text{eq.6}]$$

$$k_{fuel\_N} = \exp \left\{ \left( 0.99 \frac{F}{F_{00}} - 1.05 \right) \times (13.8 - H) \right\} \quad [\text{eq.7}]$$

Where  $k_{fuel,N}$  and  $k_{fuel,M}$  are the fuel composition correction factors and  $F/F_{00}$  is the engine thrust setting expressed in decimals. The equations are only valid for a H range of 13.4 to 14.3%; therefore, estimating  $\Delta nvPM EI_n$  for SAF with high blend ratios ( $H > 14.3\%$ ) could lead to predictions with high uncertainty.

A comparison between the work of Brem [3], ICAO [2], and Teoh [4] is shown in Figure 6 and shows the correlation between the percent change in nvPM  $EI_n$  vs. the change in hydrogen mass content (%) at increasing thrust level. The shaded pink areas represent the extrapolated regions of each model from the experimental data, up to predicted  $\Delta nvPM EI_n$  (%) values of  $\Delta H = 1.5\%$ . The work of Teoh et al. covers a broader range of  $\Delta H$  values (experimental values up to 1.1%), which corresponds to higher blends of Jet A-1 and SBC (up to 70%).

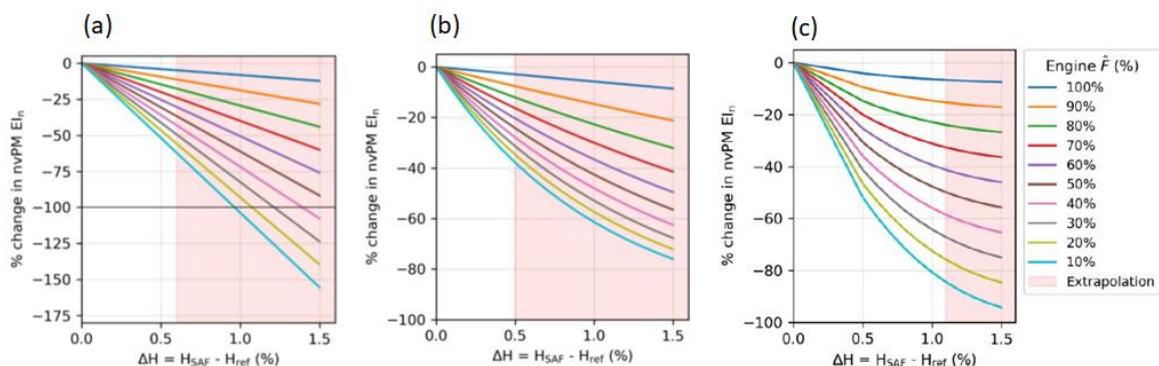


Figure 6: The percent change in nvPM  $EI_n$  as a function of  $\Delta H$  and engine thrust calculated using the (a) Brem et al., (b) ICAO, and (c) Teoh et al. models. The shaded pink region indicates that the extrapolations are estimates made from available measurements (Adapted from Teoh et al. figures in supporting information [15])

## 4. Fuel Hydrogen Content Analysis Method Uncertainty

To assess the impact of fuel on nvPM emission indices, accurate hydrogen quantification becomes vitally important. For aircraft engine certification testing, as discussed ICAO Annex 16 Volume II allows fuel composition with a Hydrogen content between 13.4 and 14.3 mass per cent [2]. There are four ASTM standards for hydrogen quantification of jet fuel, namely, D3343, D5291, D3701, and D7171. As stated in the Concawe report [12], Standards D3343 and D5291 are not recommended for accurate jet fuel hydrogen quantification and are based on estimation of hydrogen from physicochemical properties and combustion products, respectively. The D3701 and D7171 standards rely on nuclear magnetic resonance techniques (NMR) and have far lower uncertainties in the hydrogen content quantification. The D3701 standard suffers from inherent biasing; therefore, the D7171 standard, which is a low-resolution pulsed nuclear magnetic resonance (NMR) spectroscopy technique, is currently the most accurate ASTM analytical method with a reproducibility standard deviation of 0.11 mass %, equivalent to a nvPM standard deviation of 6.2 % [18]. However, it is evident that these measurement uncertainties are still rather large after considering the sensitivity of the nvPM emission indices on hydrogen content. Therefore, at present, it is difficult to explain, with a high degree of confidence, variations in nvPM emission indices at any given engine certification test, due to determination of fuel hydrogen content.

A summary of standard testing methodologies to determine hydrogen content and their ASTM stated uncertainties are shown in Table 7. In agreement with [12] ASTM D5291 is specifically not recommended by ICAO Annex 16 Volume II for use for Jet A-1 fuel hydrogen determination due to the higher uncertainties in this fuel application. However, in contradiction to [Concawe ref] D3343 is recommended by ICAO for use.

Also, it is stated by Thom [18], that the measurement instrument in ASTM D3701 is not manufactured anymore. This means that only two standard methods available to be currently used are ASTM D3343 and D7171. Since the number of global laboratories that provide ASTM D7171 method are very limited, currently for practicality reasons ASTM D3343 tends to be the preferred fuel hydrogen method used for ICAO nvPM emissions data reporting, with its known bias stated in Table 7 below.

ASTM D3343 and ASTM D7171 are based on archaic technologies (more than three decades old). Current benchtop high-resolution NMR can produce rapid (< 5 minutes), inexpensive (< 50 Euros) analyses [19], [20] that are likely to have improved uncertainty compared to ASTM D7171 low resolution NMR method. A new ASTM standard would be needed, and ideally could be performance based, to allow use of future NMR technology improvements.

Research test campaigns investigating impact of fuel on aircraft emissions, often use two-dimensional gas chromatography (often referred to as GCxGC) to provide a very detailed composition breakdown, which enables determination of fuel hydrogen content. This method coupled with mass spectrometry is considered to be the scientific optimum with expected uncertainty lower than any of the ASTM methods. However, there is no shared standardised methodology for GCxGC analysis across laboratories, thus the reproducibility is currently unknown. Global development of a standardised GCxGC fuel analysis method has been initiated, with activities in the US towards standardisation and several inter laboratory studies underway, but will likely take a number of years to develop. It is perceived that a future standardised GCxGC fuel

hydrogen analysis should be considered for inclusion into ICAO Annex 16, when its uncertainty is shown to be equivalent or lower than current techniques.

*Table 7: Uncertainties of different methods to measure hydrogen content of aviation fuels (ASTM). D3701 is not shown as this measurement device is not produced anymore*

<i>ASTM</i>	<i>Method</i>	<i>Repeatability (k=2)</i>	<i>Reproducibility</i>	<i>Bias</i>
<i>D3343</i>	<i>Correlation</i>	<i>0.03%</i>	<i>0.10%<sup>1</sup></i>	<i>0.16%</i>
<i>D5291</i>	<i>LECO/Flash analyser</i>	<i>0.43%</i>	<i>0.86%<sup>2</sup></i>	<i>Unknown due to no reference material available</i>
<i>D7171</i>	<i>Low resolution pulsed nuclear magnetic spectroscopy</i>	<i>At 40 °C: 0.12%</i>	<i>At 40 °C: 0.30%<sup>2</sup></i>	<i>Unknown due to no reference material available</i>

It is not often that the same fuel samples are analysed by multiple fuel test methods. Below in Table 8 is a limited dataset from various research campaigns where either the identical fuel was analysed in the same laboratory by different methods, identical fuel was analysed by different labs using different methods or same fuel sampled at two locations analysed by the same laboratory by different methods.

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<sup>1</sup> Does not include the effect of original data scatter used in the correlation, therefore there is possibility that the error is larger than stated

<sup>2</sup> At 13.8% fuel H content

Table 8: Comparison of Jet A-1 and SBC with Jet A-1 fuel Hydrogen content measured by different techniques

ID	Fuel blend	GCxGC MS	ASTM D3343	ASTM D5291 (not recommended by ICAO)	ASTM D7171	Data confidence info
1	<b>100% Jet A-1</b>	13.97	13.64	13.21		same lab, same sample
2	<b>100% Jet A-1</b>	14.17	13.88			same lab, same sample
3	<b>100% Jet A-1</b>	14.11	13.78			same lab, same sample
4	<b>100% Jet A-1</b>	14.3	14.03			same lab, same sample
5	<b>50% SBC 50% Jet A-1</b>	14.72	14.54			same lab, same sample
6	<b>30% SBC 70% Jet A-1</b>	14.48	14.27			same lab, same sample
7	<b>100% SBC</b>	15.17	15.27	14.92		same lab, same sample
8	<b>100% Jet A-1</b>	14.06		13.99	14.02	different labs, same sample
9	<b>100% Jet A-1</b>			12.69	13.68	different labs, same sample
10	<b>100% Jet A-1</b>			13.72	12.86	different labs, same sample
11	<b>100% Jet A-1</b>	13.72	13.61	13.01	13.65	different labs, same sample
12	<b>100% Jet A-1</b>	14.17	13.95	12.91	14.08	different labs, same sample
13	<b>100% Jet A-1</b>	14.10	13.98	14.60	14.04	different labs, same sample
14	<b>100% Jet A-1</b>			14.06	14.43	different labs, same sample
15	<b>100% Jet A-1</b>		13.75	13.8		different labs, same sample
16	<b>30% SBC 70% Jet A-1</b>	13.53			13.60	different labs, same sample
17	<b>30% SBC 70% Jet A-1</b>	14.54	14.47	14.23	14.51	different labs, same sample
18	<b>30% SBC 70% Jet A-1</b>	14.71		14.58		different labs, same sample
19	<b>49% SBC 51% Jet A-1</b>	14.45	14.46	13.82	14.40	different labs, same sample
20	<b>50% SBC 50% Jet A-1</b>		14.53	14.5		different labs, same sample
21	<b>100% SBC</b>	15.24		15.36	15.31	different labs, same sample
22	<b>100% SBC</b>	15.47		15.5		different labs, same sample
23	<b>100% SBC</b>	15.36	15.41			same lab, D3343 fuel tank sample, GCxGC engine sample

Figure 7 and Figure 8 below show the sensitivity impact that the differences in fuel H determination has on  $k_{fuel\_N}$  &  $k_{fuel\_M}$  as defined in Section 3.3, when using the different analytic fuel methods. The blue shade shows the allowable ICAO range of fuel H content, assuming GCxGC to be the reference data. The 7% and 100% LTO conditions are shown, and it is observed that the variability in derived H from different fuel methods has a higher impact at the low engine power taxi point than the high power take off point, this observation is in direct correlation with the ICAO fuel correction which predicts minimal impact of fuel hydrogen content on nvPM at high engine thrusts and increasing

impact as engine thrust reduces. As would be expected at high engine power all the points are comfortably within  $\pm 10\%$  except for D5291 for nvPM mass.

The data variability for ASTM D5291 is clearly the highest and thus agrees with the ICAO recommendation that this fuel analysis method should not be used for determination of fuel H content.

ASTM D3343 and D7171 are fairly consistent compared to GCxGC. With D7171 being the most consistent especially in the allowable ICAO H fuel content range.

It appears to be clear that for simpler hydrocarbon composition fuels as typically exhibited in higher SBC blends in SAFs, with higher H content, the fuel analysis methods agree better. However, as the H fuel content decreases, the variability between fuel methods increases, which supports that the lower limit of hydrogen content permissible as defined in ICAO Appendix 16 for engine emissions testing is raised from the currently permitted 13.4%.

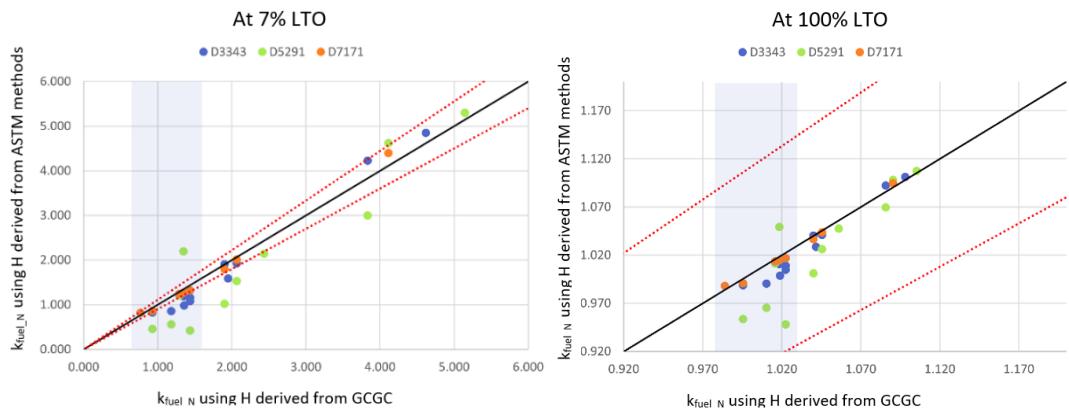


Figure 7: Comparison of fuel correction factors for nvPM number emissions at idle and take-off LTO conditions, derived from different H values of different fuel analysis methods. The black line is unity and the red dotted lines show  $\pm 10\%$  band. The blue shade indicates the allowable H range for ICAO engine certification on the x-axis

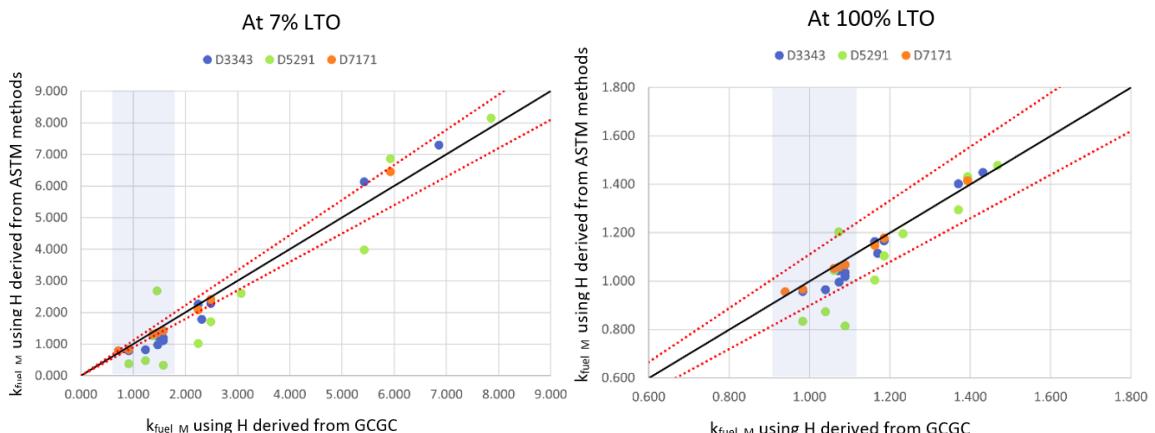


Figure 8: Comparison of fuel correction factors for nvPM mass emissions at idle and take-off LTO conditions, derived from different H values of different fuel analysis methods. The black line is unity and the red dotted lines show  $\pm 10\%$  band. The blue shade indicates the allowable H range for ICAO engine certification on the x axis

In comparison to the fairly high nvPM number and mass measurement uncertainties ( $\sim 15$  to  $20\%$ ), the uncertainties in the fuel correction values witnessed above between ICAO allowed fuel measurement methodologies (D7171 and D3343) are not significant for small fuel correction factors found at high engine power (100%). However, especially for nvPM number, at low engine power variabilities between fuel H determination methods are shown to be more significant, with up to 20% observed. There is potential to reduce this variability by specifying D7171 or a new

standardised GCxGC method. However, with the commercial scarcity of D7171 availability, it is recommended to support GCxGC standardisation to improve nvPM reported data uncertainty due to fuel analysis in the future.

GCxGC analysis tends to be fairly expensive (~1000 Euros) compared to other ASTM H fuel analysis methods (~150 Euros). Consideration could be given to using industry best practice where fuel densities are often used as a proxy to show that multiple samples of the same fuel have the same properties (i.e., will have the same H content). Thus, for example, if three fuel samples are obtained from the same fuel supply over the course of engine testing, if the density analyses are very close to each other, then a single fuel sample could be sent for standardised GCxGC analysis in order to confirm its hydrogen content.

However, it should also be noted that the ICAO fuel correction may also contain embedded uncertainties regarding fuel hydrogen content, associated with the data from which the empirical data was generated. Therefore, it should be considered that prioritising the reproducibility of fuel hydrogen content measurements, rather than absolute precision, could enhance fuel correction methods in the future. By specifying a highly reproducible hydrogen analysis technique and using it to generate the data for developing a fuel correction correlation, accurate  $k_{fuel}$  values could still be determined. This approach would remain effective as long as the same technique is consistently applied in subsequent engine testing, even if the hydrogen content measurement for the tested fuel lacks high precision.

## 4.1. Summary

As with all analyses and corrections, there is a level of uncertainty associated with quoted values. Therefore, in order to fully understand the potential impact of the ICAO permissible range of hydrogen content, an appreciation of uncertainties associated with the determination fuel hydrogen content is required. Similarly, assessment of the current ICAO correction methodology across this wide-ranging fuel hydrogen content is recommended across a number of engine technologies, to inform as to its usefulness in comparing reported regulatory nvPM Emission Indices (EIs) and in predicting the likely impact SAF adoption will have on the fleet.

Therefore, at present, it is difficult to explain, with a high degree of confidence, variations in nvPM emission indices at any given engine certification test, due to determination of fuel hydrogen content.

## 5. Assessment of Fuel Correction Methods with Contemporary Data

The ICAO fuel composition correction was developed based on nvPM emission tests from 24 representative engine types, including turbofans, turboshafts, and turboprops. However, some of the measurement systems used in these tests did not fully comply with ICAO Annex 16, Vol. II, Appendix 7. The fuels tested had Final Hydrogen Content (FHC) values ranging from 13.6% to 15.6%, but the methodologies used to determine FHC varied between tests, and in some cases, FHC values were not reported.

Within the database, the agreement between measured emissions and model-predicted values was within  $\pm 10\%$  for most data points. ICAO also assessed the impact of not applying a fuel correction factor, finding discrepancies of up to 35% for nvPM number emissions and 55% for nvPM mass emissions. The two primary influencing variables identified were engine thrust condition and FHC. The uncertainty in the fuel composition correction factor for both nvPM number and mass emissions was estimated at 12%, based on a 95% confidence interval (equivalent to two standard deviations from the mean).

The ICAO correction is intended to be universally applicable across all engine types, as developing separate models with different coefficients for specific engine types would not satisfy the need for a generalised correction applicable to all nvPM emissions data.

Since the ICAO fuel composition correction was developed, additional Jet A-1 and SAF emissions datasets have been collected using the Swiss and EUR nvPM reference sampling and measurement systems on engines where the correction had not yet been validated. In these new datasets, FHC was measured using ASTM D7171, D3343, D5291, and GCxGC methods.

These datasets, presented below, provide an opportunity to further evaluate the effectiveness of the existing ICAO fuel composition correction across a broader range of engine sizes, from 17 kN to 241 kN. Specifically, nvPM EI number and mass reductions were estimated by calculating the percent difference between the emissions measured with the different fuels ( $reduction_{measured} = (emission_{jet-A} - emission_{SAF})/emission_{jet-A}$ ). The ICAO fuel correction was estimated comparatively as  $reduction_{ICAO} = 1 - 1/k_{fuel}$  with  $k_{fuel}$  the fuel composition correction factor found in A16V2 [2] and presented in Section 3.3. It is noted that  $k_{fuel}$  is normally calculated by comparing the fuel used to a “standard” Jet A-1 fuel with a hydrogen content of 13.8% but in this case the  $\Delta H\%$  between the Jet A-1 and SAF of interest was used.

First, as already discussed in the SAMPLE IV deliverable 3 and 5 reports, nvPM and gaseous emissions from ALF502 and ALF507 engines were characterised while burning two Jet A-1 fuels and two 50% SBC blends (ID 20 to 23 in Table 8). The nvPM EI number and mass reduction introduced by switching from a given Jet A-1 to a SBC blend are shown in Figure 9, and compared to the correction for fuel composition proposed by ICAO. Given the uncertainty discussed in Section 4, the fuel hydrogen content was measured using various techniques: the first pair of fuels (Figure 9 (a) (b)) was analysed with ASTM D5291 and D3343 while the second pair of fuels (Figure 9 (c) (d)) was analysed with D3343 and GCxGC. Given each techniques yielded to slightly different fuel hydrogen contents (ID 20 to 23 in Table 8), the ICAO fuel composition correction is shown for each technique, with error bands corresponding to the rounding error ( $\pm 0.1\%$  FHC).

For nvPM EI number, the measured reductions typically agree with the ICAO correction using D3343 for the first pair of fuels (Figure 9 (a)), however the ICAO correction appears to consistently

underpredict reductions for the second pair of fuels by approximately 10% on average (Figure 9 (c)). For nvPM EI mass, the measured reductions are consistently higher than that from the ICAO correction for all FHC measurement methods and both pairs of fuels (Figure 9 (b)&(c)).

At low power (engine thrust  $\leq 7\%$ ), the measured reductions in nvPM EI number and mass show significant scatter. This variability is likely due to repeatability uncertainty in engine conditions at low power and rapidly changing nvPM emission characteristics within this range. For example, thrust variations between 3% and 8% correspond to  $T_{30}$  temperatures ranging from 109–124°C for the ALF 507 and 94–123°C for the ALF 502. These fluctuations result in changes of up to 70% in regulatory nvPM EI number and 79% in regulatory nvPM EI mass <sup>3</sup>. When excluding the low idle point and considering only thrust levels between 6–8%, these variations decrease to 38% for nvPM EI number and 40% for nvPM EI mass. Another possible reason for the scatter in nvPM EI mass reduction at low power is that the measurement was near LOD, with the lowest measured nvPM mass being  $\sim 6 \text{ ug/m}^3$  on ALF 507 and  $\sim 2 \text{ ug/m}^3$  on ALF 502, both at low idle ( $\leq 4\%$  thrust) when burning SAF.

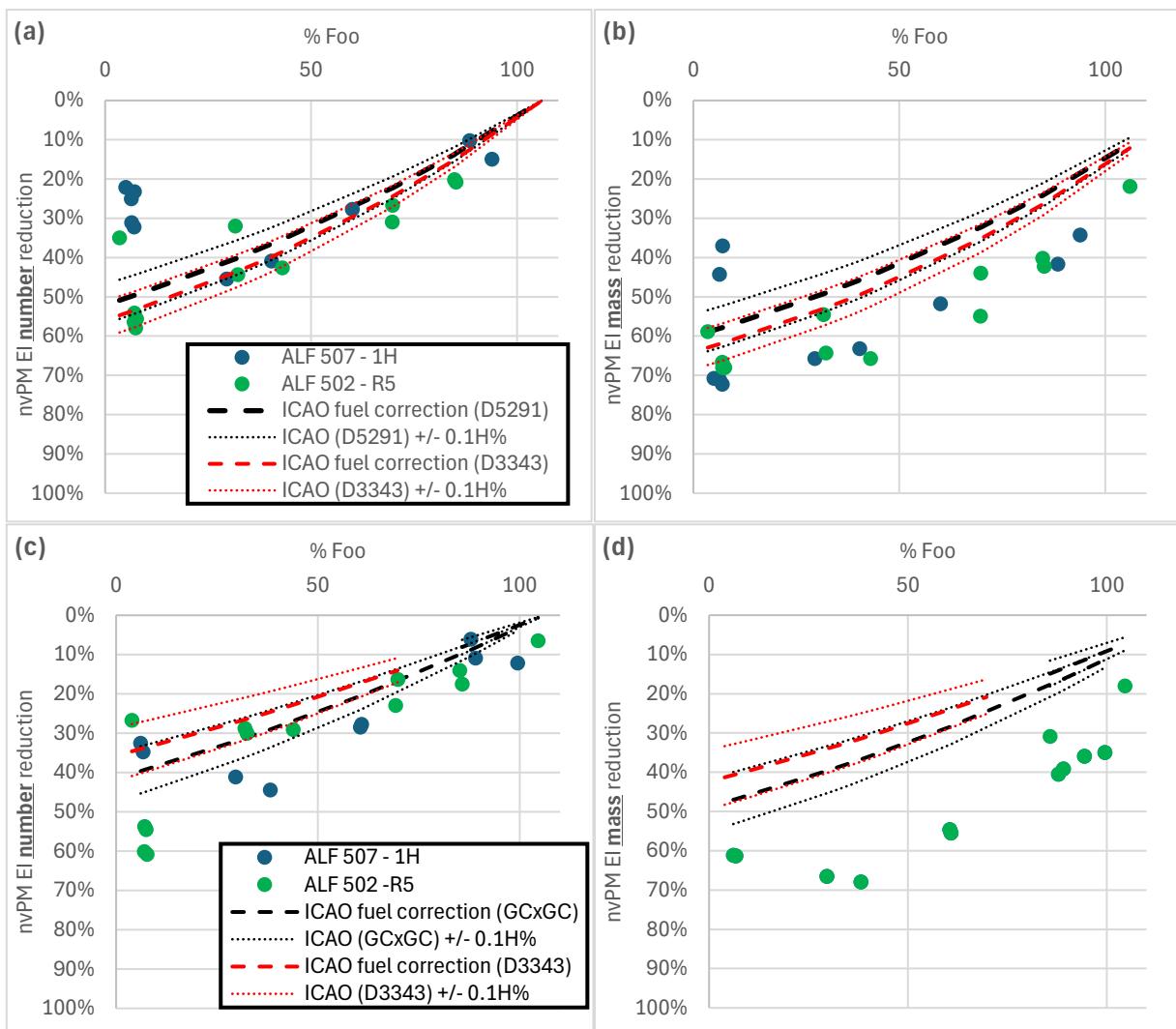


Figure 9: Reduction in regulatory nvPM EI number (a & c) and mass (b & d) emissions measured using the European nvPM reference system on the ALF 502 (30kN) and 507 (31kN) engines burning two Jet A-1 fuels compared to a blend of SAF and Jet A-1 ((a & b) -  $\Delta H 0.7\% D5291$  or  $0.78\% D3343$ ; (c & d) -  $\Delta H 0.42\% GCGC$  or  $0.51\% D3343$ ) and plotted against ICAO fuel composition correction

<sup>3</sup> See Sample IV deliverable 5

The second dataset originates from the H2020 AVIATOR programme in which the emissions of a Rolls-Royce Trent 500 were characterised. The measured EI nvPM reductions, shown in Figure 10, typically correlate better with the ICAO fuel correction using D3343. Again, significant scatter is seen at low power, likely driven by engine condition repeatability uncertainty (potentially due to changing ambient conditions). At 80% thrust, the nvPM EI mass reduction is overpredicted by the ICAO correlations. When comparing with the ALF 502 and 507 engines at similar thrust (Figure 9 (b)&(d)), this suggests that different engine technologies and sizes may yield to different EI nvPM mass reduction at high power. There could be a nvPM size dependency, since larger GMDs were observed on the Trent 500 than the ALF engines at high power.

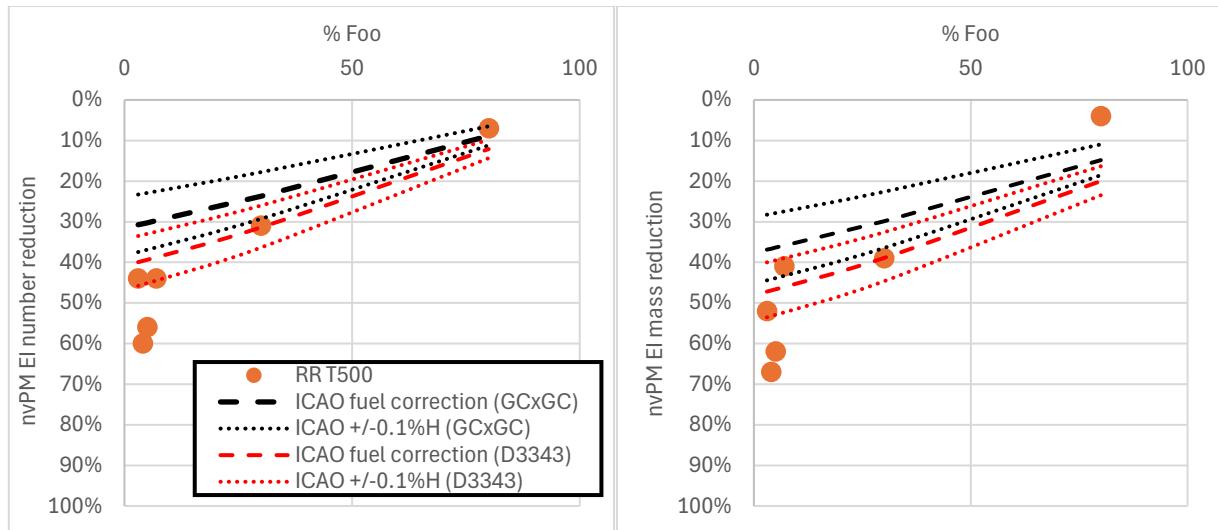


Figure 10: Reduction in regulatory nvPM EI number (left) and mass (right) emissions measured using the European nvPM reference system on a Rolls-Royce Trent 500 (249kN) engine burning Jet A-1 and a SBC blend (top -  $\Delta H$  0.36% D3343 or 0.50% GCxGC) and plotted against ICAO fuel composition correction

All the reported nvPM EI reductions in Figure 9 and Figure 10 were derived using “regulatory” nvPM emissions, which do not include size-dependent system loss corrections [21]. However, the switch from Jet A-1 to SAF is known to reduce nvPM size, number, and mass [22], [23], [24], potentially impacting the calculated nvPM EI reductions. To assess this effect, nvPM EI reductions calculated using “regulatory” nvPM emissions were compared to those obtained from fully loss-corrected nvPM emissions (using the  $PSD_B$  method), with results presented in Figure 11.

At thrust levels above 7%, including size-dependent loss corrections has a negligible impact, with differences typically within  $\pm 2\%$ . However, at thrust levels below 7%, the uncertainty increases to  $\pm 10\%$  for nvPM EI number, and a bias of up to 20% is observed for nvPM EI mass.

While not correcting for size-dependent loss (i.e., current regulatory nvPM emissions) introduces a non-negligible uncertainty at thrust levels below 7%, this uncertainty remains minimal compared to the uncertainty associated with estimating fuel hydrogen content using different methods (see Section 4) and the variability in engine condition reproducibility at low power. Therefore, regulatory nvPM EI values were used for the remainder of this analysis.

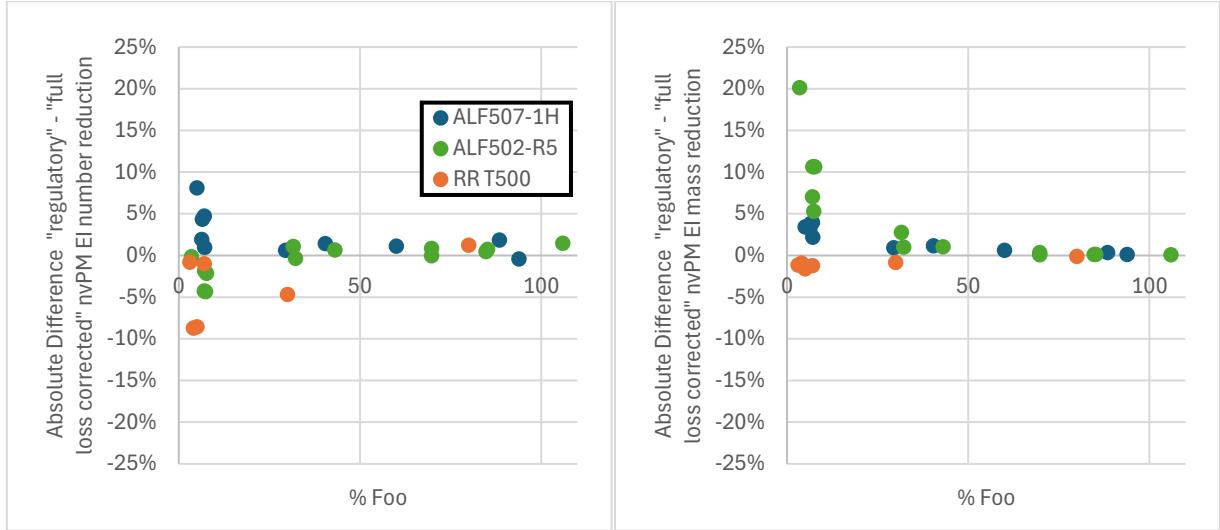


Figure 11: Comparison of nvPM EI number (left) and mass (right) reduction when using either regulatory or fully-loss corrected (method PSDB [21]) Els

The third dataset reports the nvPM EI reductions from a small unregulated turbofan engine, the PW545A with a rated thrust of 17kN. The results are shown in Figure 12 and highlights a relatively good agreement between nvPM EI mass and the ICAO fuel correction with method D7171, while the ICAO method typically seems to overpredict reductions for nvPM EI number by approximately 10%.

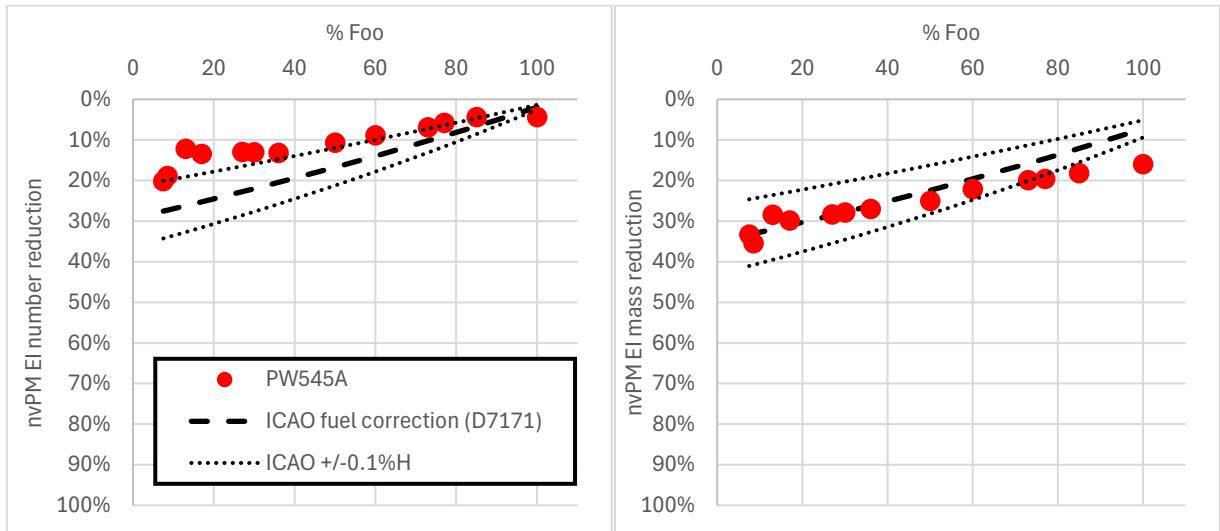


Figure 12: Reduction in regulatory nvPM EI number (left) and mass (right) emissions measured using the Swiss nvPM reference system on a PW545A (17kN) engine burning Jet A-1 and a SBC blend ( $\Delta H$  0.33% D7171) and plotted against ICAO fuel composition correction

The fourth dataset reports the nvPM EI reductions from a CFM56-7B26 engine burning various blends of the same Jet A-1 and SBC, in a study reported in the literature [24], with the results shown in Figure 13. On average, the ICAO fuel correction using D7171 correlates well with the measured nvPM EI number and mass reductions, although there is significant scatter in the measured nvPM EI reductions, partly attributed to variation in ambient conditions. It is noted that data when the measured nvPM mass is below LOD was not included.

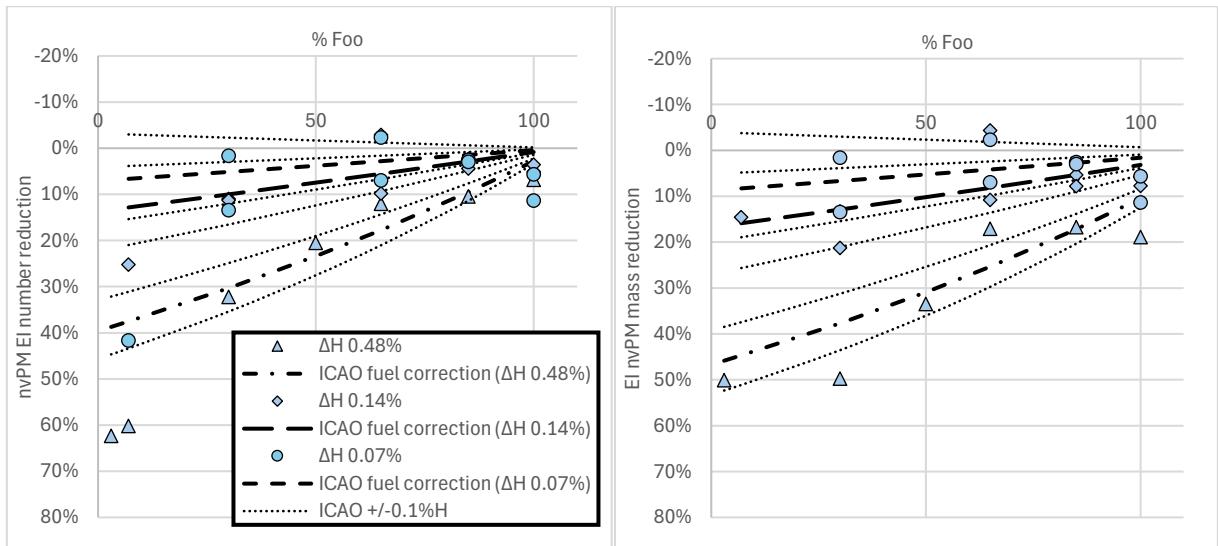


Figure 13: Reduction in regulatory nvPM EI number (left) and mass (right) emissions measured using the Swiss nvPM reference system on a CFM56-7B26 (117kN) engine burning Jet A-1 and three SBC blends ( $\Delta H$  0.48%, 0.14% and 0.07% D7171) [24] and plotted against ICAO fuel composition correction

To summarise the outputs of this chapter, the four datasets presented above (Figure 9–13) were combined with the work of Brem et al. [3] to produce Figure 14, which shows the difference between measured and ICAO-predicted nvPM EI reductions across various engine types and FHC measurement methods. Figure 14 consists of four subplots: the left panels show nvPM number reductions, while the right panels depict nvPM mass reductions. The distinction between the top and bottom panels corresponds to the FHC method used to determine  $\Delta H$  between Jet A-1 and SAF: The top panels represent methods recommended by ICAO (D3343 and D7171), whereas the bottom panels correspond to methods not currently recommended (D5291 or GCxGC). Additionally, Figure 14 includes a black dashed line representing the maximum perceived uncertainty due to uncorrected fuel composition effects and was calculated based on the maximum permissible difference in FHC ( $\Delta H = 14.3\% - 13.4\% = 0.9\%$ ) [2].

The results show that the agreement between measured nvPM EI number and mass reductions and ICAO fuel corrections hovers around 0% and scatters typically within  $\pm 20\%$ . At low power the scatter is higher as has been previously discussed. Overall, using the ICAO fuel correction therefore decreases the uncertainty in comparing results of nvPM when using fuels of different hydrogen content. This improvement is seen to be up to 60% at low power, reducing down to  $<10\%$  at take-off power, where the impact of fuel composition on nvPM formation is observed to be minimal. However, there remain significant uncertainties in accurately and consistently measuring the fuel hydrogen content and in reproducing the exact same engine condition when burning different fuels, on different days.

No differences were observed between the different methods of deriving fuel hydrogen content, likely because the same method was consistently used to measure each Jet A-1 and SAF pair. This ensured that any method-specific bias did not affect the  $\Delta H\%$ . However, if two fuels were measured using different analysis methods, the uncertainty would likely increase, underscoring the importance of repeatability in measured hydrogen content analysis.

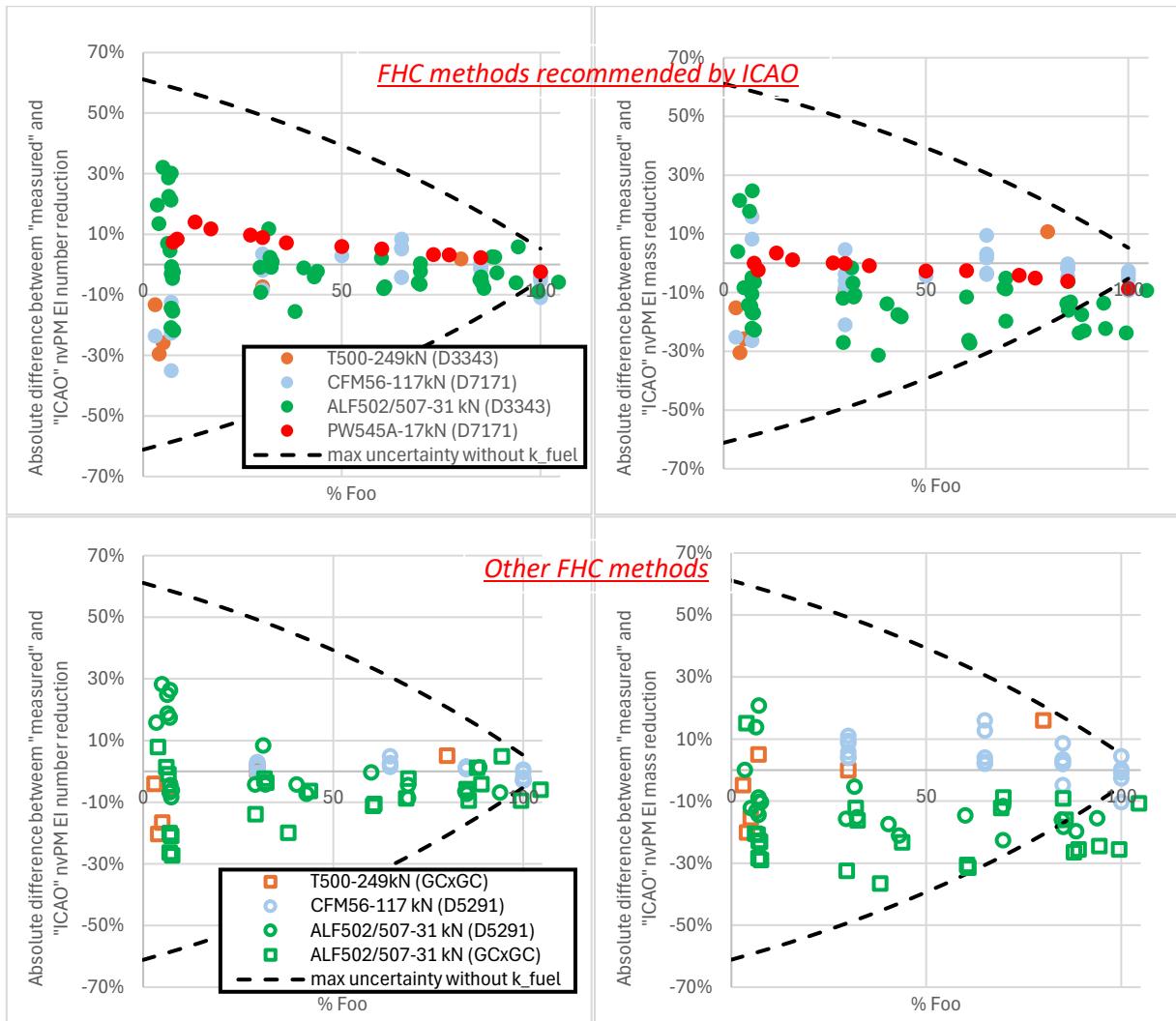


Figure 14: Absolute difference between measured and ICAO-predicted ( $k_{fuel}$ ) nvPM EI number (left) and mass (right) reduction from fuel composition (i.e., difference between ICAO fuel correction and measured nvPM reductions from Figures 9 – 14)

It can be observed in all datasets shown above (Figure 9-14) that SAF has a larger impact on nvPM mass EI reduction than nvPM EI number which is consistent with the observations of GMD reductions and with other older studies described above. Generally, it is seen that the ICAO fuel correction for nvPM EI typically agrees to within  $\pm 20\%$  for all engine types, with higher scatter at low power engine conditions ( $\pm 30\%$ ). Different engine types also displayed different bias between measured and predicted nvPM EI reductions.

## 6. Conclusions and Recommendations

From the work reported above, it can be concluded that there are significant variations in fuel composition permissible within the ASTM specifications which result in significantly different nvPM emissions being exhibited from a given engine, with reported reductions inversely correlating with fuel hydrogen content. Conventional Jet fuels typically exhibit fuel hydrogen contents from 13.5 – 14.2% (with outliers up to 14.8%). Since SBC in SAF typically has zero aromatics and high hydrogen content (as high as 15.4%), SAF with Jet A-1 and SBC typically exhibits higher hydrogen content ranges of 13.7-14.7%. Hence a trend of increasing fuel hydrogen content is expected as SAF adoption becomes more prevalent in the future.

However, the current ICAO Annex 16 fuel specification for engine emissions certification allows fuels exhibiting fuel hydrogen concentrations from 13.4-14.3%, with the 'standard' fuel to correct to at 13.8%. Given the lower end of this range is outside the typical conventional Jet fuel range, there could be an argument for increasing this value, in order that a tighter specification would mean there is a smaller range of hydrogen content over which correction is required. This is supported by the findings that the uncertainty associated with the determination of fuel hydrogen content is typically highest when measuring fuels of lower hydrogen content. However, if this was an adopted strategy then it would also potentially make sense to also increase the 'standard' 13.8% in order that average corrections were minimised across the permitted range of fuel hydrogen content. A rise in this value would also potentially move the hydrogen content to be more representative of fuels of the future which will likely contain more SBC and hence have a higher hydrogen concentration. As an example, one could consider modifying the ICAO engine emissions certification range to 13.9 to 14.5% and set the 'standard' value for fuel corrections to 14.2%. This would accomplish goals of increasing the 'standard' fuel hydrogen content to be more representative of current and future fuels, practical fuel availability and narrowing the uncertainty associated with fuel corrections for nvPM emissions. There would, in addition, either need to be an ICAO fuel specifications change in the allowed fuel maximum Smoke Point (increased) and minimum aromatics (decreased) or a removal of both these limits (which would then be the same as ASTM allowed Jet fuel specification) since the fuel hydrogen content range would 'standardise' certification fuel for nvPM emissions.

There is currently significant uncertainty and potential bias introduced by the numerous ASTM approved methods for fuel hydrogen content determination, which leads to uncertainty in both developing and using fuel correction methodologies. The ICAO recommended methods (D3343 and D7171) appeared to offer the best performance, with the impact of fuel H content determination method seen to be within 10% except for nvPM number at low power (within ~20%). However, since the vast majority of reported engine emissions data uses D3343 and the methods tend to be more precise within a method than accuracy between them, variability is likely within 10% for all engine powers. The GCxGC method appears to offer benefits, particularly if a standardised approach is developed moving forwards. It is noted that currently the GCxGC method is still relatively expensive and complicated, hence it maybe that cheaper fuel analysis techniques (e.g., fuel density) are used to determine stability and consistency of a fuel across a given test programme, with a singular GCxGC used to determine the fuel hydrogen content. Modern high-resolution NMR could also be considered in the future (as a replacement for ASTM D7171) but would also require a new ASTM standard method to be developed.

The ICAO Fuel composition correction model was shown to reduce the uncertainty in comparing reported nvPM from any given engine burning fuels of different hydrogen content within the allowable ICAO range of 13.4-14.3%. Bias improvements of 60% for engines at low powers are achieved when compared to not applying a fuel correction. This benefit reduces with increasing engine power as it is seen that at take-off type powers reductions in nvPM associated with hydrogen content are minimal.

Fuel correction methods based on hydrogen content are therefore beneficial in two ways:

- I) They allow comparison of engine technology across their power range at different testing times
- II) They help to understand the impact of the adoption of SAF fuels on non-CO<sub>2</sub> emissions

However, SAF blend usage towards 100% SAF means that H content is often well outside the ICAO allowable range, thus there will need for further improvements in correction models to fully assess the non-CO<sub>2</sub> benefits of SAF adoption.

With regard to current fuel composition correction models, there are a number of limitations which include: (1) research has only focused on rich-burn technology and this needs to be expanded to lean-burn engines, (2) very limited experimental validation data is available on high pressure ratio engines, and (3) a limited range of fuel types was used for the development of the correction models, hence they are likely cannot be fully extrapolated to understand the impact of 100% SBC in SAF adoption.

Recommendations for subsequent actions are therefore as follows:

Firstly, it should be further assessed whether the lower bound of fuel hydrogen content, currently permitted in ICAO Annex 16 (13.4%) should be increased to be better aligned with current conventional fuels and SAF blends which are likely to be widely adopted in the foreseeable future. Should this value be raised, it likely warrants also a similar raising of the 'standard' fuel hydrogen content (13.8%) in order to reduce the average uncertainty in correction, whilst making the reported certification EI's more representative of real-world emissions witnessed today and particularly in the future. Raising the upper bound (14.3%) should also be assessed for practical supply of certification fuel, since it will become more and more difficult to obtain commercially available low H content fuel as aviation fuel H content increases.

To improve uncertainty in fuel nvPM correction methods, further work is required towards reducing the uncertainty associated with fuel hydrogen content determination. If the hydrogen content is only required for nvPM fuel correction, then potentially specifying only one highly reproducible test method. This method should then be used to develop correction correlations over a very broad range of fuel hydrogen concentrations (inclusive of 100% SAF) and different engine technologies, including lean burn. There may be uncertainty benefit to use a combustion correlatory metric instead of thrust, and nvPM size (at engine exit) should also be assessed as a partial correlatory parameter. This specified method should then be used to determine the fuel hydrogen content at any given engine test.

One method which may offer this high reproducibility is GCxGC, but in order to adopt this approach, first an internationally accepted standardised method should be developed, in order there is confidence that there is not potential significant laboratory bias. Another potential method is high resolution NMR which also needs an internationally accepted standardised method.

## APPENDIX

### Effects of Blending Jet A-1 with SAF on Emissions Levels

#### *Laboratory Testing*

This section shows results of an experimental test comparing emissions results of a 100% JETA1 and a 100% SAF combusted in a bespoke liquid fuelled Combustion Aerosol Standard (CAST) Generator. In this aerosol generator a propane flame is used to pre-heat the liquid fuel that is then vaporised to generate the diffusion flame, which should therefore be treated with caution when trying to compare to studies of full engines burning SAFs [18] but offer insight into the likely fuel trends driving combustion derived emissions.

In the ALTERNATE study, the selected SBC was Alcohol To Jet (ATJ), manufactured using a catalytic conversion process to create a drop-in fuel, however as discussed previously and seen in Table x currently a 100% ATJ is not permitted for aviation and hence does not meet the ASTM specifications, but gives insight into potential emissions signatures of future SAF. As alcohols, some which can be obtained from a wide range of biogenic feedstocks via thermochemical and biochemical processes then they can be termed as SAF. However, it is noted that ATJ characteristics can differ from those of standard fossil-derived Jet A-1, particularly in terms of:

- a) Density: The density of the ATJ, used in the experiment (around 760 kg/m<sup>3</sup>) is lower than typical Jet A-1 densities defined in the relevant fuel standards (775 - 840 kg/m<sup>3</sup>).
- b) Viscosity: ATJ viscosity is always higher than Jet A-1, with the difference increasing as temperature decreases. For example, at -40 °C ATJ viscosity is up to 60% higher than Jet A-1.
- c) Cetane number of ATJ is very low and this may affect the operability of the injection system and the combustion chamber.
- d) Aromatics: ATJ is fully paraffinic and does not contain any aromatics, hence will have a higher hydrogen content. As aromatics are well established soot precursors, this difference is very important because use of this fuel should significantly reduce nvPM emissions.
- e) Boiling point: The value range of ATJ boiling point is much narrower due to its simpler chemical composition compared to Jet A-1

#### *Basic findings about the impact of SAF on particles emission*

In the laboratory combustion experiment, the change from Jet A-1 to ATJ [19] assessed a number of impacts including; changes to the main structure of the flame, change in measured nvPM emissions and change in the potential to form vPM in exhaust plume.

As expected, the combustion of 100% SAF reduced the concentration of nvPM, with respect to both number and mass, compared with the fossil-based Jet A-1. These reductions, resulted in a corresponding reduction in nvPM particle size, as shown in Figure 15, with the Jet A-1 distribution peaking at circa 4 times higher number counts at a GMD of circa 150 nm compared to 90 nm in the case of the ATJ.

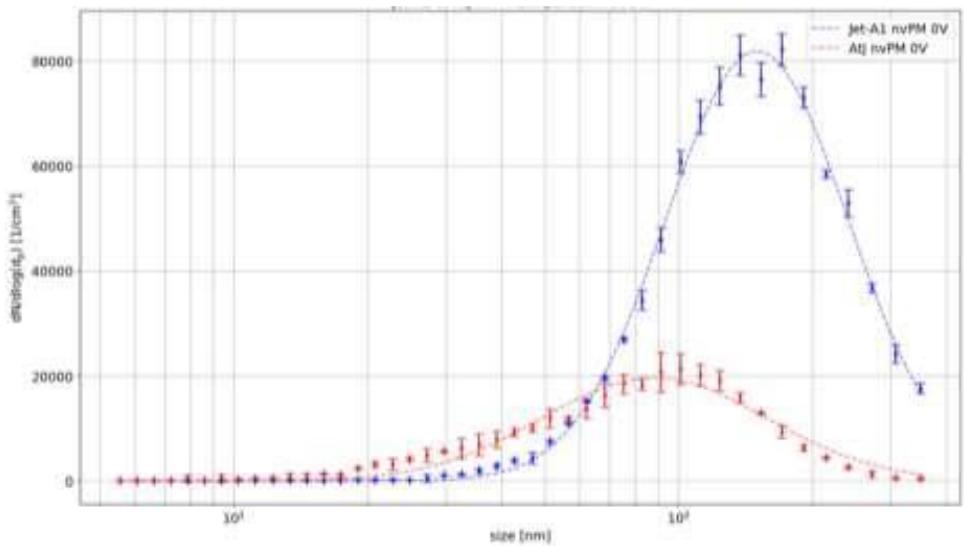


Figure 15: nvPM particle size distribution for Jet A-1 (blue) and ATJ (red) [25]

However, in the case of currently unregulated vPM, there was a smaller difference in observed comparing the emissions from the standard fossil-based Jet A-1 and ATJ fuels, as shown in Figure 16. with it observed that the ATJ produced more vPM than the corresponding Jet A-1 case. It is however noted that the sulphur content in ATJ was close to zero, indicating the possibility that UHCs in the ATJ exhaust maybe acting as potential precursors for vPM. In agreement with previous work, it is noted that the vPM mode is witnessed at smaller sizes than the nvPM, indicative of nucleated particles being formed.

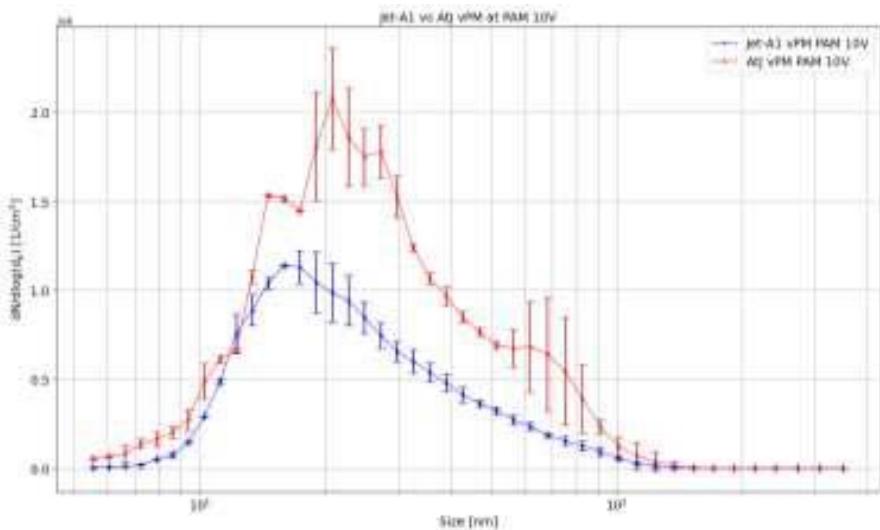


Figure 16: vPM particle size distribution for Jet A-1 (blue) and ATJ (red) [25]

Considering both the nvPM and vPM, it is noted that the nvPM decreases observed in the case of ATJ were much greater than the relative increase in vPM emission, as such the net result suggests a considerable diminishing of total PM (tPM), as represented in Figure 17.

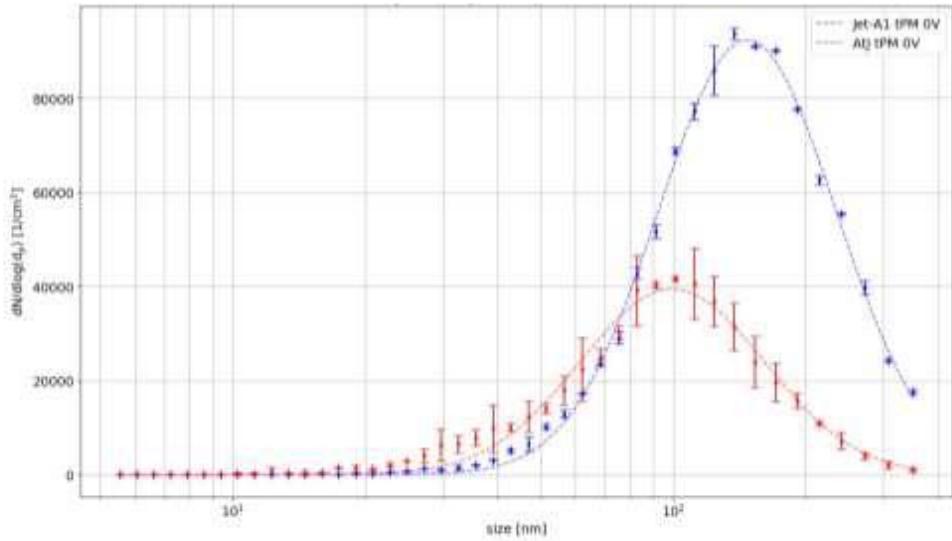


Figure 17: Total PM particle size distribution for Jet A-1 (blue) and ATJ (red) [25]

### Rig and Engine Testing

Additional studies are found in the literature which describe the impact of technology and fuel composition on emissions, with reviews of these provided in studies such as Owen et al. [26] and Moore et al. [27]. However, it is noted that many studies investigating a wide range of fuel blends are undertaken on either small-scale combustion rigs or unregulated small engines (e.g. APU's). Historically it has been difficult to source enough volume of SAF to perform test campaigns on large engines. Recently a number of studies have been performed on large engines on multiple airframes and engine OEMs. Publications from these studies is expected fairly shortly and will help to improve understanding of the impact of SAF, blends and composition on nvPM and volatile emissions.

Several examples of publicly available datasets are shown below. They all show reductions in nvPM number and mass, however, not all to the same extent and it is difficult to compare them due to caveats in the combustion source or measurement setup.

An example of a small-scale rig trial dataset is presented by Harper et al. [22] as part of the EU Horizon 2020 funded JETSCREEN programme which in agreement with other studies saw reductions in nvPM.

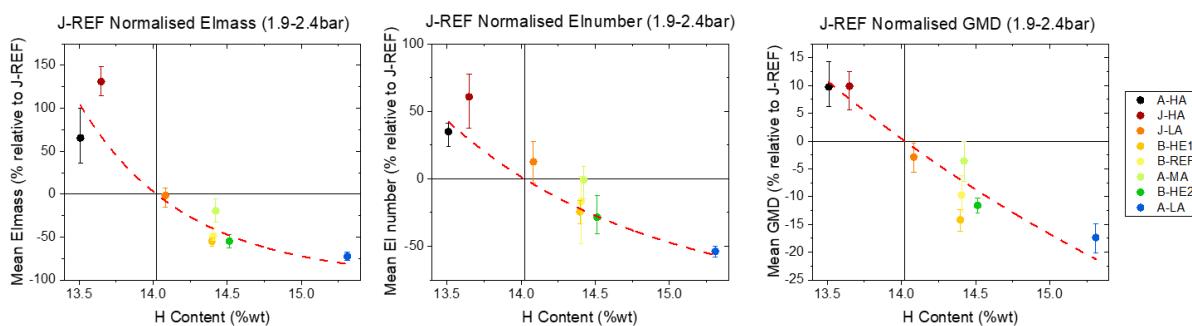


Figure 18: Example of nvPM number and mass reductions in a small-scale combustor rig [22]

Similarly, Durand et al. [23] assessed two datasets collected on the same APU.

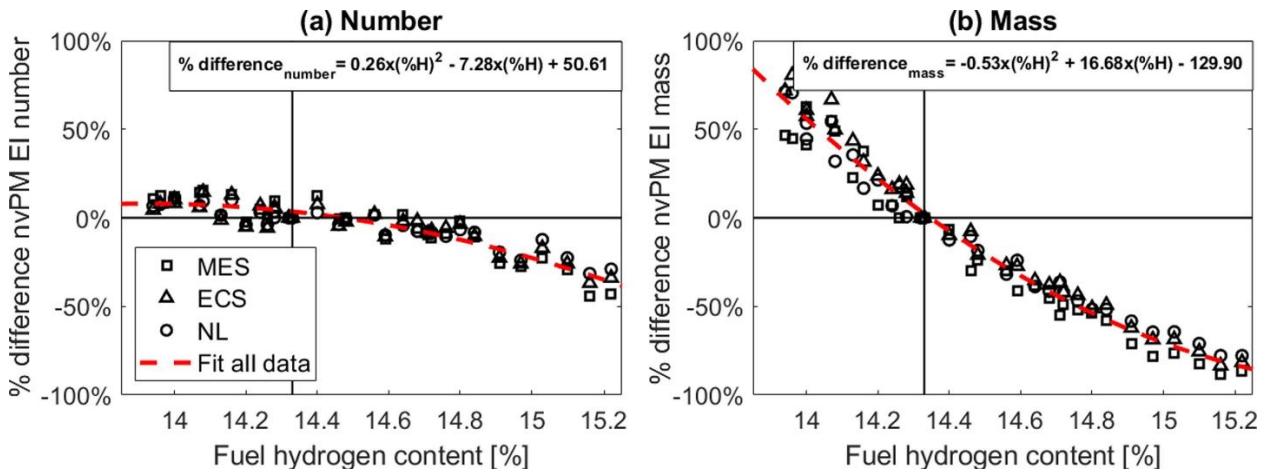


Figure 19: nvPM number and mass reductions on an APU [23]

And Schripp et al. [28] also showed reductions in nvPM mass and number on a large turbofan engine.

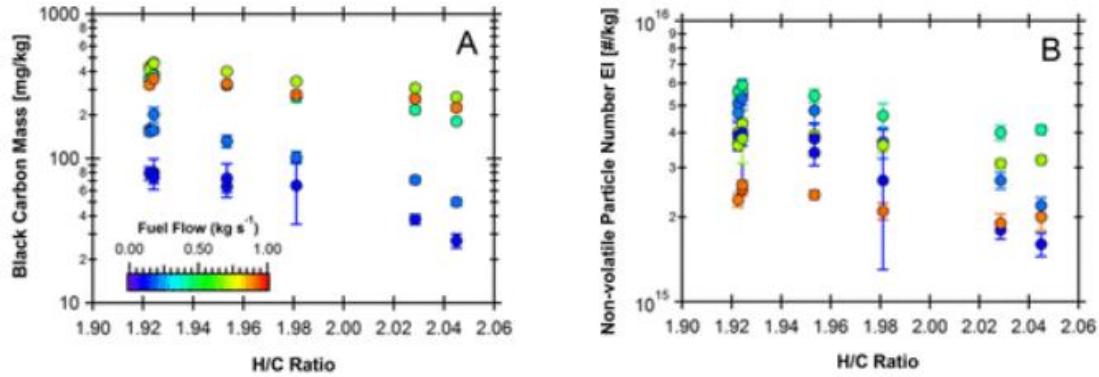


Figure 20: Reductions in nvPM mass and number at all power settings for a large turbofan engine [28]

Reductions in inflight nvPM number using SAF was observed by Voigt et al. [29].

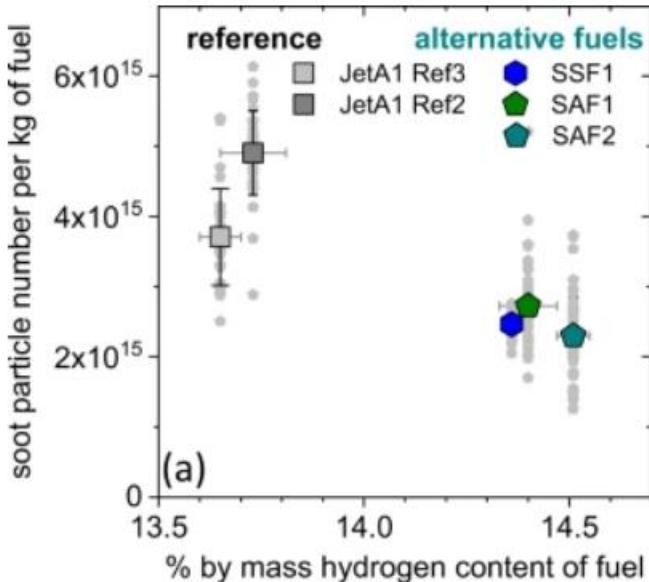


Figure 21: Inflight nvPM number emissions reduction due to SAF use in a large turbofan engine [29]

#### *Numerical predictions and validation of the impact of SAF on soot emissions*

A lab burner experiment was developed to compare the differences in soot production when Jet A-1 is replaced by ATJ. The aim of the work was:

- Gain insight on soot formation for both fuels spray flames using measurements and calculations.
- Widen the predictive capabilities of numerical tools for the use of SAF.

Evaluate and validate the numerical approaches for soot prediction in comparison with experimental data. This is made through performing Large Eddy Simulation (LES) for the same operating conditions using either Jet A-1 or ATJ

Due to data confidentiality, it is difficult to share data in this report. It is the author's opinion that the conclusions of the experiment are:

The fuel/air mixing and the flame heat release. Passing from Jet A-1 to ATJ does not modify significantly nor the spray distribution nor the flame stabilisation process. However, the different physical properties of these two fuels modify the flame heat release

The soot distribution in both cases looks similar in size with the ATJ number magnitude being significantly smaller, with averaged measured values near the detection limit. This agrees with other studies and a consequence of the different chemical composition of ATJ which as discussed exhibited a lower aromatic content and hence higher hydrogen concentration.

The use of LES for a comparative approach shows good results in the analysis of macroscopic characteristics of the flow field but is not able to correctly retrieve the reduction of soot volume fraction when Jet A-1 is replaced by ATJ. More work is needed in this area.

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