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Aviation fuel composition changes to reduce non-CO_2 emissions: European refinery impacts & effects on fuel quality

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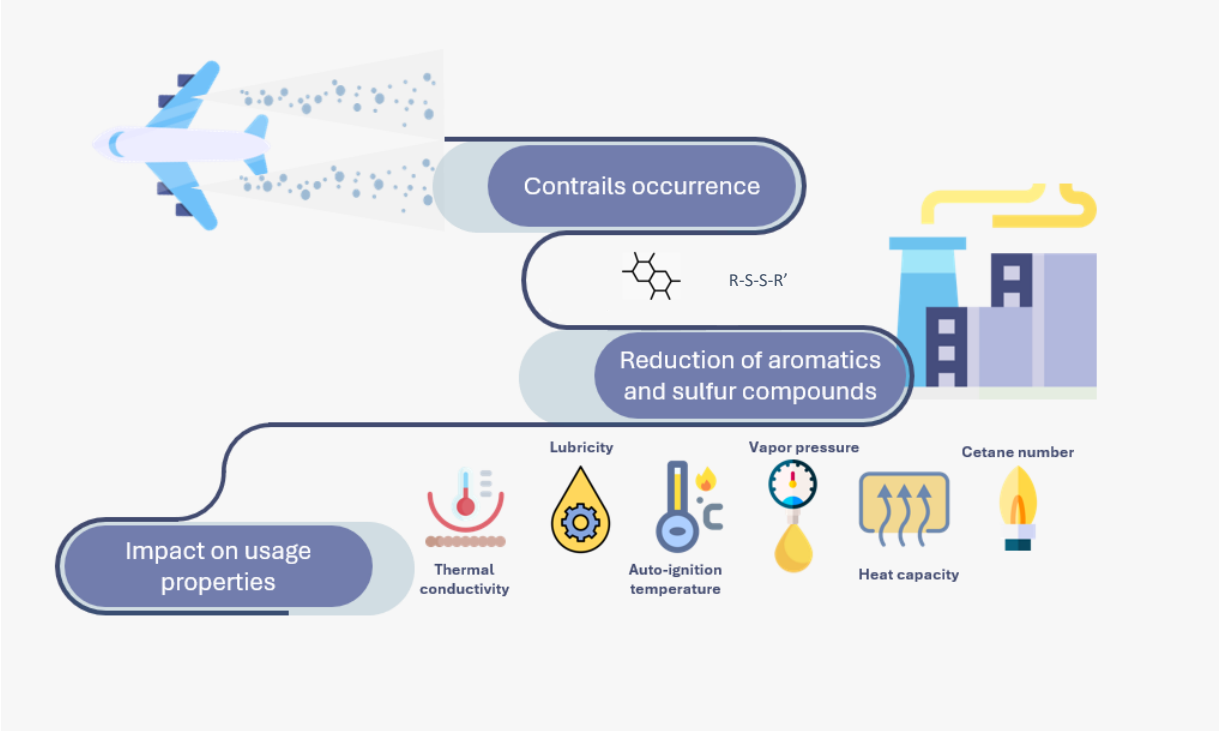

Aviation fuel composition changes to reduce non-CO_2 emissions: European refinery impacts & effects on fuel quality

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EXECUTIVE SUMMARY

In the context of ongoing research on the non-CO_2 effects of aviation on climate change and the possible actions to mitigate them, this report focuses on fuel-related impacts. These include potential benefits from the reduction of aromatics, naphthalenes and sulphur in fuel, leading to a reduction in particulate emissions which may reduce contrail formation and their persistence. Contrails form under certain conditions of air humidity and freezing temperatures in the higher troposphere or lower stratosphere. The reduction of carbon particulate emissions and possibly of contrails formation could contribute to mitigate the non-CO_2 impacts on shorter term climate change caused by aviation. This study explores the technical, economic and security of supply implications for European refineries producing aviation turbine fuels (Jet A, Jet A-1) considering hypothetical scenarios of more restrictive jet fuel specifications. The focus is on reducing levels of aromatics, naphthalenes and sulphur.

Adapting to a change in fuel specifications is not trivial: this is possible in the best case by pushing the production process to higher severity and more energy intensive operations or by constraining crude selection towards more expensive raw materials but in the worst case the only solution is large scale investment in new production units.

European refinery survey:

Based on a survey amongst Concawe's members, 31% of the EU refineries rely mainly on Merox units to produce jet fuel. This technology is unable to influence the parameters under assessment in this study and these refineries would therefore not be able to achieve any reduction in sulphur, aromatics and naphthalenes without major investments or major de-optimisation. A loss of 30% of Jet fuel production units in the EU refining system could result in security of supply issues in the EU Jet supply system, however this was not evaluated as part of this study.

Modelling the magnitude of the impact of specification changes on European refineries:

Using the data from the survey and Concawe's Linear Programming (LP) refinery model and IFPEN database, the study evaluates the capacity of the European refining system to meet progressively more stringent aviation fuel specifications using various petroleum kerosene hydrotreatment options. Results can be summarised in two groups:

[A] If the new specifications are achievable using existing hydrotreater and hydrocracker units and the Merox unit jet production is out of specification and minimised, the effects of a theoretical massive reallocation of the production would be an increase in OPEX by 0,5 – 0,9 billion EUR/y (excluding logistics and CO_2 cost) and additional CO_2 refinery emissions of 1,3 – 2,1 Mt/y (26-45 kg CO_2/ T jet).

[B] If the new specifications are so challenging that no refinery could achieve them with existing units, moving all jet production to brand new high-pressure kerosene hydrotreaters would require 5,0 – 11,8 billion EUR of CAPEX (excluding investments in an additional H_2 production plant) and the effects would be an increase in OPEX by 0,6 – 0,9 billion EUR/y (excluding logistics and CO_2 cost) and additional CO_2 refinery emissions of 1,4 - 4,5 Mt/y (30-93 kg CO_2 / T jet).

Because of the methodology used (LP model where all EU refining units are integrated in one refinery), these results are not representative of the reality for individual refineries, and the costs mentioned will be substantially underestimated in many cases.

Product Quality evaluation of reduced aromatics, naphthalenes and sulphur:

To further evaluate the product quality and fit-for-purpose implications of low aromatic and low sulphur aviation turbine fuels, this study investigates their sensitivity to selected fuel properties.

A literature review was performed, and seven properties were identified as potentially sensitive, and selected for the study: Lubricity, Derived Cetane Number (DCN), Auto-Ignition Temperature (AIT), Thermal Conductivity, Surface Tension, True Vapor Pressure (TVP), and Heat Capacity. The Dielectric constant was also noted to vary with aromatic content and important for aircraft operation but was not measured in this study.

An experimental campaign was then performed relying mainly on four jet fuels and their blends to vary total aromatics, naphthalenes and sulphur content. Of the four base fuels, two were from the market and two were obtained following mild and more severe hydrotreatment. Given the limited number of investigated blends, general conclusions may not be established. However, the fuel matrix results highlight trends that support the identification of risks or operational changes due to the reduction of aromatics, naphthalenes and sulphur content in a jet fuel. The main observations are summarised below for each fuel parameter:

Lubricity deteriorated with hydrotreatment and was particularly sensitive to naphthalene variations. At low naphthalene content, the wear scar diameter (WSD) measured closely approached the maximum WSD limit permitted by the DefStan 91-091 of 0.85mm.

Cetane number (DCN), Lubricity, Heat Capacity, and TVP were sensitive to the aromatic content. A DCN increase was observed with decreasing aromatics. Although there is no maximum limit for DCN, the values obtained with the variation were not significantly outside the range compared to the fuels surveyed in the market [1]. Regarding heat capacity, a decrease in total aromatic content reduced the heat capacity with the selected fuels. However, a comparison of heat capacity versus the temperature of a blend containing 7% total aromatics revealed a higher specific heat capacity than the average Jet A-1 market fuel survey result published in CRC 2006 [1]. A decrease in total aromatic content led to a decrease in TVP. Therefore, the reduction in total aromatics should not cause problems such as vapor lock or cavitation in the fuel pump or injectors.

Finally, lubricity and DCN are confirmed to be sensitive to sulphur content, but no clear trend was identified. A sulphur increase appears to be associated with a slight reduction in DCN. However, this trend may be influenced by other fuel parameters as no similar variation was observed with the hydrotreated fuels. Regarding Lubricity, The WSD remained about 0,2 mm below the maximum allowable limit. A more in-depth study on the effect of hydrotreating on jet fuel lubricity, and all affected fuel properties, is necessary if changes to specifications are considered. Fuel dielectric constant (permittivity) should also be featured in such studies as literature data indicates a significant influence of aromatics on this property, an attribute important for aircraft fuel gauging systems.

Neither thermal conductivity, AIT nor surface tension were measurably affected in this study by the total aromatics or naphthalene variations explored.

KEYWORDS

Non-CO_2 emissions, aviation fuels, LP Modelling, aromatics, naphthalenes, sulphur

This report is available as an Adobe pdf file on the Concawe website (www.concawe.eu).

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1. INTRODUCTION

This study is part of a larger initiative that Concawe launched to address the non-CO_2 effects of aviation fuels. The first part consisted of an extensive review[1] of the available literature on the influence of aviation fuel composition on the formation and lifetime of contrails, in the reduction of aromatics, naphthalenes and sulphur.

The second part, that is consolidated in this report, assessed the capability of the European refining system to produce Aviation turbine fuel with a lower concentration of aromatics, naphthalenes and sulphur. This study also aims to identify fuel physical and chemical properties potentially sensitive to these changes with a dedicated experimental campaign.

As a starting point to understand European refinery capabilities, a survey was conducted among Concawe members to map the available production plants and their basic characteristics.

Building on this, several theoretical scenarios with different sets of specifications in aromatics, naphthalenes and sulphur were evaluated to assess the effect of potential stepwise improvements in jet fuel quality. This study considers conventional petroleum-based jet fuel only; blending of sustainable blending components and the coprocessing of sustainable feedstocks are not considered at this stage. The ReFuelEU Aviation regulation requires 2% vol. minimum SAF at EU airports in 2025, increasing progressively to 70% vol. minimum by 2050. It is expected that this mandate will reduce overall jet fuel aromatic content over time through the use of paraffinic bio-SAF and e-SAF.

To achieve the reduction in aromatic and naphthalene content, several options for conventional petroleum kerosene processing using hydrotreatment are evaluated. These options consist of various combinations of pressure, LHSV[2] and catalyst activity. Each of these options results in different aromatics, naphthalenes and sulphur reductions, depending on the final specifications that are targeted. For each option, investment costs (CAPEX) and operating costs (OPEX) are estimated, allowing an assessment of the economic impact of the solutions on the European refining system. The extra CO_2 emissions of production due to the additional consumption of energy and hydrogen are also calculated for each option.

These findings are combined with a literature review highlighting the potential effects on jet fuel physical and chemical properties. These findings led to the blending of a fuel matrix with the three parameters variations (i.e. total aromatics < 5% vol, naphthalenes < 0,3% vol and sulphur content < 100 ppm wt). Several properties are then analysed to identify the expected trends if such a specification were to be applied.

An important disclaimer should be made before entering into the details of the assessment. The study focused only on jet fuel production at EU refineries. Europe imports yearly 10-11 Mt of aviation fuel: despite that all conclusions related to the capabilities of different technologies will be valid no matter the location of such installations, no assessment was made on the imported quality and the capabilities (and willingness) of current and potential additional importers to adapt to revised requirements.

[1] Influence of aviation fuel composition on the formation and lifetime of contrails – A literature review - Concawe

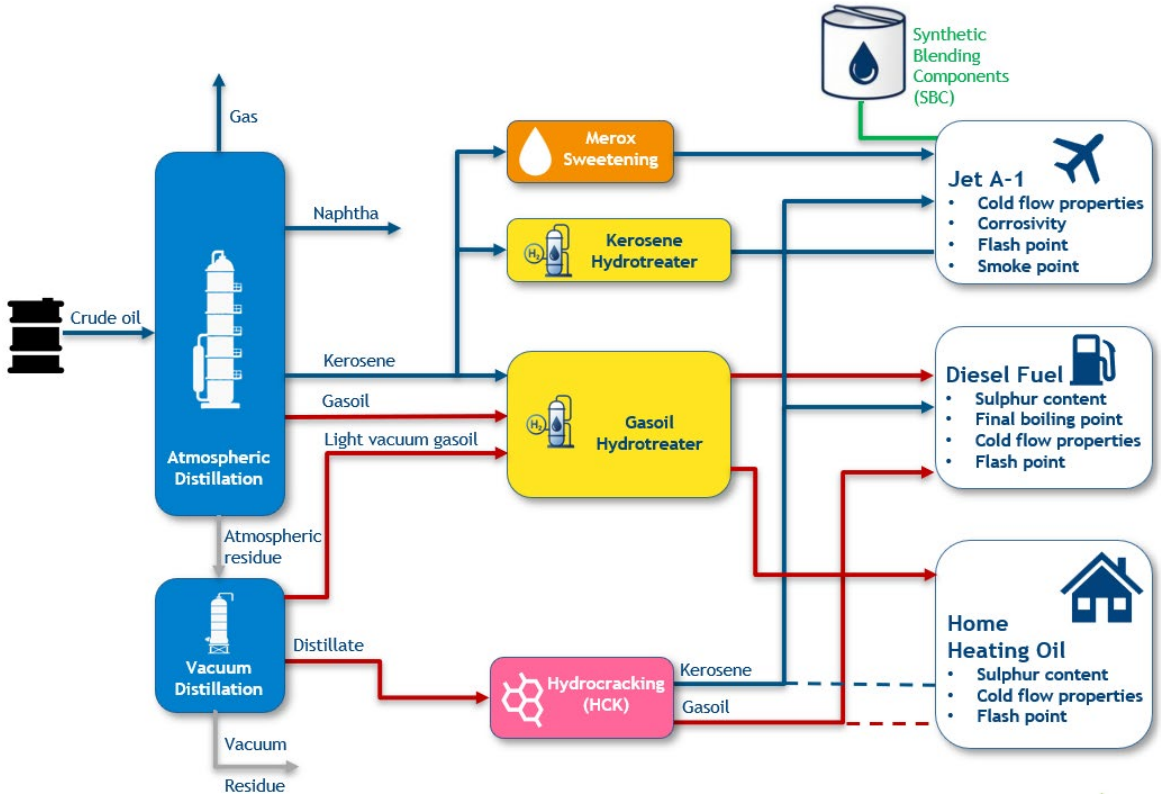
[2] Liquid hourly space velocity. It is equal to volume of feed to the process unit per hour divided by the volume of catalyst in the reactor. It is an indication of the residence time of feed in the reactor. The lower the LHSV, the higher the residence time and the higher the reactions occur.

2. IMPACTS ON EUROPEAN REFINERIES – TECHNO-ECONOMIC ASSESSMENT

2.1. SIMPLIFIED OVERVIEW OF JET FUEL PRODUCTION

When crude oil is processed in the atmospheric distillation unit (first main unit of every refinery), only around 10% of the barrel becomes kerosene, the basic component of jet fuel. This is because kerosene is a relatively narrow cut consisting of C_{10} - C_{13} hydrocarbon molecules. This straight run kerosene requires some further processing to ensure that jet fuel quality is in line with specifications, so refineries have adopted different configurations to achieve this goal.

Figure 1 *Simplified refinery scheme (focus on Jet fuel production)*



The most common contributors to jet blending are streams coming from these units:

- **"Merox" or "Sweetening" unit**
  It processes kerosene by converting mercaptans (Merox in fact stands for mercaptan oxidation), a common sulphur compound, and/or hydrogen sulphide into di-sulphides. It is a low CAPEX and OPEX process because it does not require hydrogen, but it cannot reduce the sulphur content nor affect nor improve any other property of the feedstock. Jet fuel can be produced with a Merox sweetening unit alone to meet current jet fuel specifications, and therefore many refineries only have this unit installed for jet fuel production.

- **"Hydrotreatment" or "Hydrodesulphurisation" unit (HT)**
  Hydrotreaters use hydrogen to significantly reduce sulphur of kerosene and can reach ultra-low sulphur specifications (i.e. below 10 ppm like in case of diesel). Depending on

design they can reduce naphthalenes and, to some extent, aromatics. The extent to which an existing hydrotreater could reduce aromatics will depend on its design pressure and catalyst type as main design parameters, noting that most hydrotreaters are designed for desulphurisation only. Therefore many kerosene hydrotreaters may have very limited ability to reduce aromatics. Refineries many not necessarily have a kerosene hydrotreater installed at all, or the hydrogen capacity to operate one. For refineries that have invested in kerosene hydrotreatment, sometimes a Merox unit is not used.

- **"Hydrocracker" unit (HCK)**
  Differently from the previous two units, its feedstock is not kerosene but heavier streams like vacuum gasoil. By using hydrogen and operating at higher temperatures and pressures than a hydrotreater (therefore relying on a more expensive process), this unit produces lighter and more valuable molecules, including kerosene (although usually it is not the main product as it represents only 10%-20% of the actual yield), with low sulphur and a low level of impurities. It also reduces naphthalenes and, to some extent, aromatics in a stronger way compared to a hydrotreater. Again, a refinery does not necessarily have a hydrocracker (in EU roughly 50% of refineries don't have a hydrocracker), as it represents a large capital investment that may only be feasible for some refineries.

This description highlights that each refinery can differ significantly in their capacity to produce jet fuel of varying qualities. One can therefore never give a definitive statement as to what it would cost to achieve lower aromatic, naphthalene or sulphur specifications, as each refinery would likely have to undertake varying degrees of capital investment to achieve the specification in question, which may also extend to hydrogen production capacity.

The survey of European refineries in this study will give some insight as to the differing capacities of the various refinery designs in Europe and what percentage of them could achieve increasing levels of specification severity. This study will also be useful to indicate the order of magnitude of investments required to achieve the various specification scenarios considered, but the impact on individual refineries may be more severe, possibly resulting in shut down or a decision not to produce jet fuel in certain cases.

2.2. REFINERY SURVEY AND ITS OUTCOME

Given the strong link between available units and the possibility to influence the product quality with respect to aromatics, sulphur and naphthalenes, a survey was conducted, amongst Concawe members, to collect information on their assets.

More specifically the collected information, related to 2024, covered the following items:

- refinery configuration and available units
- pressure level (for hydrotreaters and hydrocrackers only)
- typical blending recipes in 2024
- average fuel quality in 2024

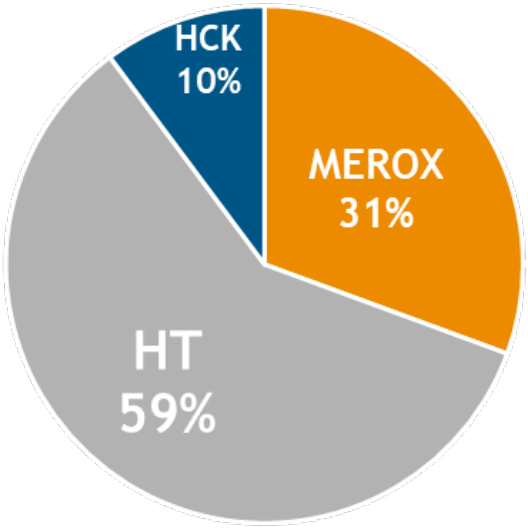
The main goal was to assess how many refineries would be capable of meeting aromatic, sulphur and naphthalene specification changes and to what extent.

Concawe received data from 49 refineries which represents 67% of the jet-producing sites in EU27+3.

2.2.1. Main unit contributing to jet production

Thanks to the data on available units and typical blending recipes, it was possible to divide the respondents into three groups according to the main components used in jet fuel production.

Figure 2 *Survey results of European refinery main jet production unit types*



Among the respondents, as exclusive or primary source of jet components (more than 60% in the final blend) the majority have hydrotreaters either fully dedicated to kerosene processing or for kerosene and gasoil treatment, 31% rely exclusively on Merox units and only 10% use mainly hydrocracker-generated components.

This Merox group raises serious concerns as 3 out of 10 sites do not have the units to influence kerosene quality with respect to aromatics, naphthalenes and sulphur and would need to resort to changing the crude oil selection (and increase the amount of light and sweet crudes) or invest in new production units to achieve a reduction in levels of these parameters.

It is important to point out that changing the crude has massive implications for a refinery: the first is the cost because it implies moving to more expensive crudes. The second is the de-optimisation of the flow of intermediate materials within the refinery and therefore the level of utilisation of secondary units, all due to one product, jet fuel, that usually represents only 10% of the total output. Economically, this might mean that the jet fuel cost recovery would have to bear the cost of the de-optimisation of the other products in addition to its own additional cost of production.

2.2.2. Alternative sets of aviation fuel specifications

To evaluate the effect of potential stepwise changes, progressive specification scenario sets have been defined. This increasing severity determines the level at which the specifications would likely trigger large investments for the European refining system.

The table below lists all the scenarios considered in this study:

***Table 1** Jet fuel specification scenarios*

Cases	Aromatic content vol%	Naphthalene content vol%	Sulphur content ppm wt
ASTM D1655[3]	≤ 25	≤ 3.0	≤ 3000
SET 1	≤ 20	≤ 0.5	≤ 1000
SET 2	≤ 16	≤ 0.4	≤ 1000
SET 3	≤ 12	≤ 0.3	≤ 1000
SET 4	≤ 8	≤ 0.2	≤ 500
SET 5	≤ 4	≤ 0.1	≤ 100

2.2.3. Current production vs alternative sets of specifications

By comparing the survey data (average produced quality in 2024) against hypothetical sets of reduced specifications, there are some important conclusions confirming the concern with "Merox only" refineries.

Reported in the table below are the sets of specifications and the percentage of refineries in each group that had jet fuel production with average quality in line with those specifications.

There is an important disclaimer to emphasise before analysing the data. The three specifications under consideration limit the maximum values of these properties but do not prescribe anything regarding average fuel quality. Comparing an average quality against a specification gives a simplified snapshot on the potential feasibility of being compliant with those limits. In real operations, qualities are measured on every individual batch of production: an average quality over time like a yearly average has no legal meaning. If specification maximum limits were reduced to the average values, assuming a normal distribution, 50% of the product volume would be out of specification. It follows that tighter specifications would very likely lead to lower jet fuel volume yields.

***Table 2** Average produced quality of jet fuel in 2024 vs fuel specifications scenarios.*

SET	SPECIFICATIONS			REFINERIES			
	ARO	NAP	SUL	MEROX	HT	HCK	TOTAL
ASTM D1655	<25 vol%	<3.0 vol%	<3000 ppm wt	100%	100%	100%	100%
SET 1	<20 vol%	<0.5 vol%	<1000 ppm wt	7%	52%	80%	41%
SET 2	<16 vol%	<0.4 vol%	<1000 ppm wt	0%	21%	60%	18%
SET 3	<12 vol%	<0.3 vol%	<1000 ppm wt	0%	0%	40%	4%
SET 4	<8 vol%	<0.2 vol%	<500 ppm wt	0%	0%	0%	0%
SET 5	<4 vol%	<0.1 vol%	<100 ppm wt	0%	0%	0%	0%

Note: all percentages are referred to the total for that group, only the last column considers all respondents.

Almost all refineries that rely on Merox are not able, even on an annual average, to produce jet fuel in compliance to the Set 1 specification and even this small reduction of sulphur, naphthalenes and aromatics would require costly and lengthy investment in new process units. This raises serious concerns about the security of supply of jet fuel in the European market that already relies significantly on imported products. Despite not being covered by this study, a

[3] In ASTM D1655 (Standard Specification for Aviation Turbine Fuels), aromatics limitations are specified as both 25% and 26.5%, depending on the testing method used: maximum of 25.0% by volume when using ASTM D1319 or ASTM D8267 and maximum of 26.5% by volume when using ASTM D6379. To avoid confusion, the study referenced only the first one.

strong reduction, on a long-term or permanent basis, of domestic production will likely bring large disruptions in the European aviation sector and reduce cost competitiveness as there is no assurance that importers will be in the position to have product in line with reduced specification in volume sufficient to continue current supply and to compensate for the reduction in domestic production.

While historical data shows that refineries with kerosene hydrotreaters and/or hydrocrackers only partially meet the Set 1 specification, it is expected that a lot of them could meet the specifications, although at a much higher cost caused by modification of the crude processed and/or by adapting their HT runs to kerosene at the cost of gasoil production.

Set 2 poses a more significant challenge and the large majority of the HT refineries would likely require investment to adapt their production.

HCK refineries are the ones which are the best suited to produce jet fuel with lower aromatics and sulphur (some achieve Set 3 specifications), however they are the least numerous.

Overall, Set 3 and beyond would need significant investment (new unit for the whole jet fuel production) for almost every refinery.

It is worth mentioning that there are instances in each group of refineries (including Merox) that show excellent performance in one specification parameter, however it is very common that the combination, when all three specification parameters are tightened at the same time, is more difficult to meet.

2.3. GENERAL METHODOLOGY OF THE ECONOMIC ASSESSMENT

As mentioned earlier, six sets of aromatic, naphthalene and sulphur specifications were assessed, ranging from those as written in DefStan 91-091 Issue 18 to some highly restrictive specifications. The compliance to the evolving jet fuel specification sets in Table 1 was evaluated through modification of operations of and/or investment in hydrotreatment units.

Despite other options being potentially available, no other technological solution was considered (e.g. dedicated hydrocracking or aromatic extraction): hydrotreating is a mature and wide-spread technology and its integration in any refinery can be commonly considered feasible, although requiring significant investment cost and additional considerations on the availability of hydrogen and utilities and other practical requirements. This decision was also taken to limit the complexity of the assessment by avoiding the introduction of a large number of additional assumptions (e.g. for aromatic extraction new products would be generated and therefore market data on demand and price would be necessary).

The Concawe LP model is used as a framework to evaluate the kerosene hydrotreatment solutions selected. This LP model optimises the economic operation of the European refining system under specific constraints. The main constraints of refining LP models are product demand, product specifications, crude slate and other feedstock availability, process unit capacities and the economic environment of the system (feed, product and utilities pricing).

The Concawe Linear Programming (LP) model was used to assess the impact in a current single refinery configuration, in which the capacities of all EU27+3 refineries have been included.

The driver for optimisation was to calculate cases that achieve an expected set of specifications for aromatics, naphthalenes and sulphur, while no properties connected to use (i.e. lubricity) were assessed. The results combine OPEX from the LP model and CAPEX provided by IFP-EN which were then reviewed by Concawe members to reach a unified economic impact assessment.

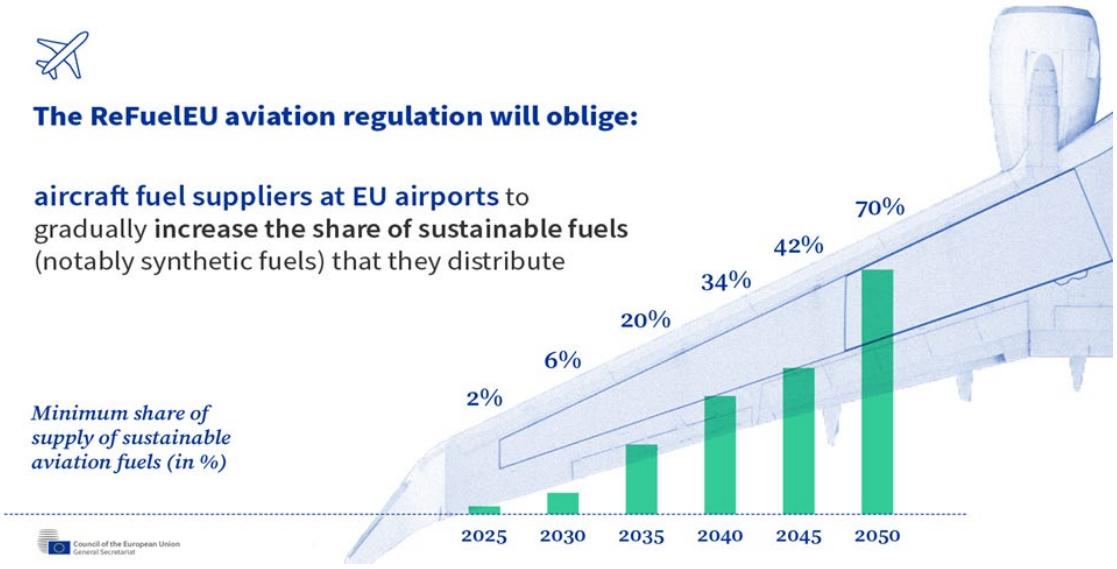
2.3.1. Synthetic Blending Components (SBC)

Before describing the economic assessment in detail, another additional important assumption needs to be presented: the focus of this study is only on conventional fossil streams. The blending of Synthetic Blend Components (SBCs) and the coprocessing of bio-feedstock to manufacture Sustainable Aviation Fuel (SAF), were not taken into account as possible solutions to lower aromatics, naphthalenes and sulphur. SAF is a general term referring to renewable jet fuel molecules derived from non-fossil sources. Specific types of these components as specified for blending in ASTM D7566 are called SBCs. Blending of paraffinic SBC's will reduce these properties significantly over time in proportion to the volumes that become available.

The availability of SBCs is growing gradually and it is fair to assume that they will play a significant role in jet fuel manufacture in the future. It is however also true that, at current or immediate future expected blending rates, their impact is marginal.

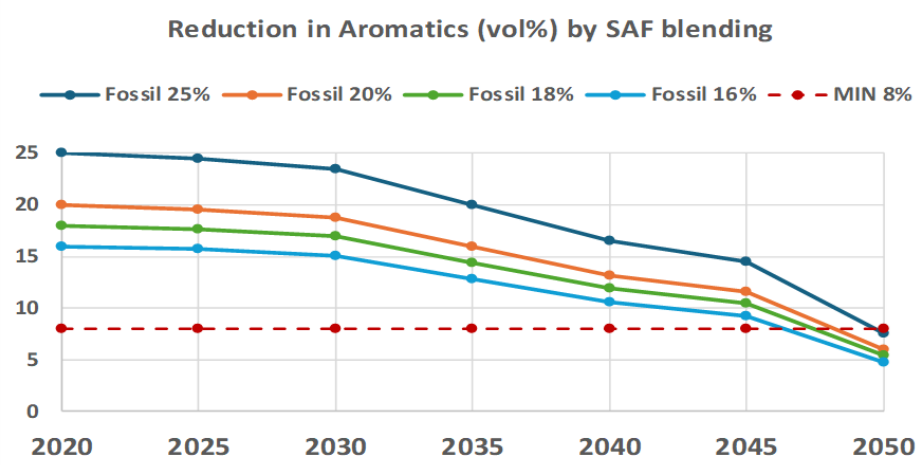
The European Union is actively promoting and regulating the use of sustainable fuels. Under ReFuelEU aviation regulation, clear SAF mandates are defined and enforced.

Figure 3 *SAF targets as per ReFuelEU aviation regulation*



The effect of the increased use of SBCs will also impact the properties of jet fuels, including those addressed by this study. Taking for example a HEFA SPK-based SBC (at the moment the most developed and most commonly available on the market) The aromatic, naphthalene and sulphur content is practically zero, so in the chart below, there is a simplified projection on the effect on the aromatic content of jet fuel assuming the fossil quality stays constant, SBCs contain no aromatics and the EU SAF mandates are achieved (this projection does not include co-processed SAF which would not necessarily reduce aromatics).

Figure 4 Projected reduction in jet fuel aromatic as SAF volumes increase



From 2035 the blended amount of SBCs has a significant contribution with a 20% reduction in aromatics compared to the original fossil blend. This effect grows significantly over time until 2050 when the overall blend will not meet the 8% minimum volume aromatics specification that is currently in place for jet fuels containing synthetic blending components (ASTM D7566). This specification also allows most SBCs to be blended up to 50% in volume, which would require a minimum aromatic content of the fossil component to be 16% in order to achieve the 8% minimum.

It follows that aromatic content will reduce anyway over time, but it is also critical that fossil jet fuel retains sufficient aromatics to enable compliant SAF blends, however this is not in the scope of this study. (Note that some SBC's may contain aromatics, but currently these are not produced in any significant volumes and are unlikely to be in the next decade at least.)

2.3.2. Hydrotreater representation

IFPEN provided a large amount of data related to Kerosene Hydrotreatment performances when processing kerosene from 6 different reference crude oils. They have evaluated 8 levels of pressure, 5 different Liquid Hourly Space Velocity and 3 levels of catalyst activity, resulting in 720 sets of data. Each set assesses the hydrotreated product qualities and the related OPEX and CAPEX.

Table 3 IFPEN data characteristics

Data sets	720
Estimated total pressure, barg	26.7 / 53.4 / 71.2 / 89.0 / 106.8 / 142.4 / 178.0 / 213.6
LHSV, hr^{-1}	0.5 / 1 / 2 / 3 / 4
Catalyst Activity	Low / Medium / High
Crude source	Arabian Light, Ekofisk, Forcados, Maya, Statfjord, Tengiz

It should be noted that the catalyst activity Low / Medium / High corresponds to different metal-based catalysts (CoMo and NiMo based).

The level chosen to define the lowest reference for pressure (26.7 barg) is representative for the actual units in operation: in the survey Concawe received, 27 out of 30 hydrotreaters had a similar pressure level. This also confirms that the first level above the base (53.4 barg) would be achievable only with the investment in a new unit as such delta level cannot be reached by revamping an existing unit or by switching a higher capability diesel hydrotreater to kerosene service, with a loss of diesel production and potential crude rate reduction.

IFPEN datasets that achieved compliance were selected for each fuel specification set listed in Table 2. Ranges of operation for the Kerosene Hydrotreatment parameters (pressure, LHSV, catalyst activity) were then defined with the resulting ranges narrowed to give realistic solutions. For example, if a targeted fuel specification set could be reached with a unit pressure of 71 barg, there is no need to evaluate a solution at 142 bar, as it will result in much higher costs that will not be compensated by improvement on the other parameters (LHSV, catalyst activity).

Given that the Concawe LP model represents the overall European crude slate through 23 crude assays, IFPEN crude dependent data (6 crude oils) cannot be used directly. Consequently, for each combination of pressure, LHSV and catalyst activity, Concawe has performed multi-linear regression on Kerosene Hydrotreatment performance (aromatics, naphthalenes and sulphur reductions, opex, capex) as a function of unit feed qualities (aromatics, naphthalenes and sulphur contents, specific gravity). These regressions shifted the focus from crude-origin dependence to dependence on kerosene quality.

These regressions are implemented in a dedicated Kerosene Hydrotreatment unit in the Concawe LP model. Practically, it is not possible to provide an optimal set of Kerosene Hydrotreatment operating parameters at this stage due to the inaccuracy of the economic impact of each independent parameter. Instead, each compliant set of parameters is evaluated separately, allowing to have a set of possible solutions with associated costs.

The final LP model results confirm a range of operation parameters which achieve the targeted specifications and allow an estimate of the corresponding costs

2.4. STUDY CASES – SPECIFICATION AND HYDROTREATMENT OPTIONS

2.4.1. Kerosene Hydrotreatment options

For each of the specification sets mentioned in table 2, several Kerosene Hydrotreatment options have been selected among the 120 combinations of Pressure, LHSV and catalyst activity provided by IFPEN. The table below lists all the combinations implemented in the Concawe LP model.

Table 4 Kerosene Hydrotreatment options

Cases	Specifications	Estimated total pressure, barg	LHSV, hr^{-1}	Catalyst activity
ASTM D1655 (current)[1] *No new units*	Aro max 25% vol Nap max 3% vol Sul max 3000 ppm wt	26.7	3.0	Low
SET 1[1] *No new units*	Aro max 20% vol Nap max 0.5% vol Sul max 1000 ppm wt	26.7	3.0	Low
SET 2[2] *No new unit but catalyst change in existing units*	Aro max 16% vol Nap max 0.4% vol Sul max 1000 ppm wt	26.7	3.0	Low
		26.7	3.0	Medium
		26.7	3.0	High
SET 3[3] *New units required*	Aro max 12% vol Nap max 0.3% vol Sul max 1000 ppm wt	26.7	0.5	Medium
		26.7	0.5	High
		53.4	3.0	Medium
		53.4	3.0	High
		53.4	4.0	High
SET 4[3] *New units required*	Aro max 8% vol Nap max 0.2% vol Sul max 500 ppm wt	53.4	1.0	Medium
		53.4	1.0	High
		71.2	2.0	Medium
		71.2	2.0	High
		89.0	3.0	Medium
		89.0	3.0	High
		106.8	4.0	Medium
		106.8	4.0	High
SET 5[3] *New units required*	Aro max 4% vol Nap max 0.1% vol Sul max 100 ppm wt	89.0	0.5	Medium
		89.0	0.5	High
		106.8	1.0	Medium
		106.8	1.0	High
		142.4	2.0	Medium
		142.4	2.0	High

[1] *No new Kerosene Hydrotreatment unit is considered, but the existing EU refining Kerosene Hydrotreatment capacity has been calibrated assuming this set of operating parameters.*

[2] *No new Kerosene Hydrotreatment unit is considered, only change of catalyst in existing EU refining Kerosene Hydrotreatment capacity.*

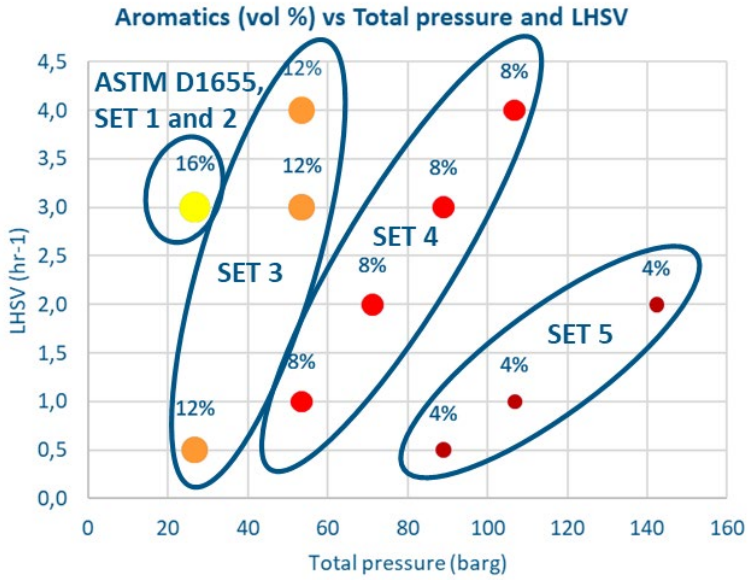
[3] *New Hydrotreatment units mandatory, in addition or to replace existing capacity.*

When new units are required (sets 3, 4 and 5), low catalyst activity is never considered, as it is most likely that Refiners will use more advanced catalysts. When medium catalyst activity is sufficient, high catalyst activity is also evaluated as the difference in catalyst cost may not be a driver in the investment decision.

Although increasing the unit pressure raises investment costs, high-pressure options with higher LHSV are still evaluated because they reduce catalyst load and, therefore, unit size.

All cases (represented by dots in Figure 4) satisfy the aviation fuel specifications of the considered set. Figure 4 shows a summary of the Kerosene Hydrotreatment conditions required to achieve the targeted specifications. Aromatic content is shown as a representative for aviation fuel specifications, as it is the most difficult quality to reach.

Figure 5 *Kerosene Hydrotreatment conditions to meet Aromatic content specifications*



2.5. RESULTS AND DISCUSSION

2.5.1. Optimisation trend

The Concawe LP model was run for each of the cases listed in table 4 The optimisation used the existing Kerosene Hydrotreatment capacity, but not necessarily to produce aviation fuel if the specification scenario was too constraining (treated kerosene can be routed to Diesel product).

Where existing unit performance was not sufficient, the optimisation allocated kerosene to the more performing but more energy intensive new unit to reach the fixed demand in aviation fuel. The utilisation of the new unit corresponded to EU required capacity investments to satisfy this 2024 level of aviation fuel demand (46.56 MTPY).

In addition to the Kerosene Hydrotreatment performance, blending of the different kerosene streams could also be optimised (high/low sulphur crude oil kerosene, Hydrocracking Kerosene, Resid Hydrocracking mainly). The impact of this blending optimisation was secondary compared to the Kerosene Hydrotreatment capacity and performance, but it could lead to potential over-optimisation for refineries where several kerosene streams are not available for blending.

It should also be noted that revamping of existing units was not considered in this study, as it would be too dependent on the precise characteristic of each individual unit.

2.5.2. Economic evaluation

The results can be summarised in two groups, according to the need of including new units.

Set 1 and 2 could be labelled as “Kerosene streams reallocation”. The two sets of specifications are achievable by existing HT and HCK units, but Merox units’ jet production is out of specification (if taken standalone) and therefore minimised. The results provided by the model may represent an answer to the question on what if production could be reallocated to those refineries with HT and HCK units.

The outcome of these calculations is:

- OPEX: +0,5 – 0,9 billion EUR/y (excluding logistics and CO_2 cost)
- Extra CO_2 refinery emissions: +1,3 – 2,1 Mt/y (26-45 kg CO_2/ T jet)

The additional OPEX costs originate from the allocation of volume from Merox unit to the more energy intensive hydrotreater and, consequently, change of the production operations and increased energy consumption. The extra emissions are linked to the increased energy requirement and the generation of additional hydrogen.

Sets 1 and 2 may be interpreted as zero CAPEX solutions (although in some cases catalyst change might be beneficial or even required), but it should be noted that what seems possible in EU average, is not possible at every single refinery level, in particular when there are no hydrotreaters available. This may have significant implications on the availability of Jet Fuels on a regional basis, including potential security of supply considerations, and would require further study. Those refineries with only Merox units would consider whether to invest into a new HT unit or to stop Jet Fuel production.

Set 3 and 4 and 5 could be labelled as “Investments in high-pressure KHT”. In these cases, almost no refinery can achieve the new set of specifications, so the only solution is to move a significant part or, in some cases, the whole production from current assets to new units. The results provided by the model may represent an answer to the question on what if all jet production would be ensured by investing in high-pressure kerosene hydrotreaters.

The outcome of these calculations is:

- CAPEX for new units: +5,0 – 11,8 billion EUR (excluding additional H2 production plant)
- OPEX: +0,6 – 0,9 billion EUR/y (excluding logistics and CO_2 cost)
- Extra CO_2 refinery emissions: +1,4 – 4,5 Mt/y (30-93 kg CO_2/ T jet)

The additional OPEX and extra emissions follow the same reasoning of the previous group. CAPEX includes estimation of ISBL (Inside Battery Limits), offsites and the first catalyst load. ISBL and offsites investments have been provided by IFPEN based on a reference capacity of 25 000 BPD and adjusted with inputs from recent projects of Concawe members. Total EU27+3 investments were estimated based on multiple units of 25 000 BPD to match the total EU capacity required to produce the quota of aviation fuel demand covered by the new units.

One should however question whether refineries would make substantial investments (several hundred million euro each) for new high pressure hydrotreaters in a market of declining fossil fuel demand because of the replacement of fossil jet fuel by SAF in compliance with ReFuelEU Aviation and other decarbonisation targets.

3. FUEL PROPERTIES EVALUATION

The previous section highlights several options to reduce aromatics and sulphur in aviation fuels. To complete this technical and economic evaluation, the objective below is to study the fuel formulation impacts on several physical and chemical properties deemed to be potentially impacted by increased hydroprocessing.

ASTM D1655 and DefStan 91-091 are the two primary technical specifications that govern the quality, safety, and composition of conventional aviation turbine fuel (jet fuel) globally. While both specifications describe essentially the same kerosene-type hydrocarbon product to ensure worldwide aircraft operability, they differ in several ways, summarised in the table below:

Table 5 Comparison between ASTM D1655 and DefStan 91-091

Feature / Property	ASTM D1655	DefStan 91-091
Fuel Grades Included	Defines both Jet A (max freeze point of -40°C) and Jet A-1 (max freeze point of -47°C).	Defines only Jet A-1 (max freeze point of -47°C).
Primary Region	United States and international markets.	UK, Europe, Middle East, Africa, and Australasia.
Conductivity & Antistatic	Static Dissipator Additive (SDA) is optional; fuel normally does not contain it unless requested.	Mandates strict conductivity requirements; SDA is standard outside the USA.
Total Acidity Level	Features a slightly higher allowable maximum limit for total acidity. Maximum 0.10 mg KOH/g.	Imposes a lower maximum limit for acidity, making it more stringent. Maximum 0.015 mg KOH/g.
Lubricity	Does not explicitly require a lubricity test for standard conventional refinery batches.	Includes a requirement for lubricity testing under specific production conditions: Measured via a BOCLE wear scar diameter limit of 0.85 mm max. Required to report percentage of non-hydro-processed, mildly hydro-processed, severely hydro-processed, synthetic components and details of the addition of additives.
Co-Processing (SAF Blends)	Historically sets standard blending limits or relies heavily on the separate ASTM D7566 for drop-in synthetic fuel blends	Recently updated to allow a up to 30% renewable co-processing (HEFA) limit to accelerate decarbonisation

Beside the specifications which mostly ensure a suitable fuel quality worldwide, ASTM D1655 and DefStan 91-091 aviation fuels are constrained in many ways. These include intrinsic “fit for purpose” properties and safety requirements which are more recently highlighted through ASTM D4054, the approval process for certification of novel synthetic fuels. The constraints also involve the aircraft itself through different systems which have been developed and optimised around a well-established petroleum jet fuel. Indeed, the latter is responsible for different functions besides the propulsion onboard. For example, lubricating high pressure fuel pumps, acting as an oil coolant and offering suitable dielectric properties for capacitance fuel gauges. In this context, any changes in the fuel composition beyond the typical aviation fuel variability should be considered with care as they could lead to impact different steps from fuel transport to flight operability.

This part of the study aims to present selected aviation fuels and a related fuel matrix to be processed and blended for an experimental campaign. A literature review is offered which presents physical and chemical properties variations when total aromatics, naphthalenes and sulphur concentrations are reduced. Finally, the experimental analysis results are presented.

3.1. FUELS AND FUEL MATRIX

3.1.1. Fuels

An experimental fuel matrix was designed to study the physical effects of total aromatics, naphthalenes and sulphur content. This matrix comprises four fuels.

Fuel 1:

Sourced directly from the market with low total aromatic and naphthalenes content.

Fuel 2:

Sourced directly from the market with typical total aromatic and naphthalenes content.

Fuel 3:

Fuel 2 following mild hydrotreatment in a pilot plant.

Fuel 4:

Fuel 2 following more severe hydrotreatment in a pilot plant.

Seven blends were then formulated based on these four fuels to target single parameter variations among:

- Total aromatics
- Naphthalenes
- Sulphur

For this study, two market fuels were selected: fuel 1 and fuel 2. Fuel 1 is characterised by its low total aromatics content of 4.5%wt and was provided by Haltermann Carless using streams to specifically target a low aromatic fuel. Fuel 2 represents a typical Jet A-1 with 19.77%wt of total aromatics and 2.77%wt of naphthalenes. The stream was obtained directly from a refinery. Fuel 2 was then used to produce two additional fuels: Fuel 3, produced by mild hydrotreatment, and Fuel 4 produced by a more severe hydrotreating. The hydrotreatment pilot plant conditions applied are detailed below. They intend to represent a typical kerosene desulphurisation unit in a refinery.

Table 6 Conditions of the hydrotreatment process

Parameter	Unit	Value
Reactor temperature	°C	230-300
Hourly volumetric flow rate	Lstd/L/h	1-4h10
ppH_2	bar	10-35

The four fuels were analysed to determine several properties listed in ASTM D1655. The results are shown in Table 7. The reduced naphthalene and sulphur content of fuel 3 and 4 demonstrate the effectiveness of the hydrotreatment.

Table 7 ASTM D 1655 specification and properties of interest of the four fuels

Property	Unit	Test methods	Limit		Fuel 1	Fuel 2	Fuel 3	Fuel 4
Density at 15°C	g/cm3	ASTM D4052		0.775 to 0.840	0.807	0.812	0.812	0.810
Distillation		ASTM D86						
10	° C		max	205	204.8	165.7	167.3	166.5
50	° C				213.9	198.7	199.4	198.9
90	° C				232.2	249	248	247.5
FBP	° C		max	300	247.1	267	266.7	266.8
Residue	% v/v		max	1.5	1	0.7	1	1.2
Loss	% v/v		max	1.5	0.4	0.8	0.1	0.1
Sulphur	ppm wt	ASTM D4294	max	3000	2.7	230.1	17.0	8.0
Freezing point	°C	ASTM D7153	max	-47	-51.0	-51.0	-50.9	-50.9
Flash point	°C	ISO 13736	min	38	68	41.5	43	43
Total aromatics	%wt	GCxGC internal*			4.5	19.8	19.7	18.6
Naphthalenes	%wt	GCxGC internal*			-	2.8	1.4	0.4
Hydrogen	%wt	GCxGC internal*			14.3	13.7	13.8	13.8
Electric conductivity	pS/m	ASTM D2624			400	5	1	2
Mercaptans	ppm	ASTM D3227	max	30		5.7	<3	<3
Viscosity at -20°C	mm2/s	ASTM D445	max	8	6.3	4.4	4.4	4.4
Smoke point	mm	ASTM D1322	min	25	37.5	22	22	23
Acid number	mgKOH/g	ASTM D 3242	max	0.015	< 0.5	0.019	0.004	0.003
Neat heat of combustion	MJ/kg	ASTM D 4529	min	42.8	43.5	43.1	43.1	43.2
Derived Cetane Number DCN	-	ASTM D 7668			52.3	42.3	44.2	43.2
Auto Ignition Temperature AIT	°C	ASTM D 659			225		235	251
Thermal conductivity	mW/K.m	ASTM D 2717			118.9			119.6
Surface tension at 25°C	mN/m	EN 14370			30.13	29.96	29.61	29.88
TVP at 25°C	kPa	ASTM D 6378				0.7		1
TVP at 38°C						1.5		1.9
TVP at 60°C						3.7		3.9
TVP at 80°C						7.6		7.6
TVP at 100°C						14.4		14.5

Heat capacity at 0°C	J/g/°C	ASTM E1269			2.06	2.14	1.86	1.81
Heat capacity at 20°C					2.15	2.25	1.93	1.87
Heat capacity at 40°C					2.25	2.37	2.00	1.95
Lubricity	mm	ASTM D5001	max	0.85	0.78	0.57	0.64	0.7

*Note: GC x GC refers to two-dimensional gas chromatography, which is a very accurate research instrument, but not a method used in jet fuel specifications.

3.1.2. Fuel matrix

The fuel matrix (Figure 6) used in the study consists of seven blends, in addition to the four fuels. The aim was to enable an independent variable analysis using at least three blends where one key property varies, while the others are held constant. To see the impact of the variation in total aromatics, Blends 3, 4, and 7 are considered, as well as Fuel 2. For the impact of the variation in naphthalenes, two sets of blends are considered. Blends 1, 2 and 3 correspond to the first set with a low total aromatic content (6 ±1%wt). Fuels 4 and 3 with blends 5, 6 and 7 comprises the second set, which has a total aromatic content in the range of 19 to 21 %wt. The remaining blends, S50 and S100, are used with fuel 2 to evaluate how sulphur content impacts the properties of interest. The physical-chemical properties of the blends are detailed in Appendix 3.

Figure 6 *Fuel matrix aiming at single parameter variations regarding the aromatic, naphthalenes and sulphur content.*

			Naphthalenes (%wt)						
			0.1	0.5	1	2	2.5-3		
Total aromatics (%wt)	4		fuel 1						
		Naphthalenes (%wt)	0.0						
		Aromatics (%wt)	4.5						
		Sulphur (ppm)	2.7						
	6		blend 1	blend 2					blend 3
		Naphthalenes (%wt)	0.00	0.5					3
		Aromatics (%wt)	7	6					7
		Sulphur (ppm)	2.7	2.7					2.6
	11								blend 4
		Naphthalenes (%wt)							3
		Aromatics (%wt)							11
		Sulphur (ppm)							2.7
	18-21			fuel 4	fuel 3	blend 5		blend 6	blend 7
		Naphthalenes (%wt)		0.4	1	2		3	3
		Aromatics (%wt)		19	20	20		21	21
		Sulphur (ppm)		8.0	17.0	16.9		2.6	16.8
							S50	S100	fuel 2
		Naphthalenes (%wt)					2	3	3
		Aromatics (%wt)					21	20	20
		Sulphur (ppm)					46.7	100.5	230.1

The different blends were formulated by mixing one of the four fuels with aromatic solvents depending on the target. **Table *8*** shows the mass fractions of each component for each blend. The total aromatic content was targeted by using solvents Solvesso 100 and 150. Meanwhile, Solvesso 200 and a naphthalene blend made of 50/50 %vol naphthalene/2-methyl naphthalene were used to vary the naphthalene content.
For the evolution of sulphur content, Fuel 2 and 3 were blended (note that Fuel 3 comes from mild hydrotreatment of fuel 2). This strategy was chosen to avoid mixing fuels that differ significantly in composition.

Table 8 *Mass fraction of fuels and solvents used for each blend.*

Blend	fuel 1	fuel 2	fuel 3	Solvesso 100	Solvesso 150	Solvesso 200	Naphthalene blend*	Aromatics (%wt)	Naphthalenes (%wt)	Sulphur (ppm)
1	98%	-	-	2%	0%	0%	0%	6.6	-	2.7
2	98%	-	-	1%	0%	1%	0%	6.0	0.5	2.7
3	97%	-	-	0%	0%	0%	3%	7.2	2.9	2.6
4	93%	-	-	0%	3%	4%	0%	11.1	3.2	2.7
5	-	-	99%	-	-	-	1%	20.5	2.3	16.9
6	83%	-	-	14%	0%	0%	3%	20.7	2.9	2.6
7	-	-	98%	-	-	-	2%	21.1	3.1	16.8
S50	-	39%	60%	-	-	1%	-	20.5	2.5	46.7
S100	-	14%	85%	-	-	1%	-	20.3	2.6	100.5

* 50/50 %vol naphthalene/2 -methyl naphthalene

Only Blend 5 and 7 were formulated using fuel 3 derived from the hydrotreatment of fuel 2. Their composition, especially the aromatic chemistry, differs from the blends formulated with fuel 1. This distinction will be considered in the analysis of the results.

Given the limited number of blends investigated, definitive conclusions may not be established. However, the primary objective of the fuel matrix is to identify key trends that can guide discussion about the potential impact of reducing aromatics, naphthalenes and sulphur content in a petroleum Jet A-1, should such a pathway be explored. Accordingly, the fuel matrix included both market fuels and compositional variation tailored to enable this type of analysis.

3.2. LITERATURE REVIEW OF SELECTED PROPERTIES

3.2.1. Fit for purpose and safety properties

Identification of relevant properties to evaluate the impact of total aromatics, naphthalene and sulphur content was based on the properties listed in ASTM D1655 and tier 2 of the ASTM D4054 standard, also named “fit for purpose properties”. Both standards are necessary for evaluating changes to aviation fuel. ASTM D1655 specifies the requirements for petroleum fuels such as Jet A-1 for flight while ASTM D4054 provides a framework for the approval of new production processes or new additives. The analysis of listed properties in these standards is essential to assess the fuel composition with the operational and safety behaviour.

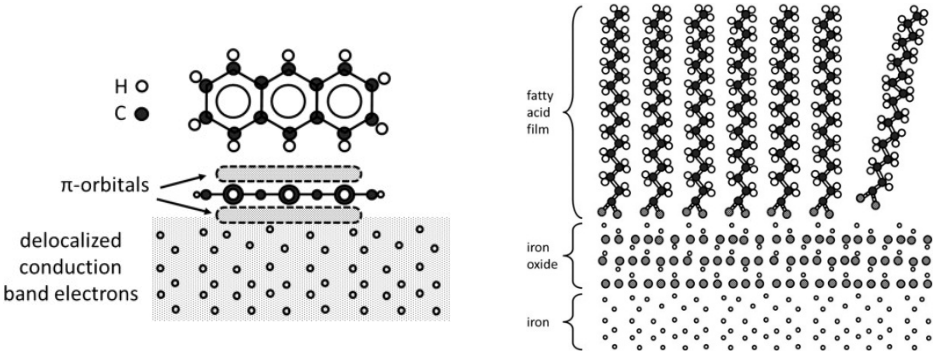
To identify relevant properties to be investigated, a literature review was conducted. This review evaluated the impact of total aromatics, naphthalenes and sulphur content on these properties.

3.2.2. Lubricity

Lubricity is the ability of a fuel to reduce friction and wear between two moving surfaces. This property ensures the proper functioning and durability of fuel system components. Low lubricity can lead to premature wear in the fuel system, particularly in high-pressure pumps and injectors [2]. This wear increases the frequency of maintenance, leading to higher operational costs. More importantly, component failure may compromise flight safety and engine reliability.

The protection of two metal surfaces in contact is based on the formation of a protective layer, either from molecules naturally present in the fuel or through the addition of a lubricity improver additive. In additive-free kerosene, this layer is mainly formed by heavy aromatic compounds [3] which have delocalised π orbitals capable of interacting with the conduction electrons of metal surfaces, promoting their adsorption [4] (*Figure 7*). Lubricity improver additives, such as fatty acids and their derivatives, as well as inorganic additives such as zinc dialkyldithiophosphates, used as extreme pressure additives [5] may be used as guided in specifications with OEM approval. These additives have a polar head containing heteroatoms (N, O or S) that allow them to adsorb onto the oxidised layer of the metal, while their non-polar chain ensures the formation of a protective film [4] (Figure 7).

Figure 7 *Mechanism of protective layer formation by aromatics (left) and molecules contain heteroatoms (right) [4]*



During hydroprocessing, sulphur, nitrogen and oxygen compounds that may be present in trace amounts in Jet A-1 are removed, leading to a decrease in the intrinsic lubricity of the fuel. Therefore, lubricity improvers may be necessary to enhance the fuel lubricity, but this is not without additional risks to manage. Unnecessary or excessive hydroprocessing is therefore not advisable in the production of aviation fuel.

DefStan 91-091 Issue 17, F.3.2 states that the chemical and physical properties of jet fuel cause it to be a relatively poor lubricating material under high temperature and high load conditions. Severe hydroprocessing removes trace components, resulting in fuels which tend to have a lower lubricity than straight-run or wet-treated fuels. Lubricity improver additives are widely used in military jet fuels. They have been used occasionally in civil jet fuel to overcome aircraft problems, but only as a temporary remedy while improvements to the fuel system components or changes to fuel were achieved. Because of their polar nature, these additives can have adverse effects on ground-based filtration systems and on fuel/water separation characteristics.

It should also be noted that DefStan 91-091 also has a requirement to report composition of the fuel in terms of the percentage volume of non-hydroprocessed, mildly hydroprocessed, severely hydro-processed and synthetic blend components. Severely hydro-processed components are defined as petroleum derived hydrocarbons that have been subjected to a hydrogen partial pressure of greater than 7000 kPa during manufacture. The requirement to determine lubricity applies only to fuels whose composition is made up of less than 5% non-hydroprocessed components and at least 20% severely hydroprocessed components or includes synthetic components. Fuels exceeding the maximum allowable lubricity wear scar diameter of 0.85mm would then require approved lubricity improver additives. (Table 1, Note 7, 18 DefStan 91-091)

In military aviation, certain Lubricity Improver Additives (LIA) or dual-purpose Corrosion Inhibitor/Lubricity Improver (CI/LI) additives are allowed, these are strictly evaluated and approved by aircraft and engine Original Equipment Manufacturers (OEMs). For example, such additives carry the NATO code S-1747, and the governing specification for lubricity improvers is MIL-PRF-25017.

It is important to note that additives which carry the NATO code S-1750 are part of the NATO single fuel concept. Additive group S-1750 is strictly for ground use only (eg: diesel engines). **It must not be used for aircraft.**

For civil aviation turbine fuels like Jet A and Jet A-1 (which are also widely used by international military forces as F-35), the allowable additives are controlled by Annex A of Def Stan 91-091 and Table 2 of ASTM D1655.

- Fuel suppliers can only use LIAs specifically named in these annexes.
- Approved formulations typically match those on the military QPL-25017 list (such as DCI-4A, Nalco 5403, and HiTEC 580) because they have gone through rigorous joint OEM and industry testing frameworks like ASTM D4054.
- Severe Hydroprocessing & Synthetics: Aviation specifications do not require lubricity additives for all batches. They are mandatory primarily at the point of manufacture for fuels containing synthetic components or heavily hydroprocessed materials where natural lubricants have been stripped out. [1]
- Strict Dosage Caps: In commercial and military aviation specifications, these additives have narrow concentration envelopes (typically ranging from a minimum effective dose up to a maximum limit, usually capping out near 54 g/m^3 or 24 mg/L depending on the specific product). Exceeding this cap is forbidden because it degrades the fuel's water-separation properties.

Lubricity additive use must strictly follow the relevant specifications and any additive not specified cannot be considered for use until such time as it is listed in the governing specification. However for the purpose of technical understanding, some relevant literature is described below: Other studies conducted on hydrotreated aviation fuels have shown that adding corrosion inhibitors containing fatty acid dimers (e.g., dimerised linoleic acid) can also improve lubricity [6], [7]. Ababneh et al. [8] demonstrated that the addition of 50 ppm of linoleic acid into paraffinic kerosene, led to an almost 50% reduction in the Wear Scar Diameter (WSD). Anastopoulos et al. [9] evaluated the lubricity effect of several esters on JP8, showing that adding

750 to 1500ppm reduced the WSD to around 460 µm, in compliance with the EN 590 standard. On the other hand, Karonis et al. [10] focused on F-34 military kerosene and found that adding up to 0.4%v/v of any texted biodiesel reduced WSD below 460µm.

Lubricity evaluation for low-sulphur diesel applications has been widely studied through the analysis of physical and chemical fuel properties. Wang and Cusamo [11] highlighted that the lubricity of low sulphur fuels is determined primarily by the viscosity and the di-aromatic (napthaleninc) content. Lacey et al. [12] conducted a survey on the lubricity of military fuels using the BOCLE method. They found that the fuel lubricity without additives was generally related to the levels of di- and poly-aromatic compounds, while viscosity demonstrated a weaker relationship. J. K. Appeldoorn et al. [2], reported that the addition of mono-aromatics reduces the wear scar diameter (WSD) and improves lubricity. This reduction is even more pronounced when naphthalenes are added. These findings are consistent with the results presented by Appeldoorn and Tao showing that 2% of heavy aromatics can reduce wear and friction. Moreover they showed an improvement in lubricity for aviation fuels thanks to a synergistic effect between trace oxygen and water with heavy aromatic hydrocarbons [3].

Hence, reducing the total aromatics content in petroleum aviation fuels may show negative effects in lubricity. While more recent research indicates that wear scar diameter can be estimated from kinematic viscosity, nitrogen content, and cycloparaffin concentration [13]. Barbour et al. also note that minor oxygen and nitrogen containing compounds contribute to improved lubricity in petroleum distillate fuels [14]. This finding aligns with earlier work by Wei and Spikes, who reported a reduction in HFRR wear scar diameters when 8-hydroxyquinoline and 1,4-hydroquinone were added as model compounds to a hydrotreated fuel [15].

The impact of sulphur compounds has been also studied [2]. A concentration of 500 ppm of heavy mercaptans (C_{18}) leads to a reduction of the WSD by approximatively 0.15 mm.

Consequently, lubricity is a critical property when considering aviation fuel hydroprocessing and will be analysed in this study to assess the impact of low-level sulphur concentrations, as well as the total aromatics and naphthalene variation.

3.2.3. True vapour pressure (TVP)

The vapour pressure refers to the pressure exerted by the fuel vapour in a thermodynamic equilibrium with its liquid at a given temperature. The true vapour pressure of a complex blend, such as jet A-1, is defined as the pressure exerted as this vapour/liquid ratio approaches zero [16]. A high TVP indicates a more volatile fuel.
Volatility is an important property as it is directly linked to proper functioning of fuel pumps and injectors. Under reduced pressure conditions, such as those encountered during flight, a fuel with a high vapour pressure, will evaporate even more easily. This may cause vapour lock or cavitation in the fuel pump or injectors [16],compromising their mechanical and operational functionality and the overall engine performance.

J. T Edwards et al. [17] indicate that certain aromatics exhibit vapour pressures values at 100°C similar to iso-paraffinic compounds. Despite the lack of a clear trend between aromatic content and vapour pressure, it was considered prudent to investigate the impact of aromatics on vapour pressure in this study. When referring to “aromatics”, it denotes a blend of molecules which have a carbon number ranging mainly from C8 to C12 and comprising mono-aromatics and polyaromatics structures.

3.2.4. Flash point

Volatility and flash point are closely related properties. While volatility describes how easily the fuel evaporates, flash point describes the lowest temperature at which the fuel vapour ignites

under an ignition source, such as a spark or flame. In general, as volatility increases, flash point decreases. Therefore, it is crucial to find a compromise between volatility to ensure proper engine and on-board systems operations while maintaining a flash point high enough to avoid any explosion hazard.

In the literature, M. Braun-Unkhoff et al. [18], showed that different molecular families, such as n-paraffins, iso-paraffins and naphthenes and alkyl mono-aromatics exhibit similar behaviour for the flash points. For all the chemical families, an increase in the carbon number leads to an increase in flash point, reflecting a decrease in volatility as molecular weight increases.

When considering complex blends [19], rather than pure compounds, an increase of 15% of low molecular weight aromatics compound such as styrene in a synthetic paraffin kerosene, decreases the flash point up to the ASTM D1655 limit of 38 °C. In contrast, a heavier aromatic solvent (C9-C11) contributes to slightly increase the flash point. The increase in the heavier aromatic solvent concentration, revealed no observable effect, as the response of different concentrations reached a plateau. This indicates that naphthalenes have little to no impact in contrast of mono-aromatics. Since flash point is related to volatility and the TVP was characterised, the flash point was not included in this study.

3.2.5. Freezing point

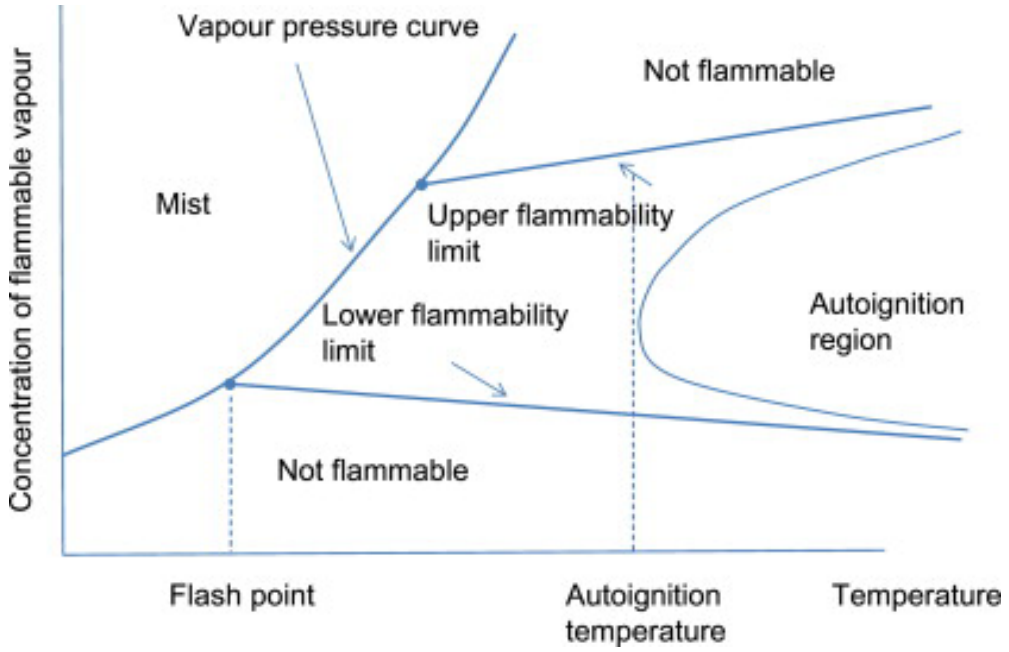
The freezing point represents the lowest temperature at which the fuel remains liquid and free of crystals. It is a critical safety property, since aircraft filters and fuel system pipes might clog due to low temperatures at high altitude (around -40°C), potentially leading to engine failure or reduced performance [16].

H. Kittel et al. [20], found that the freezing point tends to decrease with an increase in aromatic content. However, I. A. Al-Nuaimi et al. [19] suggested there is no significant difference between mono-aromatics and naphthalenes at the same concentration.
While reducing the aromatic content may negatively affect the freezing point, it has not been characterised in this study. Technical solutions commonly used in practice, can effectively prevent filter and fuel line clogging. In aircraft equipped with a heat exchanger, solidified molecules are melted, ensuring continuous fuel flow. In the absence of the heat exchangers, fuel system icing inhibitors may be used.

3.2.6. Auto-ignition temperature (AIT) – ASTM E659

The auto-ignition temperature (AIT) represents the lowest temperature at atmospheric pressure at which the vapour of a fuel spontaneously and without a source of ignition, ignites (Figure 8). A fuel with a low AIT can ignite prematurely, even before the correct combustion zone. This pre-ignition leads to the reduction of efficiency and potential damage of the fuel system or the engine [21]. It is also an important property for risk-free handling procedures, and in aircraft tank design as it can affect accidents related to the ignition of fuel within the fuel tank. Maintaining the AIT above 204°C [22] [23] is essential to ensure safe operation and efficient combustion.

Figure 8 Relationship between vapour concentration, temperature and auto-ignition temperature [24]



M. Braun-Unkhoff et al. [18] showed the behaviour of pure molecules from different hydrocarbon families present in petroleum Jet A-1. The results indicate the AIT decreases when the carbon number increases as well as a variation among the molecular structure. Mono and di-aromatics tend to exhibit the highest AITs among the other chemical families, followed by cycloalkanes [25]. This suggests that the presence of aromatics (or potentially cycloalkanes) is necessary to avoid any safety hazard. However, the related concentration remains to be assessed, and it may be affected by the base fuel composition due to complex reaction schemes. This is therefore an important property to consider.

3.2.7. Derived cetane number

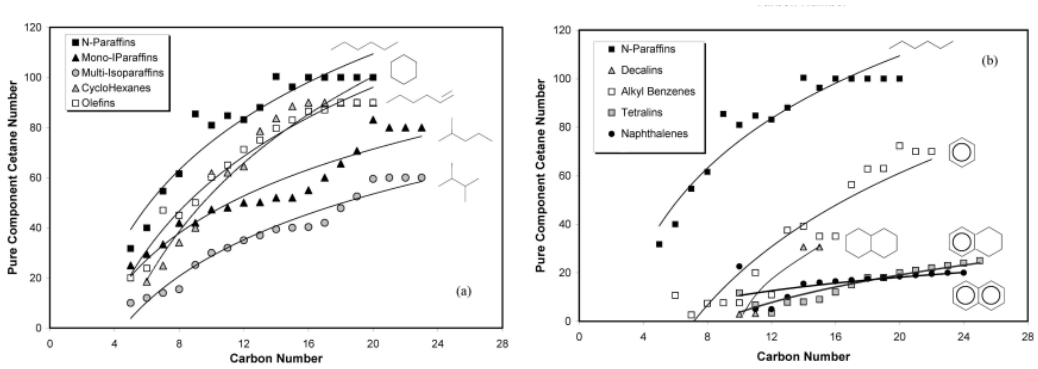
The derived cetane number (DCN) is a parameter used to characterize the auto-ignition quality of a fuel, particularly for compression ignition engines (diesel). It provides an estimate of how easily a fuel will ignite under pressure. Higher DCN values indicate shorter ignition delays and better auto-ignition.

Even though DCN is widely used in diesel application, it is not a common property controlled for aviation applications. For ground applications, a high DCN enhances cold start performance by ensuring ignition under low-temperature conditions.
For aviation applications, N. Rock et al. [26] reported that fuels with higher DCN provide greater resistance to lean blow-out (LBO) and its recovery. These phenomena are critical to maintain a stable combustion at low fuel-air ratios encountered in modern turbine engines.

The literature on pure molecules reveals distinct DCN behaviour across different chemical families [27]. DCN increases with carbon chain length and varies among molecular structures. Naphthalenes exhibit the lowest cetane numbers (
), followed by naphteno-aromatics compounds. These are then followed by tretralins and mono aromatics. It is important to note that aromatics containing between 12 to 16 carbons generally

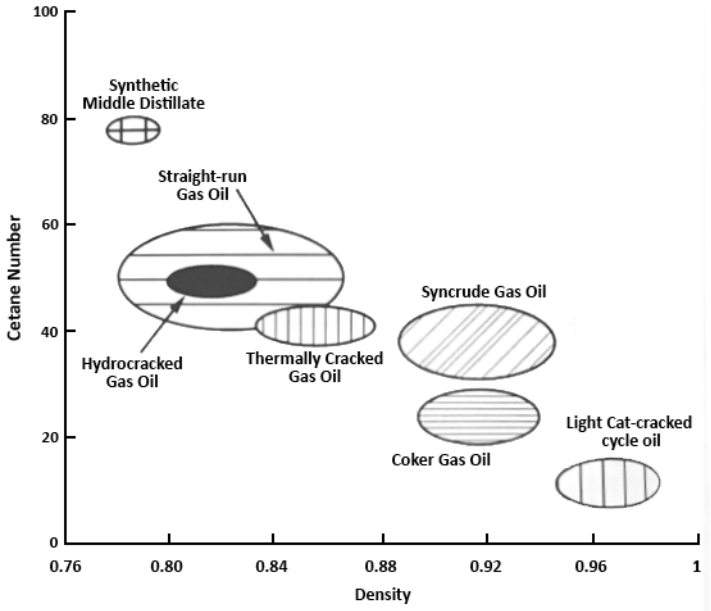
show cetane numbers of approximately 25-50. In contrast, n-paraffins present the highest cetane numbers, followed by naphthenes and then iso-paraffins.

Figure 9 *Cetane number of pure compounds [28]*



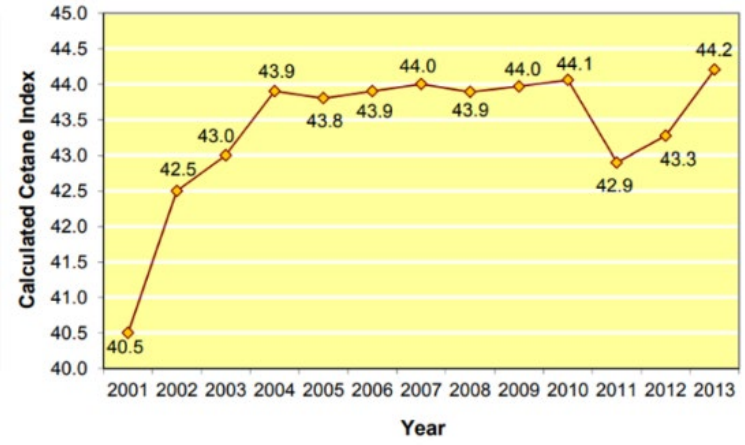
N. Brassart et al.[29] suggested that mono- and di-aromatics do not significantly impact the cetane number of a blend compare to n-paraffins, which have a strong positive impact. Additionally, it is also suggested that sulphur content may also play a role in cetane enhancement. Since DCN is not specified for petroleum aviation fuels, its characterisation in this study will be performed.

Figure 10 *Density/cetane number relationship as a function of production unit [30]*



Given the strong correlation between the calculated cetane index (ASTM D4737) and the derived cetane number (DCN), the average cetane number of 45 for JP-8 (Jet A) (Figure 11) will be adopted for comparative analysis.

Figure 11 Cetane number evolution of the JP-8 cetane number over several years [31]



3.2.8. Density

Fuel density is a key property that defines the mass of fuel per unit volume. This property is used in aircraft's weight calculation and tank design [32].

According to the findings of M. Braun-Unkhoff et al. [18], mono-aromatics and naphthalenes as pure compounds exhibit densities higher than the Jet A-1 maximum specification allows. When these components are incorporated into blends [19] no major difference is observed between low molecular weight aromatic and high molecular weight aromatics (C9+). However, data from H. Kittel et al. [20] reveals an increase of the density with the increase of aromatic content as expected. For reduced aromatics, the density may start to fall outside the lower limit of 775 kg/m3. The 8% minimum aromatic specification for SAF blends in noteworthy in this context also. This has not been specifically evaluated in the present study.

3.2.9. Specific energy and energy density

The specific energy, usually expressed in MJ/kg, refers to the amount of energy stored per unit of mass. The energy density, typically in MJ/L refers to the amount of energy stored per unit of volume. These properties are important since both affect the useful capacity of an aircraft [33]. A higher specific energy means less fuel mass required for the same amount of energy. This reduces the overall weight of the aircraft. Meanwhile, higher energy density allows more energy to be stored in a given tank. This is an important parameter to consider when designing the tank of the aircraft or when volume-limited aircraft are used, for military purposes for example.

In the literature, M. Braun-Unkhoffe al. [18], demonstrate for pure compounds, that mono-aromatics are the only chemical family present in Jet A-1 whose specific energy falls below the minimum specific energy requires in ASTM D 1655, of 42.8 MJ/kg. Furthermore, H. Kittel et al. [20], showed in complex blends, that reducing the aromatic content increases the specific energy. However, by reducing aromatic content, the energy density tends to decrease, resulting in a greater volume of fuel being required to cover the same distance.
H. Kittel et al. [20] results also revealed that a variation of up to 60% of aromatics leads to a variation of approximately 2.5 MJ/kg in specific energy and 2.5 MJ/L in energy density. However, the expected change in aromatic content in this study is much lower than this which does not require - further investigation of this property to what is in the literature.

3.2.10. Heat capacity

Heat capacity, also known as the specific heat, is defined as the amount of heat in Joules required to raise the temperature of a 1g substance by 1°C without phase change [34]. For fuels, a high heat capacity means that the fuel can absorb more thermal energy without a significant increase in temperature which is beneficial for aviation applications since the fuels is also used as a coolant that controls thermal loads [35].

Research conducted by T. J. Fortin et al.[35], with different fuels showed that the heat capacity tends to decrease as the aromatic content increases. In other words, an increase of aromatic content, tends to reduce the ability of the fuel to absorb heat effectively. However, no clear trend has been observed between heat capacity and naphthalene content. Therefore, reducing the aromatic content in fuels could enhance their heat transfer capacity and improve their efficiency in absorbing and transferring heat within the cooling system.

3.2.11.Thermal conductivity

Thermal conductivity is a property that refers to the ability of a fluid to conduct heat through conduction. For liquid fuels, this property is used to calculate heat transfer to maintain uniform temperature distribution within the system [36]. A low thermal conductivity leads to poor heat distribution, which can result in local overheating of on-board components in contact with the fuel, potentially affecting their operational functionality [37]. At low temperature, poor thermal conductivity may also cause cold spots within the fuel system. Increasing the risk of crystal formation and eventually pipelines and filter blocking.

According to W. A. Malatesta et al. [36] findings, thermal conductivity tends to increase with the aromatic content in Jet A-1. The measurements were performed using ASTM D7896, which shows a repeatability values below 0.003 W/m.K for different reference heat-transfer fluids such as glycerine, ethylene glycol and Syltherm WTL. Although these repeatability values are not established specifically for kerosene fuels, the repeatability for the fuels is likely of the same order of magnitude. Consequently, the observed variation of 0.006 W/m.K measured by Malatesta et al. remains consistent with the variability of the method. Therefore, reducing the aromatics may lead to a slight degradation of thermal conductivity, possibly with no measurable variation. Since no data was found in the literature between naphthalenes and thermal conductivity, this property will be studied. In addition, whether the naphthalenes or aromatics will exhibit the same trend even if their concentrations are reduced remains to be studied.

3.2.12.Dielectric permittivity

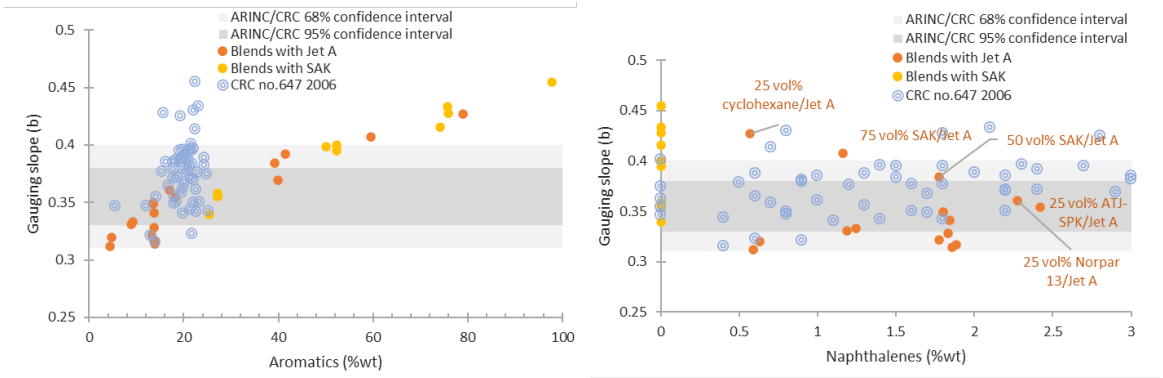
Dielectric permittivity or dielectric constant describes the ability of a material to store electrical energy in an electric field. In the aviation sector, it is used for fuel gauging during flights. However, if a variation in composition induces a variation in permittivity, the fuel gauge could provide an inaccurate reading.

Recent results from Z. Yang et al. [38], showed that aromatics and naphthalenes can have higher and lower permittivity than the average permittivity of the CRC survey 2006 [1]. Aromatics with a strong dipole moment tend to show high permittivity, while those with a weak dipole moment show values lower that the average for Jet A-1. However, these results are based on pure compounds.

Kosir et al.[39] measured permittivity and density for several fuel blends. They found that alkylbenzenes and non-alkylated aromatics exhibit a positive correlation with the gauging slope, whereas linear, iso and cycloparaffins exhibit a negative correlation. These data, together with the GCxGC results shared by Kosir et al.[39] were used to calculate the gauging slope according

to the Clausius-Mossotti equation. The resulting slopes were plotted against total aromatics and naphthalenes content (*Figure 12*).

Figure 12 *Gauging slope of various blends against total aromatics (left) and naphthalenes (right), data from [39]*



Two groups of blends are observed, those containing Jet A and those containing Synthetic Aromatic Kerosene (SAK) (*Table 9*). The slope variation with naphthalenes shows two distinct trends. For some blends, the slope decreases with increasing naphthalenes content, while it increases for others. This suggests that the influence of naphthalenes on the gauging slope is limited on its own and depends on the presence and proportion of other chemical families in the fuel. In contrast, the gauging slope decreases with decreasing total aromatic. However, based on the CRC 2006 data, the trend is no longer evident specially around 20%wt aromatic content.

Table 9 *Evaluated fuel blends tested by Kosir et al.[39].*

Fuels blended with Jet A	Fuels blended with SAK
25 vol% ATJ-SPK/Jet A	25 vol% HEFA-SPK/SAK
50 vol% ATJ-SPK/Jet A	50 vol% HEFA-SPK/SAK
75 vol% ATJ-SPK/Jet A	75 vol% HEFA-SPK/SAK
25 vol% CPK/Jet A	25 vol% ATK-SPK/SAK
50 vol% CPK/Jet A	50 vol% ATK-SPK/SAK
75 vol% CPK/Jet A	75 vol% ATK-SPK/SAK
25 vol% SAK/Jet A	25 vol% CPK/SAK
50 vol% SAK/Jet A	50 vol% CPK/SAK
75 vol% SAK/Jet A	75 vol% CPK/SAK
25 vol% cyclohexane/Jet A	SAK
25 vol% cyclooctane/Jet A	
25 vol% decalin/Jet A	
5 vol% adamantane/Jet A	
25 vol% Norpar 13/Jet A	
25 vol% Isopar M/Jet A	
25 vol% Aromatic 150/Jet A	
25 vol% Aromatic 200/Jet A	

Comparison with the 95% confidence interval of the gauging slopes measured on ARINC and CRC fuels indicates that the majority of civil aviation fuels have a gauging slope corresponding to approximately 8% aromatics.

This property is important but was not studied in this project due to the unavailability of a laboratory to perform the necessary measurements.

3.2.13. Viscosity

Kinematic viscosity is a measure of the fluid resistance to flow under the influence of gravity. It is defined as the ratio of dynamic viscosity to density. It determines how easily the fuel can flow and be pumped [32]. It also plays a role in fuel atomisation [40] and lubrication. Low viscosity fuels may not provide sufficient lubrication, which can result in premature wear of components. High viscosity fuels, on the other hand, may impede proper fuel flow, especially at low temperatures. Therefore, it is important to maintain the viscosity within the required limits for safety and optimal performance.

According to the literature, results from I.A. Al-Nuaimi et al. [19] show that increasing the mono- or di-aromatic content in a SPK/Jet A-1 blend by adding more Jet A-1, tends to raise the kinematic viscosity. This trend was also observed by J. T Edwards only for petroleum fuels [17].
Despite the importance, kinematic viscosity will not be studied in this project, as established viscosity limits are provided in the ASTM D1655 standard and other properties were prioritised.

3.2.14. Surface tension

Surface tension is the cohesive force at the surface of a liquid, resulting from intermolecular interactions. In aviation fuels, surface tension may have an impact in fuel-air mixing, water separation, and cavitation.
A low surface tension can promote a better dispersion of water in the fuel [41], which can form emulsions that may generate combustion instabilities. It can also lead to cavitation [42], a phenomenon where vapor bubbles form and collapse in the fuel system, potentially causing damage to pumps and injectors. An optimised surface tension is required to enhance fuel atomization [43], which is critical for combustion efficiency and emissions reduction.
According to J.J Jasper [44] , naphthalenes have the highest surface tension among the pure compounds examined across different chemical families within hydrocarbons.
For fuels, surface tension tends to increase by about 3 dynes/cm with the increase of aromatics up to 15%, and then decreases as aromatic content continues to rise [17]. This supports an effect of the aromatic content which is also discussed when synthetic aviation fuels are used. However, such a property can be affected by low concentration components and nonlinear effects may be observed. It is considered as a relevant property to be investigated in this study.

Among all the properties described, only the properties listed in Table 10 will be investigated. These properties were selected based on the relevance of their reported trends with aromatic content in the literature and on the availability of the corresponding analytical methods. A detailed description of the analytical methods is provided in the Appendix 3.

3.2.15. Properties selected for further analysis in this study

Table 10 Overview of selected fuel properties

Property	Method	Expected trend with decreasing aromatics
Lubricity	ASTM D5001	Wear Scar Increase
Derived cetane number (DCN)	ASTM D7668	Increase
Auto-ignition temperature (AIT)	ASTM E659	Decrease
Thermal conductivity	ASTM D2717	Slight decrease to no variation
Surface tension	EN 14370	Decrease
True vapour pressure (TVP)	ASTM D6378	No clear trend
Heat capacity (Cp)	ASTM E1269 & IFPEN method	Increase

3.3. RESULTS AND DISCUSSION

The properties listed above were measured on the various blends shown in Figure 13. In this figure, blends are arranged according to increasing the aromatics and naphthalene content and distinguished by a colour code. The red blends allow assessment of the effect of varying the naphthalene content at low aromatic concentration, while the blue blends allow the same assessment but with a higher aromatic content. The green blends illustrate the impact of varying the aromatic content when naphthalenes are kept constant, and the orange blends allow observation of the variation of sulphur with aromatics and naphthalenes being constant. This colour code is consistently applied across most of the figures. Error bars represent the repeatability of the employed methods.

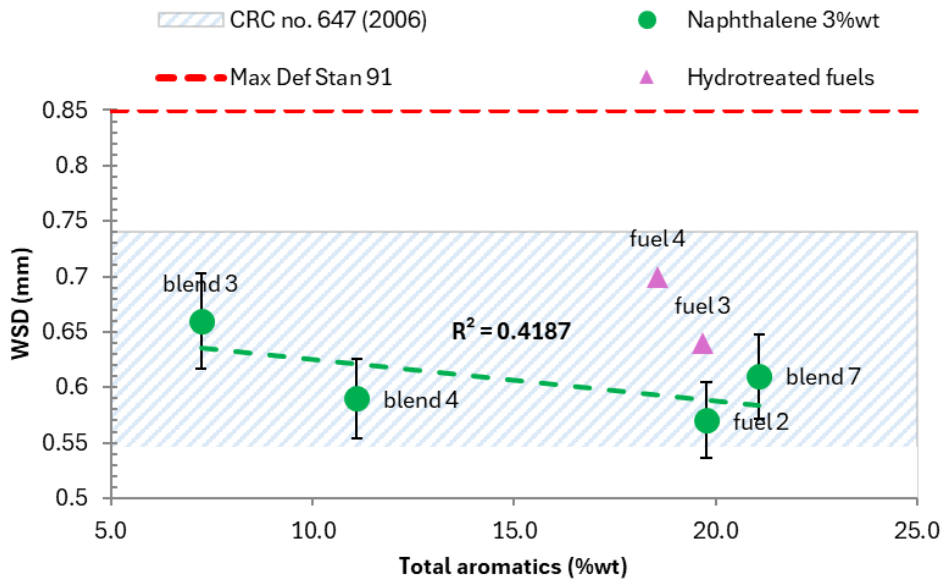
***Figure 13** Fuel matrix aiming at single parameter variations regarding the aromatic, naphthalenes and sulphur content*

			Naphthalenes (%wt)						
			0.1	0.5	1	2	2.5-3		
Total aromatics (%wt)	4		fuel 1						
		Naphthalenes (%wt)	0.0						
		Aromatics (%wt)	4.5						
		Sulphur (ppm)	2.7						
	6		blend 1	blend 2					blend 3
		Naphthalenes (%wt)	0.00	0.5					3
		Aromatics (%wt)	7	6					7
		Sulphur (ppm)	2.7	2.7					2.6
	11								blend 4
		Naphthalenes (%wt)							3
		Aromatics (%wt)							11
		Sulphur (ppm)							2.7
	18-21			fuel 4	fuel 3	blend 5		blend 6	blend 7
		Naphthalenes (%wt)		0.4	1	2		3	3
		Aromatics (%wt)		19	20	20		21	21
		Sulphur (ppm)		8.0	17.0	16.9		2.6	16.8
							S50	S100	fuel 2
		Naphthalenes (%wt)					2	3	3
		Aromatics (%wt)					21	20	20
		Sulphur (ppm)					46.7	100.5	230.1

3.3.1. Lubricity – ASTM D5001

The wear scar diameter (WSD) results in relation to total aromatic content (*Figure 14*) indicate that the wear scar tends to increase as the total aromatic content decreases. The increase in the WSD is observed through the linear correlation, suggesting a reduction of lubricity with decreasing aromatic content, as expected from the literature.

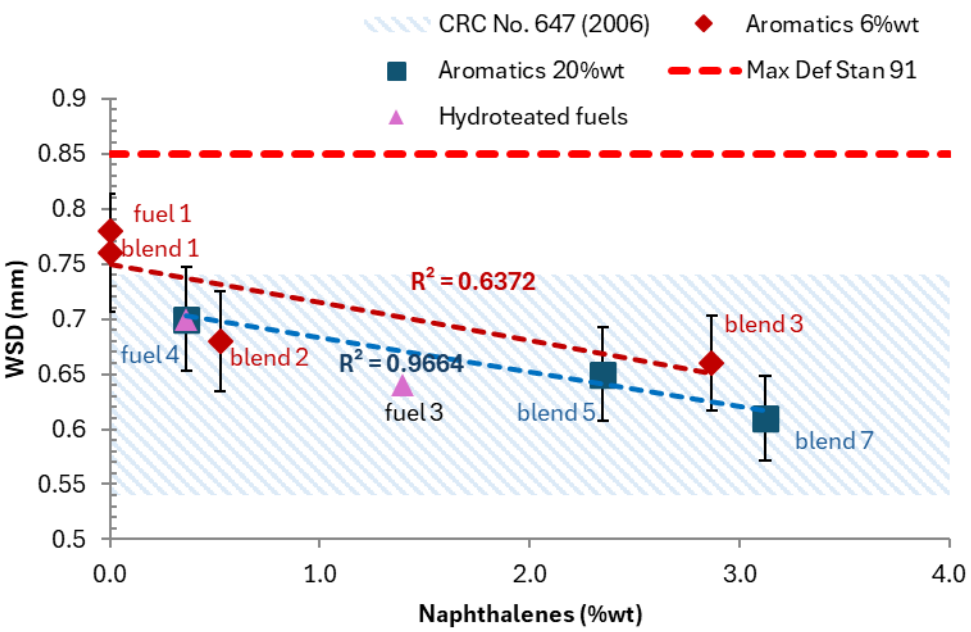
Figure 14 *Wear scar diameter as function of total aromatic content*



	fuel 2	fuel 3	fuel 4	blend 3	blend 4	blend 7
Total aromatics (%wt)	19.8	19.7	18.6	7.2	11.1	21.1
Naphthalenes (%wt)	2.8	1.4	0.4	2.9	3.2	3.1
Sulphur (ppm)	230.1	17.0	8.0	2.6	2.7	16.8

The variation of the WSD as a function of naphthalenes is presented in Figure 15. The results highlighted that a decrease in naphthalenes tends to increase the WSD and deteriorate lubricity. It is noteworthy that a naphthalene content approaching 0% results in a WSD that nearly reaches the maximum allowable limit of 0.85 mm (a difference of 0.1 mm). Naphthalenes appear to have a larger effect on lubricity than total aromatics. As reported in the literature, heavy aromatic compounds contain a higher number a double bonds, which facilitates and strengthens their interaction with metal surfaces compared with mono-aromatics [4], emphasizing the need for caution with respect to lubricity if the naphthalene content decreases significantly.

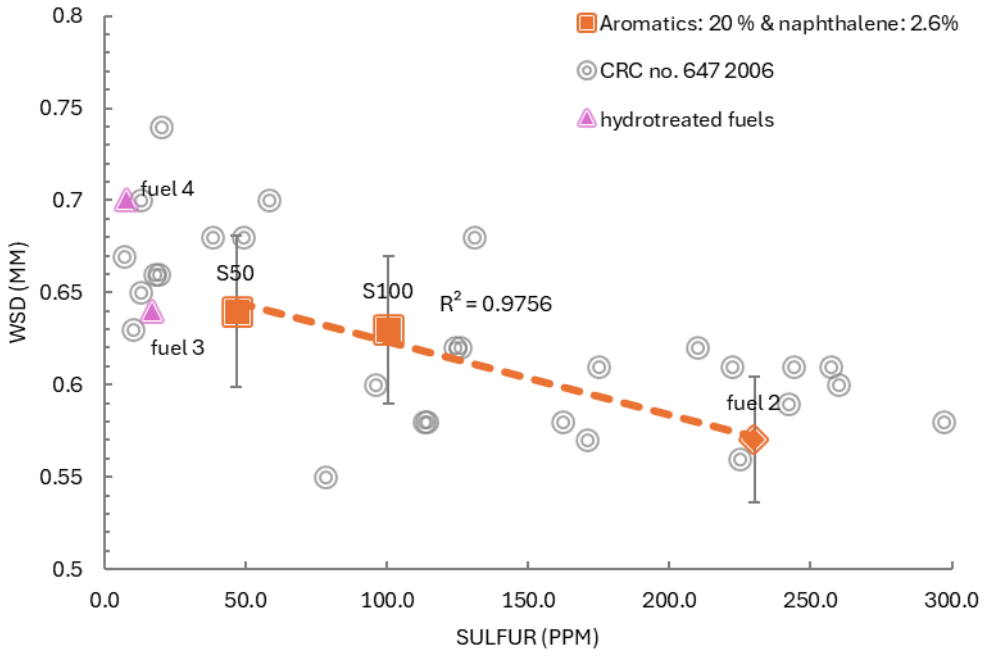
Figure 15 Variation of the WSD as a function of naphthalenes



	fuel 1	fuel 3	fuel 4	blend 1	blend 2	blend 3	blend 5	blend 7
Total aromatics (%wt)	4.5	19.7	18.6	6.6	6.0	7.2	20.5	21.1
Naphthalenes (%wt)	-	1.4	0.4	-	0.5	2.9	2.3	3.1
Sulphur (ppm)	2.7	17.0	8.0	2.7	2.7	2.6	16.9	16.8

The lubricity results with a variation in sulphur content (Figure 16) reveal that a decrease in sulphur content negatively impacts lubricity as indicated by an increase of the WSD. However, at 50 ppm of sulphur, the increase in the WSD remains approximately 0.2 mm below the maximum allowable limit.

Figure 16 WSD as function of the sulphur content



	fuel 2	fuel 3	fuel 4	S50	S100
Total aromatics (%wt)	19.8	19.7	18.6	20.5	20.3
Naphthalenes (%wt)	2.8	1.4	0.4	2.5	2.6
Sulphur (ppm)	230.1	17.0	8.0	46.7	100.5

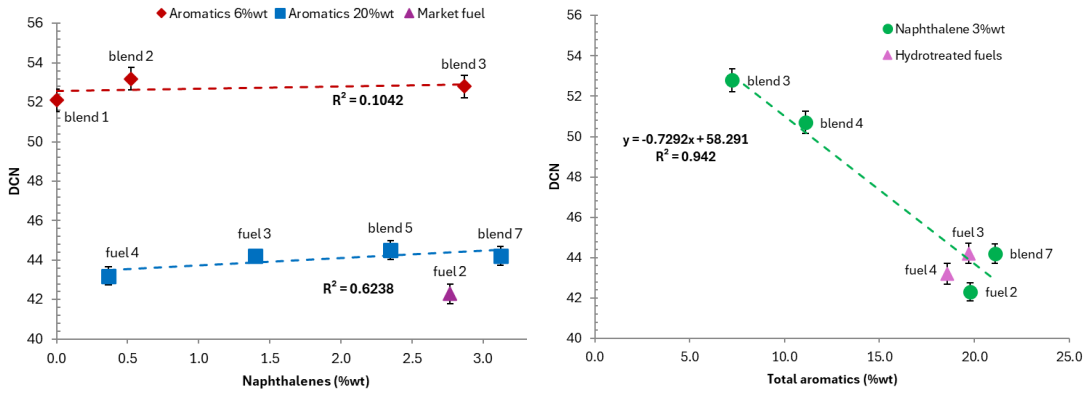
In addition, the three values were compared with the data from 2006 CRC survey [1]. This comparison indicates that there is no significant difference between the two blends representing the lowest sulphur content (S50) and the highest sulphur content tested (Fuel 2). Additional data points would be required to confirm the trend observed and validate the limited effect of sulphur within this range of variability. It is however noted from literature that lubricity is more affected by the hydrotreating process, particularly the reduction of heavy aromatics, than sulphur itself.

As with most other properties, a trend is clearly visible, but the differences between the results are not large enough to exceed the repeatability of the measurement. However, caution is advised if naphthalene levels approach zero, as lubricity improver additives may have to be considered.

3.3.2. Derived cetane number (DCN) – ASTM D7668

Figure 17 shows the variation of DCN as function of naphthalene and total aromatics. For the naphthalene variation, two sets of blends were tested. The set with low total aromatic content (tot. aro: 6 %wt, red diamonds) and the set with a representative content of total aromatics (tot. aro: 20 %wt, blue squares). For both sets, results show a stable and flat trend with no significant changes among the blends. Based on these results, naphthalenes do not seem to show the expected impact on DCN as reported in the literature.
Concerning the total aromatic content, results show a strong and negative linear correlation. For every 1% increase in total aromatics the DCN is expected to decrease by 0.7 points. This result is not unexpected as paraffinic molecules significantly increase the cetane number.

Figure 17 *Derived cetane number as a function of naphthalenes (left) and total aromatics (right)*



	fuel 2	fuel 3	fuel 4	blend 1	blend 2	blend 3	blend 4	blend 5	blend 7
Total aromatics (%wt)	19.8	19.7	18.6	6.6	6.0	7.2	11.1	20.5	21.1
Naphthalenes (%wt)	2.8	1.4	0.4	-	0.5	2.9	3.2	2.3	3.1
Sulphur (ppm)	230.1	17.0	8.0	2.7	2.7	2.6	2.7	16.9	16.8

Comparison of the Fuel 2 (market fuel), and Fuel 3 and 4 shows that the difference in DCN resulting from hydrotreatment is not significant. During hydrotreatment, di-aromatics compounds are primarily hydrogenated into naphtheno-di or mono aromatic, or tretalin. However, the chemical composition of the fuels (Figure 18) shows that Fuel 2, 3 and 4 do not differ significantly in their contents of naphthenes and naphtheno-aromatic compounds. In contrast Fuel 1 and Blend 4 have higher naphthenes and iso-paraffins, and lower mono-aromatics concentrations. As reported in the literature, naphthenes and iso-paraffins exhibit higher DCN than naphthalenes and mono aromatics. This shows that the reduction of mono aromatics has an impact on DCN, however the increase observed in Figure 17 17 also highlights the effect of other chemical compounds.

Figure 18 *Chemical composition of Fuel 1, 2, 3, 4 and Blend 4*

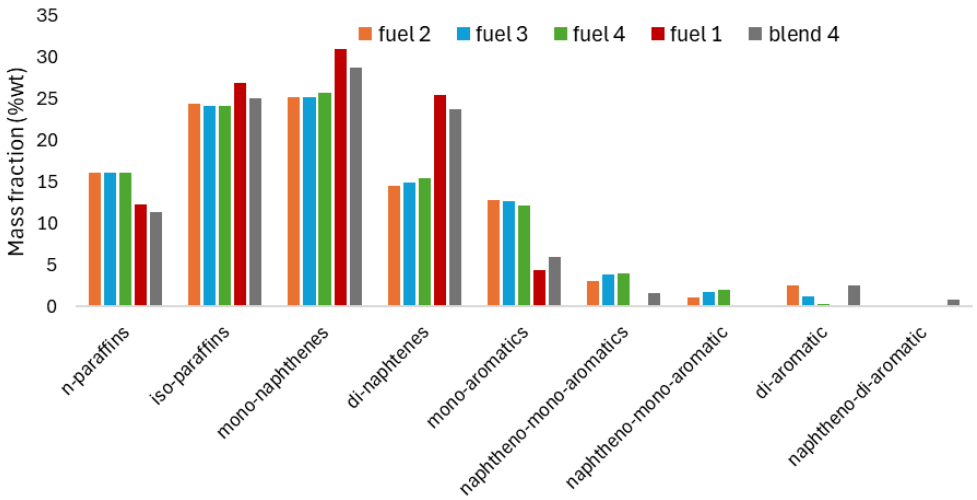
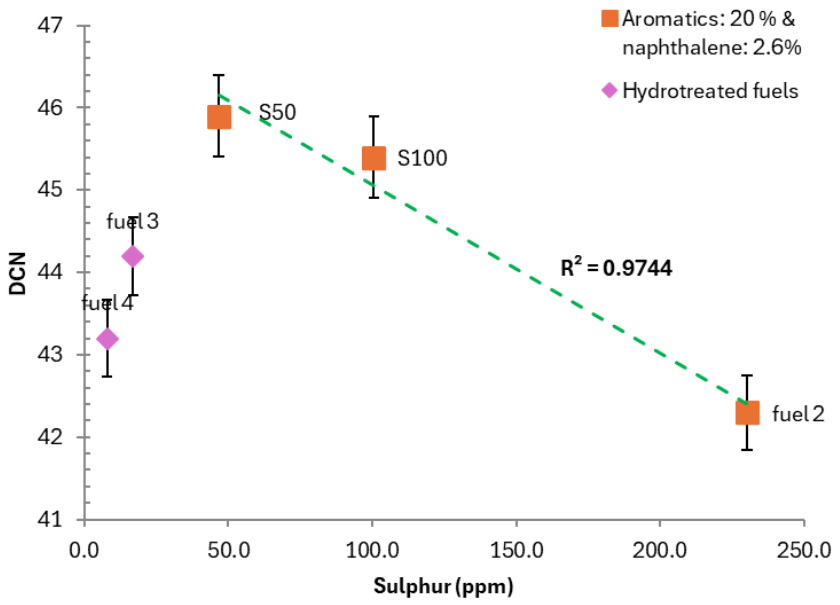


Figure 19 shows the derived cetane number values depending on sulphur variation. The graph includes the set comprising the Blends S50, S100 and Fuel 2 as well as Fuel 3 and 4 which come from the hydrotreatment of Fuel 2. During the hydrotreatment, the sulphur compounds present in the kerosene cut are converted to hydrocarbons and hydrogen sulphide [45]. Therefore, S50 (50 ppm sulphur) is expected to have a DCN similar to Fuel 3 and 4, which have sulphur contents of 17ppm and 8ppm respectively. The main results are:

- When comparing the results from Fuel 2, 3 and 4. DCN for Fuels 3 and 4 are lower than the S50. This highlights that reducing sulphur through hydrotreatment reveals no clear trend.
- When comparing the results from the formulated blends (S50, S100 and Fuel 2) an increase in sulphur content is linearly correlated with a decrease in the cetane number. However, this is more likely due to other components on the S50 S100 blends than sulphur itself.

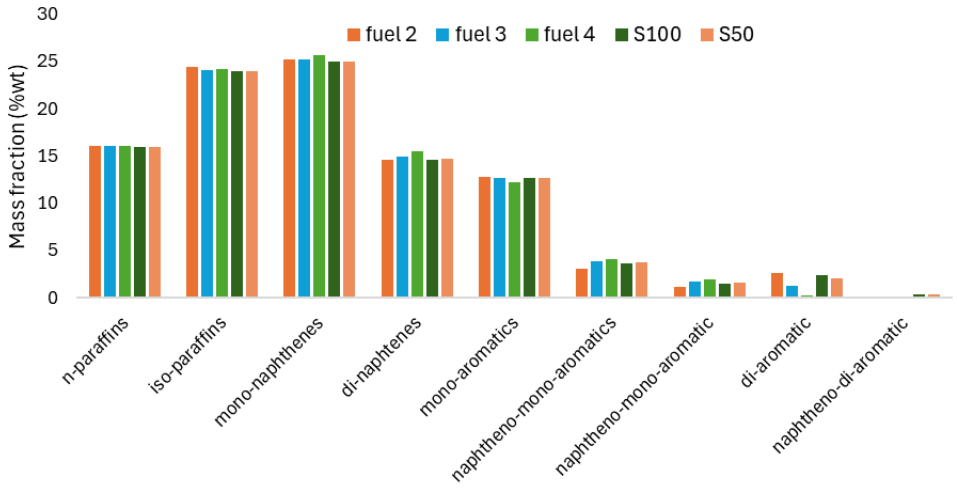
By comparing the composition of the different blends and fuels (Figure 20), no clear difference is observed that could account for these divergent trends, but cannot be concluded that sulphur has a significant impact on cetane number (DCN).

Figure 19 *Derived cetane number as function of sulphur content*



	fuel 2	fuel 3	fuel 4	S50	S100
Total aromatics (%wt)	19.8	19.7	18.6	20.5	20.3
Naphthalenes (%wt)	2.8	1.4	0.4	2.5	2.6
Sulphur (ppm)	230.1	17.0	8.0	46.7	100.5

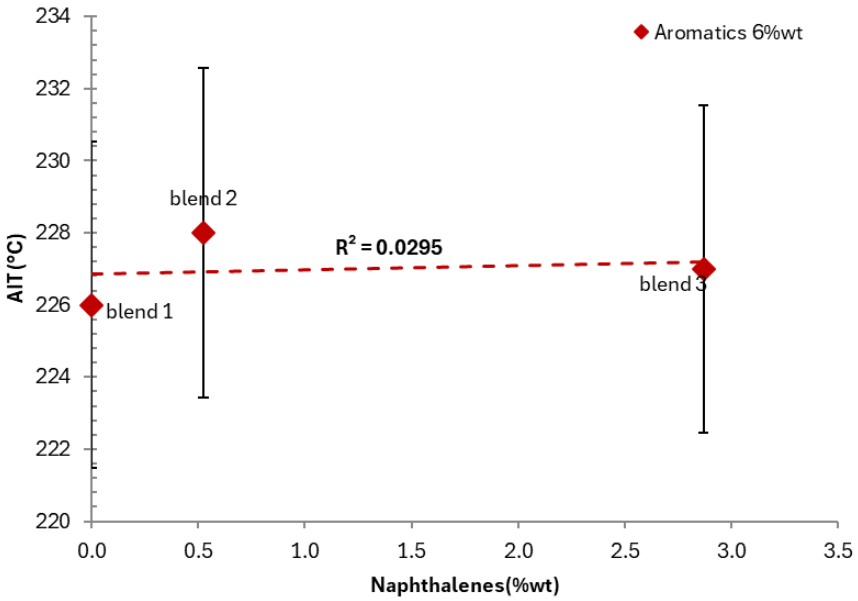
Figure 20 Chemical composition of Fuel 2, 3, 4, Blend S100 and S50



3.3.3. Auto-ignition temperature (AIT) – ASTM E659

The auto-ignition temperatures as function of naphthalenes are presented in Figure 21. No significant variation is observed, and it remains within the measurement repeatability. Naphthalenes have no impact on AIT.

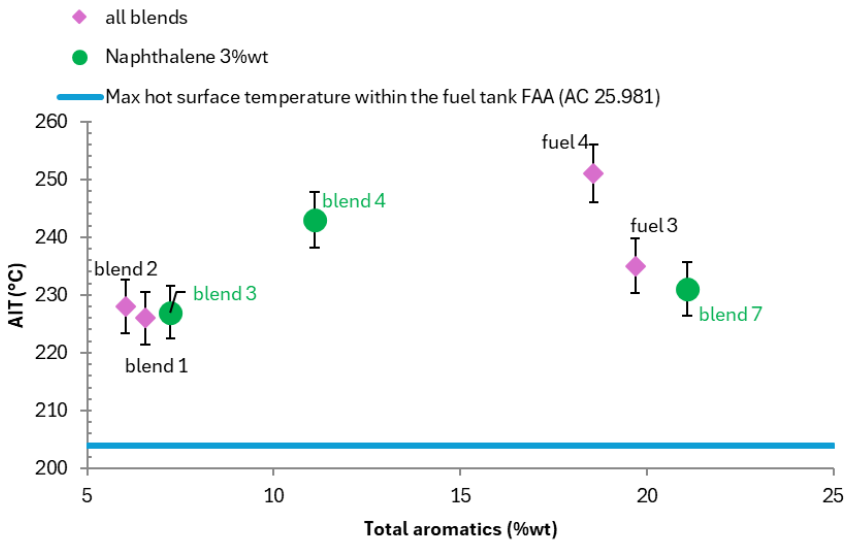
Figure 21 Auto-ignition temperature (AIT) as a function of naphthalenes



	blend 1	blend 2	blend 3
Total aromatics (%wt)	6.6	6.0	7.2
Naphthalenes (%wt)	-	0.5	2.9
Sulphur (ppm)	2.7	2.7	2.6

The auto-ignition temperatures as a function of total aromatics are presented in Figure 22. The green data points represent the AITs of the selected blend set, analysed to observe the variation in total aromatics. These three results do not show any clear trend between AIT and total aromatic content.
The pink markers correspond to additional blends from the fuel matrix that were also analysed. Since the results from Figure 21, revealed that naphthalenes have no impact on AIT, these points were plotted as well. However, no consistent trend is observed. It is important to note that, despite the lack of clear trend and the fact that the results do not align with what was expected based on the literature review, all blends exhibit an auto-ignition temperature at least 20° C higher than the Jet A-1 AIT limit (204°C)[22],[23]. This indicates that a reduction in either naphthalenes or total aromatics would not present a safety concern.

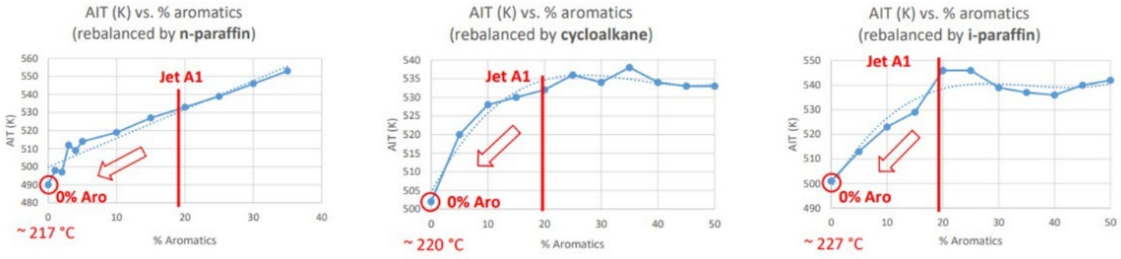
Figure 22 *Auto-ignition temperature (AIT) as a function of total aromatics*



	fuel 3	fuel 4	blend 1	blend 2	blend 3	blend 4	blend 7
Total aromatics (%wt)	19.7	18.6	6.6	6.0	7.2	11.1	21.1
Naphthalenes (%wt)	1.4	0.4	-	0.5	2.9	3.2	3.1
Sulphur (ppm)	17.0	8.0	2.7	2.7	2.6	2.7	16.8

Chemical kinetic modelling made on a surrogate base on Jet A-1 composed of 19 %vol of n-dodecane, 32 %v iso-octane, 30 %v methylcyclohexane and 19%v toluene suggests that aromatics are the primary contributors among the other chemical families. These simulations in Figure 23 also reveal that removing aromatics, decreases the overall AIT. If the reduction is done by replacing the aromatics with other families, such as linear, branched, or cyclic alkanes, a reduction is still visible, but with trends with a more pronounced decrease, particularly for linear and branched alkanes.

Figure 23 *Simulation of Jet A-1 surrogate AIT as function of aromatic content replaced by n-paraffins (left), cycloalkanes (middle) and i-paraffins (right)*

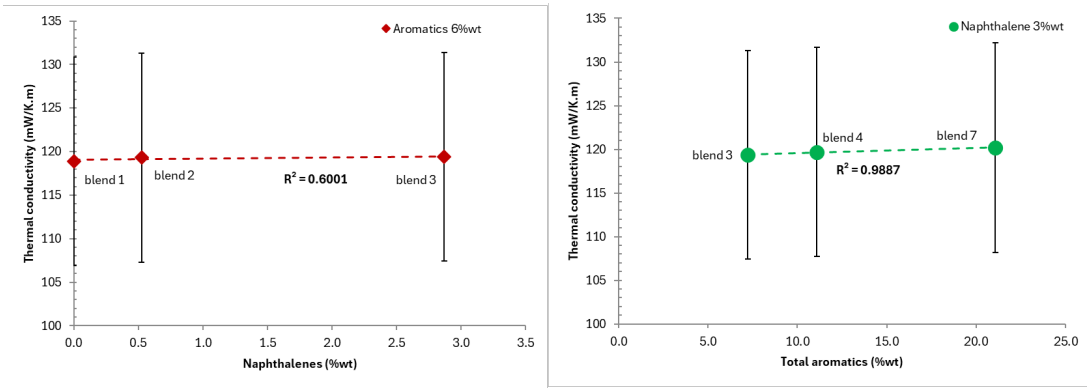


These simulations suggest that a strong non-linear relationship could be expected as the blend approaches 0% aromatics. They also indicate that the effect of reducing aromatics strongly depends on the base fuel composition, particularly on whether aromatics are replaced by iso-paraffins or naphthenes. Further experiments would thus be necessary with a more systematic variation of jet A1 to assess the impact of very low levels of aromatics.

3.3.4. Thermal conductivity – ASTM D2717

The thermal conductivity as a function of naphthalenes and total aromatics are presented in (Figure 24). The variation of both parameters, naphthalenes and total aromatics, does not exhibit significant differences in thermal conductivity as highlighted by the results of Malatesta et al. The difference observed among the results remains within the measurement repeatability. Based on the results both, naphthalenes and the total aromatic content, have no impact on thermal conductivity.

Figure 24 *Thermal conductivity as a function of naphthalenes (left) and total aromatics (right)*

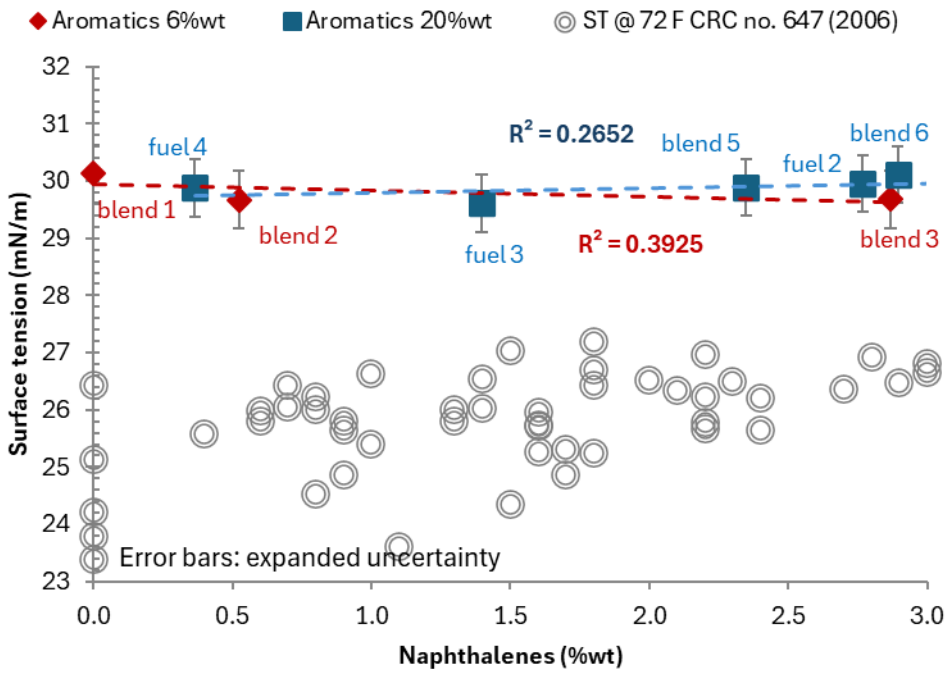


	blend 1	blend 2	blend 3	blend 4	blend 7
Total aromatics (%wt)	6.6	6.0	7.2	11.1	21.1
Naphthalenes (%wt)	-	0.5	2.9	3.2	3.1
Sulphur (ppm)	2.7	2.7	2.6	2.7	16.8

3.3.5. Surface tension - EN 14370

The surface tension results with variation in naphthalenes are illustrated in Figure 25. Two sets of blends with low and high total aromatic content were examined. Results from both sets show a weak linear correlation and no visible trend. This unexpectedly indicates that the naphthalene content has no impact on the surface tension while according to the literature, naphthalenes have the highest surface tension among the pure compounds. This potentially supports a nonlinear effect or a difference in surface tension for naphthalenes that is not significant enough compared to the measurement repeatability to assess any effect.

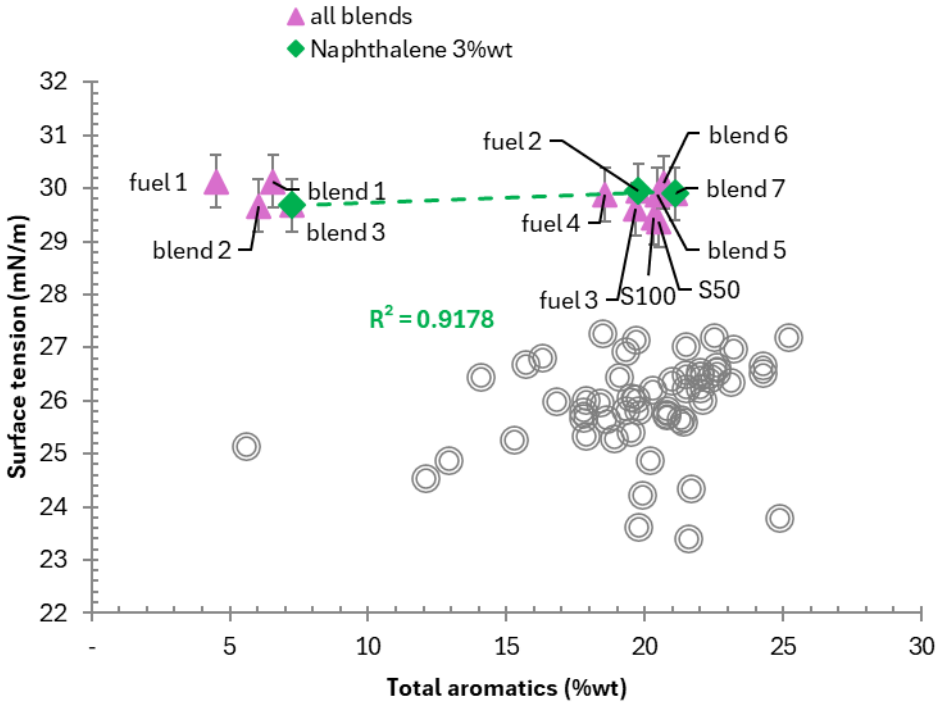
Figure 25 *Surface tension as a function of naphthalenes*



	fuel 2	fuel 3	fuel 4	blend 1	blend 2	blend 3	blend 5	blend 6	blend 7
Total aromatics (%wt)	19.8	19.7	18.6	6.6	6.0	7.2	20.5	20.7	21.1
Naphthalenes (%wt)	2.8	1.4	0.4	-	0.5	2.9	2.3	2.9	3.1
Sulphur (ppm)	230.1	17.0	8.0	2.7	2.7	2.6	16.9	2.6	16.8

For the variation of total aromatic content, two data sets were plotted (Figure 26). The first data set (green dots) was initially planned to investigate the influence of total aromatics. The results suggest a linear correlation between the total aromatic content and the surface tension. It implies that reducing the total aromatic content could lead to a lower surface tension. These results aro also inconsistent with the literature review, which reported that surface tension shows a peak behaviour, increasing to a maximum and then decreasing at higher aromatic content (>25%vol). However, a second dataset (pink markers) including additional blends and fuels from the fuel matrix were also analysed and plotted.

Figure 26 Surface tension as a function of total aromatics



	fuel 1	fuel 2	fuel 3	fuel 4	blend 1	blend 2	blend 3	blend 5	blend 6	blend 7	S50	S100
Total aromatics (%wt)	4.5	19.8	19.7	18.6	6.6	6.0	7.2	20.5	20.7	21.1	20.5	20.3
Naphthalenes (%wt)	-	2.8	1.4	0.4	-	0.5	2.9	2.3	2.9	3.1	2.5	2.6
Sulphur (ppm)	2.7	230.1	17.0	8.0	2.7	2.7	2.6	16.9	2.6	16.8	46.7	100.5

As previously mentioned, naphthalenes did not display any significant effect on surface tension. With the addition of this new data the total aromatic content also appears not to impact the surface tension in a significant manner. The lack of trend is also observed with the CRC data. For both figures, Figure 25 and Figure 26, the surface tension measured in this study remains higher than the CRC data. This is due to the temperature at which the tests were performed. CRC measurements were performed at 72 F (~ 22°C), whereas the measurements in this study were performed at 25°C.

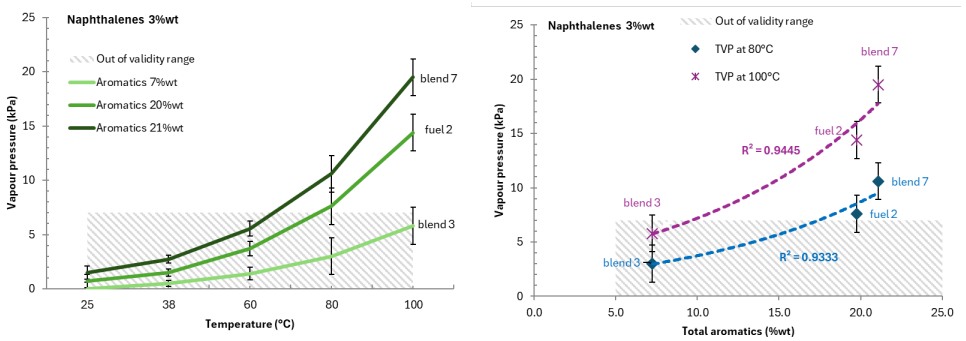
The variation observed among the measurements are relatively small (max. variation ~1 mN/m) particularly when the reproducibility of 5mN/m [46] or the expanded uncertainty of 0.5 mN/m [47] are considered. Which leads to conclude there is no significant variation of the surface tension with the total aromatic content variation proposed.

3.3.6. True vapor pressure (TVP) - ASTM D6379

The true vapor pressure results are illustrated in Figure 27. The graph on the left presents the TVP as a function of temperature and the total aromatic content, while the graph on the right displays only the data points that fall within or near the measurement's validity range as a function of the total aromatic content. Figure 27 (left) shows that TVP increases exponentially

with temperature, and that increasing the total aromatic content leads to a higher TVP. The graph on the right reveals that this increase in TVP is exponential with respect to the total aromatic concentration. It is important to note that the TVP might be affected by the boiling range, without considering aromatics, naphthalenes and their concentrations.

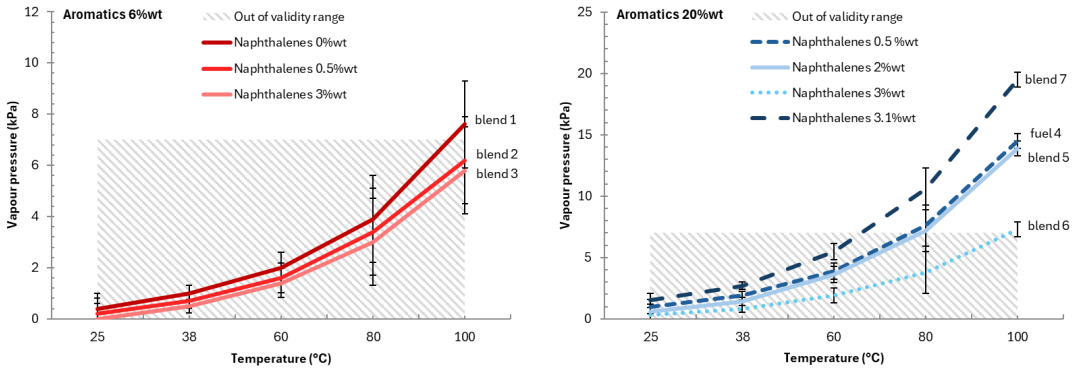
Figure 27 *True vapor pressure as function of temperature (left) and as function of total aromatics (right)*



	fuel 2	blend 3	blend 7
Total aromatics (%wt)	19.8	7.2	21.1
Naphthalenes (%wt)	2.8	2.9	3.1
Sulphur (ppm)	230.1	2.6	16.8

To assess the impact of naphthalene, TVP measurements were performed on two sets of blends: one set with a total aromatic content of 6 %wt and another set with 20 %wt.
Results for the low total aromatic content blends (Figure 28, left) indicate that increasing the naphthalene concentration leads to a decrease in TVP. However, this decrease should not be considered significant, as the difference between the three blends is smaller than the repeatability of the measurement. Additionally, all the values fall outside the validity range. For the high total aromatic content blends (Figure 28, right) no clear trend is observed. This suggests that naphthalenes do not significantly impact TVP.

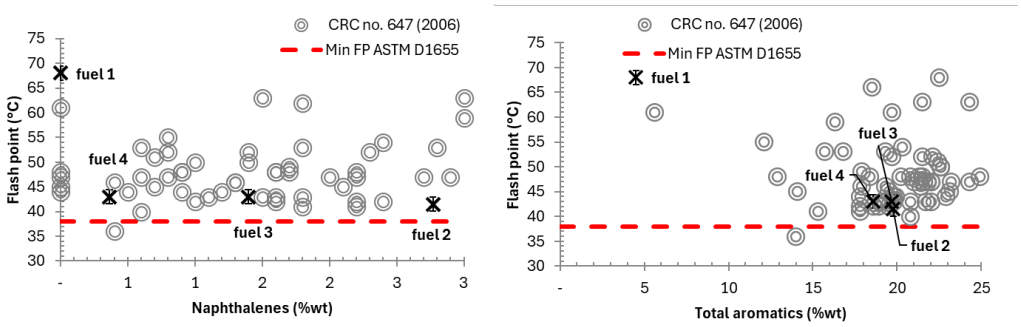
Figure 28 *True vapor pressure as function of temperature with 6% (left) and 20% (right) of total aromatic content*



	fuel 4	blend 1	blend 2	blend 3	blend 5	blend 6	blend 7
Total aromatics (%wt)	18.6	6.6	6.0	7.2	20.5	20.7	21.1
Naphthalenes (%wt)	0.4	-	0.5	2.9	2.3	2.9	3.1
Sulphur (ppm)	8.0	2.7	2.7	2.6	16.9	2.6	16.8

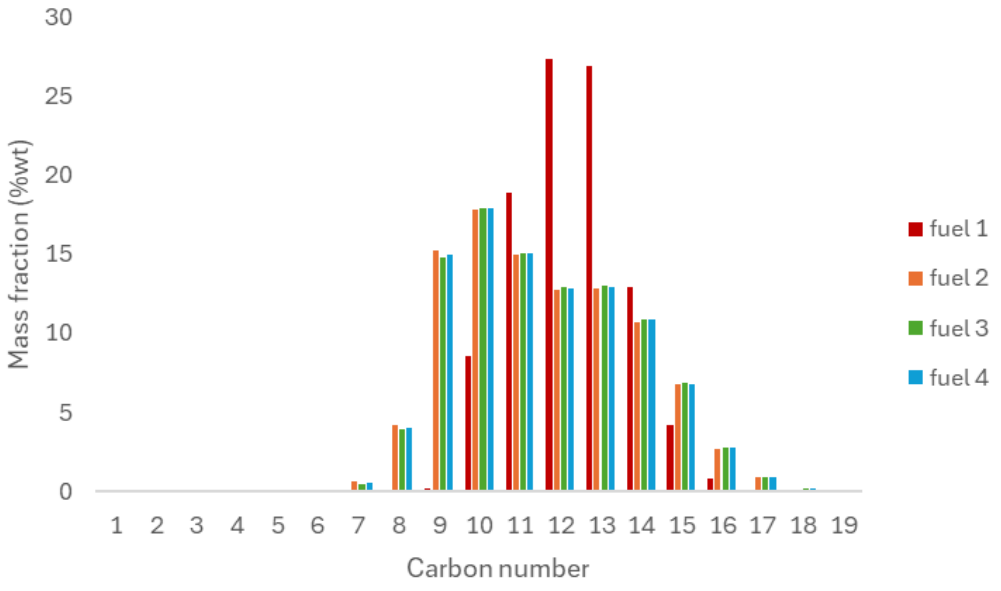
As previously mentioned, TVP is related to the flash point. A fuel with a low flash point typically indicates a high volatility, which is in turn associated with a higher TVP. Although, the flash point was not measured for all the blends of the fuel matrix, it was measured for Fuel 1, 2, 3 and 4. The results are given in Figure 29. The total aromatics and naphthalenes in Fuel 2, as well as in the hydrotreated samples Fuels 3 and 4, vary without influencing the FP, indicating a minimal impact of these factors. Consequently, the difference with Fuel 1 is mainly due to a higher molecular weight distribution as shown in . As seen in the literature review, increasing the molecular weight decreases the volatility which in turn, results in a higher flash point.

Figure 29 *Flash points of the four fuels as function of naphthalenes (left) and total aromatics (right)*



	fuel 1	fuel 2	fuel 3	fuel 4
Total aromatics (%wt)	4.5	19.8	19.7	18.6
Naphthalenes (%wt)	-	2.8	1.4	0.4
Sulphur (ppm)	2.7	230.1	17.0	8.0

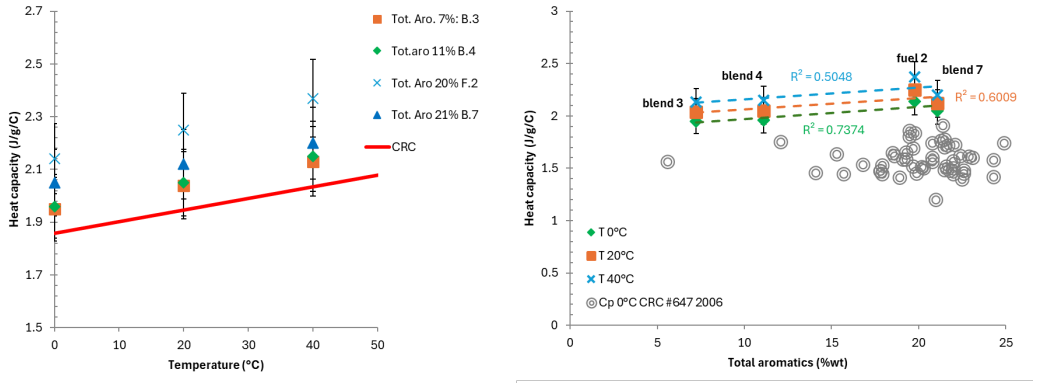
Figure 30 *Carbon distribution of the four base fuels*



3.3.7. Heat capacity –ASTM E1269 and IFPEN method

The results of the heat capacity as a function of temperature and total aromatic content show, as expected, that heat capacity increases with the temperature (Figure 31, left). Additionally, a decrease in total aromatic content tends to decrease slightly the heat capacity, in contradiction to which the previously reported literature findings, which indicates that a reduction of aromatic content shows an increase of the heat capacity. This trend is visible in Figure 31 (right) which highlights a mild to strong positive linear correlation between the heat capacity and the total aromatic content. While this trend is apparent, it should be noted that the differences between the results fall within the measurement repeatability range.
A decrease in the heat capacity is not recommended, as it prevents proper heat distribution. Nevertheless, above a total aromatic content of 7%wt, the heat capacity remains above the average value of jet A-1 from the CRC survey 2006 [1].

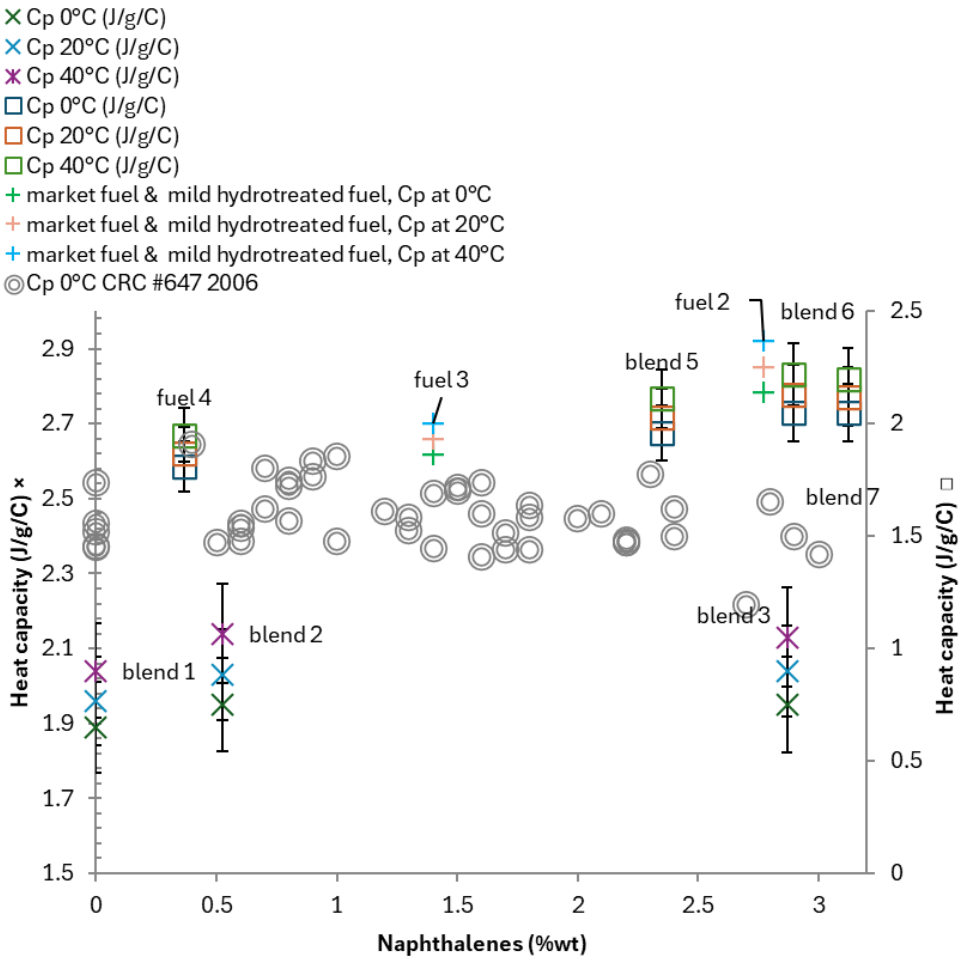
Figure 31 *Heat capacity as a function of temperature (left) and total aromatics (right)*



	fuel 2	blend 3	blend 4	blend 7
Total aromatics (%wt)	19.8	7.2	11.1	21.1
Naphthalenes (%wt)	2.8	2.9	3.2	3.1
Sulphur (ppm)	230.1	2.6	2.7	16.8

Figure 32 illustrates the variation of heat capacity as a function of naphthalene content. The first data set (cross markers) corresponds to the blends with a low total aromatic content (values to be read on the left y-axis), while the square markers represent blends with the high total aromatic content (values to be read on the right y-axis). For both sets of blends, the values are similar (~ 2 J/g/C), and the variation is within the repeatability range. This indicates that there is no significant variation in heat capacity with respect to the naphthalene content. This is also observed with the CRC report no. 647 (2006) data.

Figure 32 Heat capacity as function of naphthalenes for the blends with 6% (cross markers) and 20% (circle markers) of total aromatic content



	fuel 2	fuel 3	fuel 4	blend 1	blend 2	blend 3	blend 5	blend 6	blend 7
Total aromatics (%wt)	19.8	19.7	18.6	6.6	6.0	7.2	20.5	20.7	21.1
Naphthalenes (%wt)	2.8	1.4	0.4	-	0.5	2.9	2.3	2.9	3.1
Sulphur (ppm)	230.1	17.0	8.0	2.7	2.7	2.6	16.9	2.6	16.8

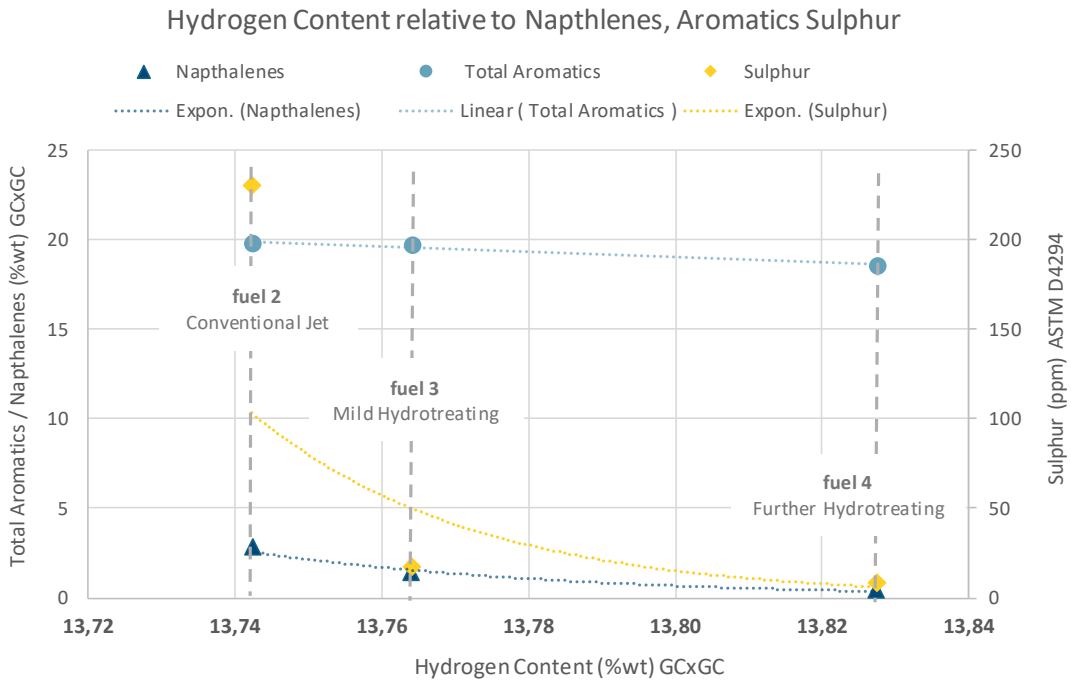
3.4. FUEL HYDROGEN CONTENT

The fuel hydrogen content has become a measure of interest as it correlates with non-volatile Particulate Matter (nvPM) engine test results. Typically, emissions tests show reduced Particulate Matter emissions with fuels of various reduced levels of aromatic, naphthalene or sulphur contents. It is difficult to correlate the measured effects to each individual fuel property, but hydrogen content directionally reflects all three and has therefore become popular in academic studies to correlate the results more simply. Fuels with higher hydrogen content show lower aromatic, naphthalene or sulphur content, or reduced levels of all three in different proportions. Reduction in each of these properties may result in lower nvPM emissions. While the details of these emission tests are not in the scope of this study, in this context it is of interest to present the hydrogen content related data of the fuel samples blended and analysed for this study. For context, the hydrogen content of typical petroleum jet fuel is 13.5-14 wt%, with SAF blends between 14-15 wt% and fully paraffinic synthetic jet fuel is typically 15-15.2 wt%.

Effect of hydrotreating on hydrogen content in Fuel 2, Fuel 3 and Fuel 4

As mentioned in section 3.1, Fuel 2 is a representative sample of European jet fuel and was subjected to hydrotreating for desulphurisation, which is a possible process in some refineries for kerosene production. The resulting Fuel 3 was further hydrotreated to produce Fuel 4, which represents a more severely hydroprocessed product.

***Figure 33** Hydrogen Content of a fuel with progressive levels of hydrotreatment*



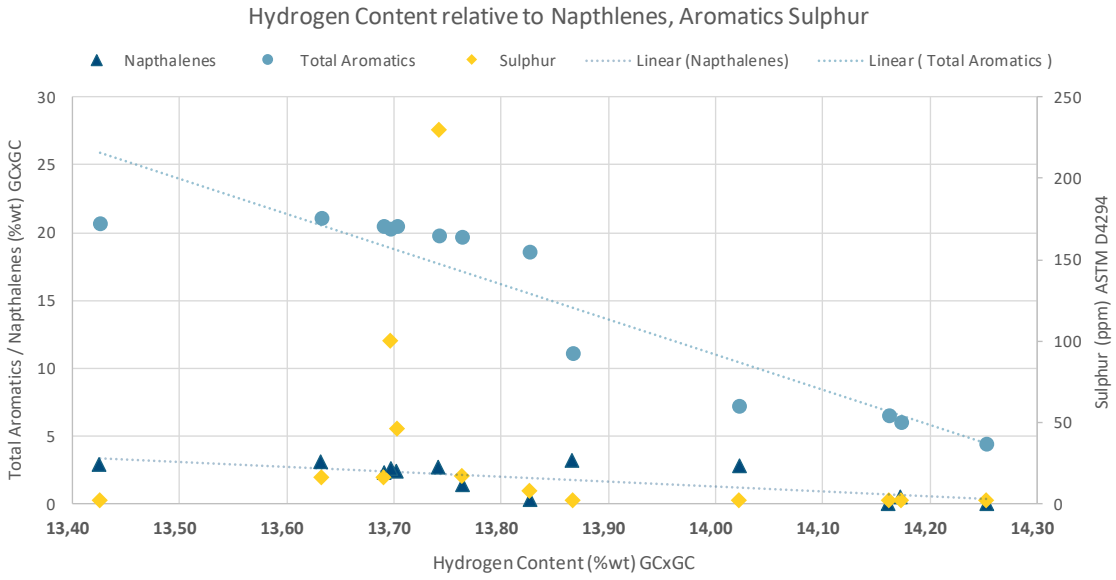
Results of the total aromatics, sulphur and naphthalene content are analysed in Figure 33. Hydrotreatment reduces sulphur effectively, while total aromatics and naphthalenes showed marginal reductions from Fuel 2 to Fuel 3. In this case Hydrogen content only slightly increases, demonstrating that during desulphurisation, some of the hydrogen is lost from the fuel in form of hydrogen sulphide gas (H_2S). More severe hydrotreating, as shown by the difference between Fuel 3 and Fuel 4, confirms that naphthalene molecules had been saturated. To a lesser degree it may also saturate some of the mono-aromatic molecules. The overall effect of hydrotreatment allows production of a fuel with low levels of sulphur and naphthalenes, a slightly reduced total aromatic content and higher hydrogen content.

It is worth noting that hydrotreating affects these three properties at different rates, which helps explain why aromatic, naphthalene, and sulphur contents do not always show a linear correlation with nvPM emissions, whereas hydrogen content often does. Hydrotreating will however directionally reduce all three, and it is not possible to leave one property unaffected if hydrotreating is done. For example, reducing sulphur and aromatics while leaving naphthalenes unaffected would not be possible.

Hydrogen content of the complete fuel matrix.

The fuel matrix was produced to perform the detailed fuel property evaluation of the previous section, with fuel samples of widely varying aromatic, naphthalene and sulphur contents. This was achieved by blending the hydrotreated fuels with other fuels containing either very low aromatic or high aromatic components. The hydrogen content of all these blends was measured.

***Figure 34** Hydrogen content of the fuel matrix*



This further shows how various combinations of sulphur, naphthalene and aromatic levels result in higher or lower hydrogen content. Fuels with higher hydrogen content, typically above 14 wt%, will have very low levels of aromatic, naphthalene and sulphur.

Hydrogen content calculation by ASTM D3343

While hydrogen content is interesting from an academic point of view in the study of non-CO_2 emissions, it is not required to be measured for fuel quality compliance, engine operability or as a safety parameter. For this reason, hydrogen content is not measured in the commercial aviation industry and does not appear on a certificate of quality for a Jet A/A-1 (ASTM D1655) or Jet A-1 (DefStan 91-091) aviation fuel.

Direct measurement of hydrogen content requires an analytical method capable of determining fuel composition and such methods are typically complex and expensive. As part of this study, comprehensive two-dimensional gas chromatography (GCxGC) was used for accurate fuel compositional analysis, including hydrogen content measurement.

In the absence of a mandatory hydrogen content measurement in commercial jet fuel specifications, parties interested in the hydrogen content can easily use ASTM D3343 - Standard Test Method for Estimation of Hydrogen Content of Aviation Fuels.

This method consists of a calculation procedure based on an empirical correlation to estimate the hydrogen content using data available on any commercial certificate of quality. The calculation procedure is described below, followed by a comparison of results from the fuel samples in this study to demonstrate the accuracy of the method.

Required Measurements (Inputs)

1. Density (D) – kg/m³ at 15 °C (Test Method ASTM D1298 or equivalent)
2. Aromatic content (A) – volume % (Test Method ASTM D1319)
3. Average distillation temperature (T) – °C:
   - Run ASTM D86 distillation.
   - Record temperatures at 10 %, 50 %, and 90 % recovered.
   - T = (T_{10} + T_{50} + T_{90}) / 3.

Hydrogen Content Formula (SI / Metric Units)

$$\%\mathrm{H} = \frac{9201.2 + 14.49T - 70.22A}{D} + 0.02652A + 0.0001298AT - 0.01347T + 2.003$$

where:

- % H = mass percent hydrogen
- T = average distillation temperature (°C)
- A = aromatics (volume %)
- D = density (kg/m³ at 15 °C)

This simple calculation was performed for the fuel blends where the input data was measured, resulting in ASTM D3343 hydrogen content results. This result can be compared to GCxGC results. The result comparison is shown in the table below, showing very good accuracy, within 1%.

Table 11 Comparison of hydrogen test methods: ASTM D3343 vs GCxGC

	ASTM D3343 Calculation			Results Comparison		
Fuel Samples	D: Density kg/m³	A: Aromatics vol%	T (Average) °C	Hydrogen Content D3343 mass%	Hydrogen Content GCxGC mass%	Difference %
fuel 1	807,00	3,93	216,97	14,25	14,25	-0,02%
fuel 2	811,80	17,14	204,47	13,66	13,74	-0,61%
fuel 3	811,50	17,17	204,90	13,67	13,76	-0,72%
fuel 4	810,20	16,25	204,30	13,71	13,83	-0,82%
blend 1	808,30	5,74	216,10	14,16	14,16	0,02%
blend 5	813,30	17,81	205,23	13,62	13,69	-0,54%
blend 6	821,10	18,14	210,73	13,52	13,43	0,66%
blend 7	814,60	18,33	205,33	13,58	13,63	-0,39%

4. CONCLUSION

This study assesses the technical and economic feasibility of producing petroleum-based aviation fuels with reduced levels of aromatics, naphthalenes, and sulphur within the European refining system. Using survey data from Concawe members, the Concawe LP model and extensive data from IFPEN, Kerosene Hydrotreatment scenarios were evaluated to meet a set of increasingly stringent jet fuel specification scenarios.

The study focused on investigating the three most critical elements when considering a change in specifications:

- Feasibility based on installed technology
- Additional emissions and production costs (including potential investments)
- Effects on fuel properties, including use-related properties

Out of the three most common production units for jet fuel components, hydrotreaters and hydrocrackers are processes which can potentially reduce aromatics, naphthalenes and sulphur. Any change in specifications requiring the reduction in average sulphur, naphthalene or aromatic content would however not be achievable by those refineries relying on Merox as the main jet fuel production unit (~31% of the EU refineries). A minor reduction may be achievable without major investments by those refineries equipped with HT and HCK units but with an increase of OPEX, refinery CO_2 emissions and a potential loss of jet fuel volume.

If new specifications are achievable by existing hydrotreater and hydrocracker units (indicatively down to 16% vol aromatics), the effects of a theoretical massive reallocation of the production to these units would be an increase in OPEX by 0,5 – 0,9 billion EUR/y (excluding logistics and CO_2 cost) and additional CO_2 refinery emissions of 1,3 – 2,1 Mt/y (26-45 kg CO_2/ T jet). These however are very conservative estimates: amalgamating all units of the EU refining system in one single refinery results in an “ideal” case which cannot be representative of the sum of the real costs which will have to be borne by individual refineries and it significantly understates the difficulty the industry would face in meeting these specification changes.

A further reduction in aromatics would need substantial capital investment (and significantly increased OPEX and CO_2 refinery emissions) for all EU refineries: such investments may not be forthcoming so they may accelerate refinery closure and risk security of supply. Importers could face the same challenges, as they might require similar technology upgrades, and this might end in lower product availability to compensate for the loss of EU production.

If new specifications are so challenging that no refinery could achieve them with existing units, moving all jet production to brand new high-pressure kerosene hydrotreaters would require 5,0 – 11,8 billion EUR of CAPEX (excluding investments in additional H_2 production plant) and the effects would be an increase in OPEX by 0,6 – 0,9 billion EUR/y (excluding logistics and CO_2 cost) and additional CO_2 refinery emissions of 1,4 - 4,5 Mt/y (30-93 kg CO_2 / T jet). One can question the economic viability to invest heavily in new units to de-aromatise fossil jet fuels in a market of declining demand for these products due to ReFuelEU Aviation.

SAF production by SBC blending in line with ATSM D7566 specifications and ReFuel EU Aviation renewable volume targets, require the fossil portion of the jet fuel pool to contain at least 16% aromatics, very close to the current average. A reduction in the current aromatic specification would further reduce this average and limit SAF blending, thus negating the desired climate benefits.

Considering the impacts of a decrease in aromatics, naphthalenes and sulphur on fuel physical and chemical properties, this study also provides an evaluation of several potentially sensitive parameters. It uses different fuel samples, some of them hydrotreated. The results aimed to

highlight any areas of concern regarding engine operability or safety with a potentially different specification for aviation fuels. It is not intended to provide an exhaustive representation of the market fuel variability and thus cannot be regarded as a conclusive study, but more indicative for further research. The main observations are:

- Some key aviation fuel properties vary significantly with changing aromatic, naphthalene and sulphur content.

- Hydroprocessing always reduces the lubricty of the fuel. The lubricity results in this study are close to the limit even with mild hydroprocessing and this needs to be treated with caution. Reducing naphthalenes had the most severe reduction in lubricity, approaching the Wear Scar Diameter limit of 0.85mm.

- Fuel volatility is affected, as illustrated by the TVP measurements for naphthalenes and total aromatics variations. While issues such as vapor lock or cavitation in the pumps or injectors are not expected, reducing fuel volatility may have effects on the combustion process.

- Reactivity related properties such as derived cetane number (DCN) are affected, especially when aromatics are reduced. Cetane numbers were significantly higher for samples with low aromatics. However, the observed trend, which leads to increased reactivity is not only due to the reduction in aromatics but also results from a synergistic effect between the decrease in aromatics and the increase in naphthenes. This reactivity increase does not translate in other properties like the auto-ignition temperature (AIT). Indeed, while a reduction could be anticipated by simple chemical kinetic modelling, the experiments do not confirm this trend. It is assumed that the fuel composition proposed prevents any clear discussion on that matter. The same applies for the sulphur effect as hydrotreatment did not display any clear trend but a DCN increase is observed for the proposed variation. This suggests that the sulphur variation performed may be coupled with other compositional effects.

- In general, higher cetane numbers would change the combustion behaviour in the various combustor designs, and engine manufacturers would have to carefully asses these affects for potential issues.

- The heat capacity was affected within the samples tested, showing a slight decrease in heat capacity with decreasing aromatics. Nevertheless, above a total aromatic content of 7%wt, the heat capacity remained above the average value of Jet A-1 from the CRC survey 2006 [1].

- Neither thermal conductivity nor surface tension was affected by total aromatics or naphthalene content variations performed in this study.

There was no evidence in this study that the formulated fuels with lower aromatic, naphthalene and sulphur content would lead to values outside of the current aviation fuel specifications for the tested properties. However, directional changes were observed and further detailed studies on fuel compatibility will be required should changes in fuel specification be considered.

Fuel dielectric constant (permittivity) should also be featured in such studies as literature data indicates a significant influence of aromatics on this property, an attribute important for aircraft fuel gauging systems.

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GLOSSARY

AC	Advisory Circular
AIT	Auto-Ignition Temperature
ASTM	American Society for Testing and Materials
BOCLE	Ball-on-Cylinder Lubricity Evaluator
BPD	Barrel per day
CAPEX	Capital Expenditures
CD	Combustion Delay
CoMo	Cobalt Molybdene catalyst
Cp	Heat capacity
CRC	Coordinating Research Council
DCN	Derived Cetane Number
DefStan	Defense Standard (UK Ministry of Defense)
DSC	Differential Scanning Calorimetry
ETBE	Ethyl Tertiary Butyl Ether
EU	European
FAA	Federal Aviation Administration
FBP	Final Boiling Point
GCxGC	Two-dimensional gas chromatography
HVO	Hydrotreated Vegetable Oil
IASH	International Association for Stability, Handling, and Use of Liquid Fuels
ID	Ignition Delay
ISBL	Inside battery limits
ISSR	Ice Super-Saturated Regions
LBO	Lean Blow-Out
NiMo	Nickel Molybdene catalyst
nvPM	non-volatile Particulate Matter
OPEX	Operating Expenditure
LHSV	Liquid Hourly Space Velocity
LP	Linear Programming
MTPY	Millions of metric tons per year
ppH2	Partial pressure of hydrogen
Px	Pressure x
SAF	Sustainable Aviation Fuel
e-SAF	Sustainable Aviation Fuel made synthetically using renewable electricity
SAK	Synthetic Aromatic Kerosene
SBC	Synthetic Blending Component
SPK	Synthetic Paraffinic Kerosene
RQL	Rich burn Quick quench Lean
TVP	True Vapor Pressure
VP	Vapor Pressure
Vx	Volume x
WSD	Wear Scar Diameter

APPENDIX

APPENDIX 1 – LP MODEL: STRUCTURE AND BASE CASE ASSUMPTIONS

STRUCTURE

Linear Programming model

The purpose of an oil refinery is to turn crude oil into marketable products in the most efficient and economical way. A particular refinery generally serves a particular market which sets the quality of the products to be supplied and to an extent the amount of each grade. Depending on the geographical location of the refinery, there can also be opportunities to export to other markets. The refinery has access to certain crude oils and other feedstocks, the range of which is a function of its location and the way it is supplied (e.g. ships or pipelines). Finally, the refinery features a certain combination of process units (generally referred to as its configuration).

Refinery operation is thus characterised by multiple real constraints arising from feedstock supply, product demand (quantity and quality) and process unit limitations. Yet there are many ways of operating within these constraints and refiners have always strived to optimise their operation in order to maximise profit or minimise costs to supply a given market demand within a given set of product prices and input costs. The tool used to that end by refiners worldwide is known as Linear Programming (LP), a mathematical technique which, given a quantity to be optimised, aims at identifying the optimum solution amongst the myriads of possible solutions to a complex problem.

In an LP model the refinery constraints are represented by a system of linear equations linking the different variables. Because there are more degrees of freedom (or variables) than there are constraints, the system has an infinite number of possible solutions. Provided that appropriate cost factors are defined as model inputs (i.e. cost of feedstocks, energy, additional plant capacity, price of products etc.), a so-called “objective function” can be derived, describing the quantity to be optimised (maximum profit or minimum cost). The LP solver then provides a pathway towards the optimum solution.

For a given set of desired products, the LP solution tells the refiner how much of each available feedstock should be processed, the level at which each refinery process units will be utilised and, more generally, which amongst all the constraints will actually be binding. Crucially it also provides information on the impact on the objective function of a marginal change in each of the binding constraints (the so-called “marginal values”).

Concawe LP model main features

Since the mid-90s Concawe has operated a refinery LP model representing the combination of all refineries operating in the European Union (EU). This model was originally developed to estimate the cost to EU refiners of EU legislation (mostly affecting product quality) and of expected changes in EU market demands. Note that the model considers all the European refineries as one system therefore conclusions need to be read in the context of this overall generalisation and may not be true for each and every individual refinery.

Model structure

The model features a full library of refinery process units represented by a number of operating modes including feedstock type, product yield structure and all relevant quality parameters. From this a refinery can be modelled with any combination of process units.

A range of crude oils is available, representing the diversity of grades available to EU refiners, and a blending module allows finished products to be prepared according to the required quality specifications from selected intermediate streams.

CO_2 emissions modelling

In response to the CO_2 emissions challenge, the model was adapted in the early years of the last decade so that it could estimate the CO_2 emissions associated with a particular operating case. This primarily requires CO_2 emission factors for combustion of refinery fuels (t of CO_2 emitted per GJ of fuel burnt), combined with fixed unit-specific energy consumption factors (GJ per t unit feed). It must also consider structural emissions arising from specific chemical reactions (notably the production of hydrogen by reforming or partial oxidation of hydrocarbons), expressed in ton of CO_2 per ton of each feedstock type processed.

Because a refinery generally uses its own feeds or products for a proportion of its fuel needs, the carbon contained in the input to the refinery is apportioned between products and fuels. In order to avoid any spurious carbon gain or loss as a result, it is therefore essential that the model be strictly carbon-balanced (i.e. that the amount of carbon entering the refinery in the form of feedstocks and possibly fuels equals the amount that leaves the refinery in the form of CO_2 and products). In order to achieve this, the model is actually carbon, hydrogen, nitrogen, oxygen and sulphur balanced across each process unit, from the crude oil to the finished products.

In order for the model to optimise CO_2 emissions, these must have an impact on the objective function. In other words, CO_2 emissions must be assigned a monetary value if the CO_2 emissions should be optimised. As mentioned in the costing section above for this study no cost has been assigned to CO_2 emissions.

LP model main variables for optimisation

Crude oil throughput: total amount processed in the EU refining system is free, but the crude oil ratios are fixed to match average EU feedstock quality (refer to Crude slate section).

Oxygenates (ETBE, Ethanol, FAME, HVO and Rapeseed oil): total amount of imported oxygenates is open, but is indirectly limited by gasoline and diesel specifications, coprocessing constraints and ETBE production capacity.

Exports: only 2 gasoline grades are allowed to be exported (US and West African grades), limited by the amount observed in the reference year (2024).

Refining operations: routings of intermediate streams, severities and utilisation of process units are the major optimisation variables of the LP model. They represent the flexibility of the refineries to respond to market demands and constraints.

Calibration

This type of model, where individual refinery data is aggregated into one single large refinery model, is subject to over-optimisation (under-constrained system), because all process unit capacities are available simultaneously, significantly increasing the degrees of freedom of the refining system. To mitigate this risk of over-optimisation, a calibration run is performed at the beginning of each Concawe study where LP is involved.

A reference year is selected, 2024 for this study, for which all the input data are publicly available (EUROSTAT, Wood Mackenzie).

The main LP model inputs required for the calibration include the European average crude oils slate, the other imported products, the finished products demand (and qualities) and the

exported products amounts. In addition, the energy efficiency of the process units is tuned to match the overall CO_2 emissions of the refining system as measured for the reference year.

A calibration run is performed with the LP model to ensure that the optimisation can meet the demand pattern with similar amounts and types of refinery feedstocks as observed in real operation. In addition, it is essential that the optimisation faces the same constraints as the actual refineries to achieve the products demand. For this purpose, marginal values associated to demand constraints have been tuned to reflect the actual market. Tuning the marginal values is performed through tuning of the process units' capacities. More constrained/relaxed specific process units capacities result in more constrained/relaxed specific finished products production, hence impacting the marginal values of these specific finished products demand in both direction (increase or reduction).

This artificial way of tuning process unit's availability allows to reduce the over-optimization inherent to aggregated models. This can be seen as a conservative approach, as it may imply that the refining assets would not adapt to the future constraints. Decades of experience in regional LP modelling showed us that it remains the best way to proceed to get results as realistic as possible.

BASE CASE ASSUMPTIONS

This section presents the main assumptions that are most likely to affect the LP modelling results. The reference year considered for this study is 2024.

Crude Slate

The crude slate is derived from the EUROSTAT database. First, EUROSTAT crude oil volumes are aggregated per country of origin (production field). Then each country is matched with one of the 23 reference crude oils in the Concawe database. Some adjustments are then performed so that the overall crude slate API and Sulphur content match the average value reported in EUROSTAT.

Other Refinery feedstocks

For this study, the import of other refinery feedstocks has been simplified. Bio ETBE can be imported to satisfy the bio content of European Gasoline finished products. Similarly, HVO (from rapeseed) and bio-FAME can be imported to blended into Diesel finished product.

Bio Ethanol is used for refining ETBE production. Rapeseed oil is used as coprocessing feed in the Diesel hydrotreatment unit.

Refining finished products demand

Historical products demand is extracted mainly from Wood Mackenzie database, though EUROSTAT is also used for very specific data (Bitumen, lubes, waxes). More specifically for the LP model, European (EU) refining production is considered to be equal to the product demand because it corresponds to the actual constraint supported by the refining system. On one hand this means that finished product imports are not accounted for because they have no impact on the refining system. On the other hand, finished products net exports are accounted for because they are actually produced by the EU refining system.

Finished product specifications

Standard finished products specifications are used for the main products. However, for some specific grades, some assumptions and intermediate calculations are required.

Oxygenates and bio components in Gasoline

According to Fuels Quality Monitoring report (EU Commission), 2023 bio ethanol equivalent content of the gasoline consumed in Europe is around 6.8 vol%. This bio ethanol volume equivalent is converted into bio ETBE equivalent, which is by simplification the only component used in the LP model to match the gasoline bioenergy content.

Bio components in Road Diesel

From Wood Mackenzie data, bio content of Diesel is about 8.7 wt% in 2024. It is then assumed that this bio content is satisfied by FAME (75%) and HVO (25%).

Process unit capacities

Concawe owns a detailed database featuring the process units operating in European refineries, their designs, and capacities (including expansion projects and closures). These capacities are aggregated to determine the LP model process unit capacities.

Prices

Feed and product prices are mainly derived from Wood Mackenzie data. As crude slate and products demand are fixed, and only gasoline export is open, this costing has a very limited impact on the optimisation. It is noted that no CO_2 emissions cost has been implemented for this study.

Specific assumptions

For this study, the aromatic and naphthalene contents of the kerosene is crucial. From external sources provided by Concawe Members, it seems that the Concawe assays average aromatic content of the kerosene (150-250°C TBP cut points, perfect fractionation) is too low, around 11 vol% when more than 20 vol% is expected. Naphthalene content is within the expected range, around 1.4 vol%.

Prior to the study, the aromatic content of the kerosene cut of Concawe assays is adjusted so as to match around 20 vol% in the average crude slate. The final kerosene aromatic content obtained is 21.3 vol% and 1.3 vol% for the naphthalene content.

LIMITATIONS OF THE MODEL AND THE SET-UP USED FOR THIS STUDY

In this study the Concawe LP model was set as “single refinery – single region”: this means that there is a single refinery representing the aggregation of all European refineries (crude intakes, process units, capacities) supplying one market where all EU market demand is concentrated. This choice brings some benefits but also carries some limitations.

Aggregating all refineries into one generates a site with an extreme variety of units installed. The flexibility within such refinery to modify the processes and react to changes in demand and specifications is way higher than what individual refineries can realistically achieve. Having a large set of different blending components makes way easier generating a new product (or a product with a new specification). Moreover, if a refinery has only one a merox unit, it cannot reduce its production and increase the hydrotreater utilisation so a situation like the one of Set 1 and 2 are infeasible.

A change of specifications, like the one analysed in this study, affects all refineries simultaneously: all product on the market must be compliant with the same rules so distinguishing regions when no market differences are present is unnecessary. The downside is that the geographical dimension is lost. Not all areas in Europe would be equally impacted as refineries with different configurations are not equally distributed.

Still on the geographical perspective, having all units aggregated creates more space for optimisation: normally units are not running constantly at maximum so there is some unused capacity. Some fragmented spare capacity brings limited benefits as the possibility to increase production might be far from where the product is needed so the benefit of the extra production might be undercut by high logistic costs to deliver the product in a distant region.

Also, all cases would imply massive logistic efforts to exchange components and deliver products around Europe: this will likely be infeasible due to logistic limitations or be extremely expensive to find alternative routes and solutions.

The last major point, which is more practical than mathematical, is that a common optimisation of all refineries does not exist. Optimisation, by definition, tries to find the optimal solution. All results imply a coordinated effort amongst all refineries to supply the market. European refineries belong to different competing companies with different priorities and independent decision-making processes. Market opportunities might be visible to everybody but the way to answer them may be extremely different depending on the subject taking the decision.

APPENDIX 2 – EXAMPLE OF MULTI-LINEAR REGRESSIONS FROM IFPEN DATA

This section illustrates how LP modelling of Kerosene Hydrotreatment performances is derived from IFPEN data. A full review of the 720 data sets has been omitted as excessive.

Assuming the following aviation fuel specifications, Aromatic content ≤ 8 vol%, Naphthalene content ≤ 0.2 vol% and Sulphur content ≤ 0.05 wt%, it can be asserted that a Kerosene Hydrotreatment operating at 53.4 bars, with a LHSV of 1 hr-1 and a high activity catalyst will allow the targeted specifications to be met.

At these conditions, IFPEN has provided performance for 6 kerosenes, derived from 6 different crude oils.

Table 12 *Extract of IFPEN Kerosene Hydrotreatment data*

Source	Arabian Light	Ekofisk	Forcados	Maya	Statfjord	Tengiz
Data set #	27	147	267	387	507	627
Estimated total pressure, barg	53.4	53.4	53.4	53.4	53.4	53.4
LHSV, hr^{-1}	1	1	1	1	1	1
Catalyst Activity	High	High	High	High	High	High
Feed qualities						
Specific Gravity	0.789	0.800	0.832	0.799	0.801	0.795
Sulphur, wt%	0.1937	0.0080	0.0365	0.7465	0.0183	0.2641
Aromatics, wt%	16.3	17.9	19.8	17.8	18.1	17.3
Naphthalenes, vol%	0.9	1.1	2.1	1.3	1.7	1.0
Performances						
Desulphurisation, % (Sulphur reduction)	99.98	99.99	100.00	100.00	100.00	100.00
Dearomatisation, % (Aromatics reduction)	60.11	59.44	50.39	59.68	59.40	59.90
Dediaromatisation, % (Naphthalenes reduction)	96.54	94.97	86.42	95.92	96.48	95.51

In the Concawe LP model kerosene comes from 23 different crude oils, consequently the Hydrotreatment unit feed is a mixture of these 23 kerosenes. To match the Concawe LP model structure, it is required to be able to predict Kerosene Hydrotreatment performance as a function of the feed mixture qualities in addition to the operating parameters of the unit. For this purpose, multi-linear regressions of unit performances are derived as function of feed qualities.

In LP modelling, it is usual to model yields and qualities prediction using a reference point as a pivot. The linear regression is then in the form of:

$$y = y_0 + \sum_i \frac{d(\Delta y)}{d(\Delta p_i)}(p_i - p_0)$$

Where *y* is the dependent parameter to predict (yield, quality), p_i the independent parameters (unit operating parameter, feed quality) and *0* index the corresponding values at the reference point. The multi-linear regressions are then in the form of:

$$\Delta y = f(\Delta p_i)$$

By convention, the reference point selected for all the regressions is the Arabian Light data set. The following table shows the results of the regressions generated from the data in ***Table 12***.

Table 13 *Example of HT multi-linear regression coefficients*

Regression parameter (Unit feed qualities)	**Δ Specific Gravity** -	**Δ Sulphur content** wt ppm	**Δ Aromatic content** wt%	**Δ Naphthalenes content** wt%
Δ Desulphurisation, % (Sulphur reduction)	-0.0067347	0.0000000	0.0001570	-0.0000324
Δ Dearomatisation, % (Aromatics reduction)	-4.1860123	0.0000000	0.0237695	-0.0011185
Δ Dediaromatisation, % (Naphthalenes reduction)	-4.5927141	0.0000001	0.0173670	0.0292383

For example, the Dearomatisation prediction equation is written in the LP model as:

$$HDA = HDA_0 + \alpha_{SPG}(SPG - SPG_0) + \alpha_{SUL}(SUL - SUL_0) + \alpha_{ARO}(ARO - ARO_0) + \alpha_{NPH}(NPH - NPH_0)$$

Where *HDA* is the predicted dearomatisation, *SPG* the feed specific gravity, *SUL* the feed sulphur content, *ARO* the feed aromatics content and *NPH* the feed naphthalenes content and *0* index the corresponding values for Arabian Light data set. Numerically:

$$HDA = 0.6011 - 4.1860123 \times (SPG - 0.789) + 0.0000000 \times (SUL - 1937) + 0.0237695 \times (ARO - 16.3) - 0.0011185 \times (NPH - 0.9)$$

It is acknowledged that the robustness of a regression based on 6 data points cannot be asserted. However, this methodology gives sufficient accuracy to predict Kerosene Hydrotreatment performance for feed qualities close to the region of IFPEN data points.

It should be noted that more Kerosene Hydrotreatment unit performance information is retrieved from the IFPEN data than is shown for the example in this section: unit hydrogen consumption, product specific gravity, power, steam and fuel gas consumptions, CAPEX, catalyst cost.

APPENDIX 3 - FUEL MATRIX PHYSICAL CHEMICAL PROPERTIES

Property	unit	Method	fuel 1	fuel 2	fuel 3	fuel 4
Density at 15°C	g/cm3	IFPEN 2427	0.807	0.8118	0.8115	0.8102
Distillation		ISO 3405				
IBP	° C	ASTM D86	192.8	144.2	146.3	144.6
5	° C		203.8	161.8	163.6	162.6
10	° C		204.8	165.7	167.3	166.5
20	° C		206.4	172	173.2	172.6
30	° C		208.4	179.1	180	179.6
40	° C		211	187.9	189.2	188.7
50	° C		213.9	198.7	199.4	198.9
60	° C		217.1	210.2	210.6	210.3
70	° C		220.7	222.6	222.6	222
80	° C		225.3	234.8	234.4	234
90	° C		232.2	249	248	247.5
95	° C		238.5	258.2	256.8	256.7
FBP	° C		247.1	267	266.7	266.8
Distillat	% v/v		98.6	98.5	98.9	98.7
Residu	% v/v		1	0.7	1	1.2
Pertes	% v/v		0.4	0.8	0.1	0.1
Sulphur	ppm	ASTM D4294	2.7	230.1	17.0	8.0
Freezing point	°C	ASTM D7153	-51.0	-51.0	-50.9	-50.9
Flash point	°C	ASTM D3242	68	41.5	43	43
Total aromatics	%wt	GC*GC internal	4.50	19.77	19.69	18.57
Naphthalenes	%wt	GC*GC internal	-	2.77	1.40	0.37
Electric conductivity	pS/m	ASTM D2624	400	5	1	2
Mercaptans basses teneurs	ppm	IFPEN 1925				
Mercaptans fortes teneurs	ppm	IFPEN 1926		5.7	<3	<3
Viscosity at -20°C	mm2/s	NF EN ISO 3104	6.31	4.36	4.40	4.39
Smoke point	mm	ISO 3014	37.5	22	22	23
Acid number	mgKOH/g	ASTM D 664A	< 0.5	0.019	0.004	0.003
Neat heat combustion	MJ/kg	ASTM D4529	43.46	43.14	43.14	43.18
Lubricity	mm	ASTM D5001	0.78	0.57	0.64	0.7
DCN		ASTM D7668	52.3	42.3	44.2	43.2
DVPE	kPa	ASTM D 5191	< 15.5	1	1	1.8
TVP at 25°C	kPa	ASTM D 6378 18a		0.7		1
TVP at 38°C	kPa	ASTM D 6378 18a		1.5		1.9
TVP at 60°C	kPa	ASTM D 6378 18a		3.7		3.9
TVP at 80°C	kPa	ASTM D 6378 18a		7.6		7.6
TVP at 100°C	kPa	ASTM D 6378 18a		14.4		14.5
AIT	°C	ASTM E 659	225		235	251
Thermal conductivity	mW/K*m	ASTM D2717 :1995	118.9			119.6
Thermal diffusivity	mm2/s	ASTM D2717 :1995	84			
Surface tension at 25°C	mN/m	EN 14370	30.13	29.96	29.61	29.88

Property	unit	Method	blend 1	blend 2	blend 3	blend 4
Density at 15°C	g/cm3	IFPEN 2427	0.8083			
Distillation		ISO 3405				
IBP	° C	ASTM D86	191.1			
5	° C		201.6			
10	° C		202.9			
20	° C		204.6			
30	° C		207.1			
40	° C		210.1			
50	° C		213.1			
60	° C		216.6			
70	° C		220.5			
80	° C		225.3			
90	° C		232.3			
95	° C		238.7			
FBP	° C		247.4			
Distillat	% v/v		98.4			
Residu	% v/v		1.1			
Pertes	% v/v		0.5			
Sulphur	ppm	ASTM D4294	2.7	2.7	2.6	2.7
Freezing point	°C	ASTM D7153				
Flash point	°C	ASTM D3242				
Total aromatics	%wt	GC*GC internal	6.57	6.03	7.24	11.10
Naphthalenes	%wt	GC*GC internal	-	0.52	2.87	3.19
Hydrogen	%wt	GC*GC internal	14.2	14.2	14.0	13.9
Electric conductivity	pS/m	ASTM D2624				
Mercaptans basses teneurs	ppm	IFPEN 1925				
Mercaptans fortes teneurs	ppm	IFPEN 1926				
Viscosity at -20°C	mm2/s	NF EN ISO 3104				
Smoke point	mm	ISO 3014				
Acid number	mgKOH/g	ASTM D 664A				
Neat heat combustion	MJ/kg	ASTM D4529				
Lubricity	mm	ASTM D5001	0.76	0.68	0.66	0.59
DCN		ASTM D7668	52.1	53.2	52.8	50.7
DVPE	kPa	ASTM D 5191				
TVP at 25°C	kPa	ASTM D 6378 18a	0.4	0.2	0	
TVP at 38°C	kPa	ASTM D 6378 18a	1	0.7	0.5	
TVP at 60°C	kPa	ASTM D 6378 18a	2	1.6	1.4	
TVP at 80°C	kPa	ASTM D 6378 18a	3.9	3.4	3	
TVP at 100°C	kPa	ASTM D 6378 18a	7.6	6.2	5.8	
AIT	°C	ASTM E 659	226	228	227	243
Thermal conductivity	mW/K*m	ASTM D2717 :1995		119.3	119.4	119.7
Thermal diffusivity	mm2/s	ASTM D2717 :1995				84
Surface tension at 25°C	mN/m	EN 14370	30.13	29.67	29.68	

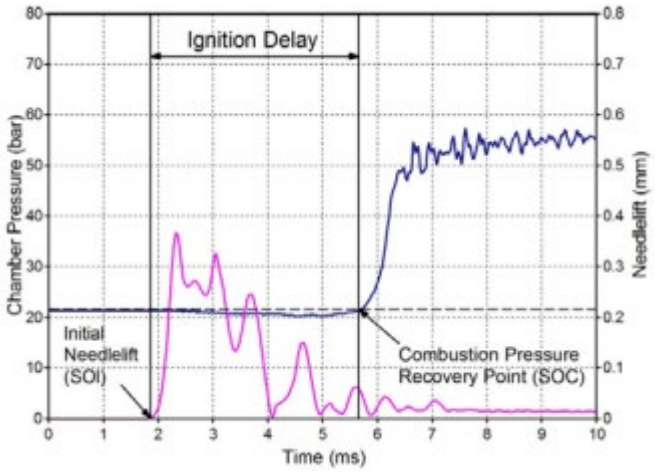
Property	unit	Method	blend 5	blend 6	blend 7	S50	S100
Density at 15°C	g/cm3	IFPEN 2427	0.8133	0.8211	0.8146		
Distillation		ISO 3405					
IBP	° C	ASTM D86	146.2	179.5	145.9		
5	° C		163.4	192.8	164.1		
10	° C		167.3	193.8	167.4		
20	° C		173.7	196.5	174.3		
30	° C		180.9	199.7	181.3		
40	° C		190.1	203.6	190		
50	° C		200.4	208	200.5		
60	° C		211.3	212.5	211.5		
70	° C		223.1	217.5	222.9		
80	° C		234.9	223	234.6		
90	° C		248	230.4	248.1		
95	° C		257.3	236.9	257.5		
FBP	° C		267.4	246.9	267.2		
Distillat	% v/v		98.6	98.6	98.5		
Residu	% v/v		1.1	1.1	1		
Pertes	% v/v		0.3	0.3	0.5		
Sulphur	ppm	ASTM D4294	16.9	2.6	16.8	46.7	100.5
Freezing point	°C	ASTM D7153					
Flash point	°C	ASTM D3242					
Total aromatics	%wt	GC*GC internal	20.46	20.68	21.08	20.51	20.33
Naphthalenes	%wt	GC*GC internal	2.35	2.89	3.12	2.45	2.59
Hydrogen	%wt	GC*GC internal	13.7	13.5	13.6	13.7	13.7
Electric conductivity	pS/m	ASTM D2624					
Mercaptans basses teneurs	ppm	IFPEN 1925					
Mercaptans fortes teneurs	ppm	IFPEN 1926					
Viscosity at -20°C	mm2/s	NF EN ISO 3104					
Smoke point	mm	ISO 3014					
Acid number	mgKOH/g	ASTM D 664A					
Neat heat combustion	MJ/kg	ASTM D4529					
Lubricity	mm	ASTM D5001	0.65	0.69	0.61	0.64	0.63
DCN		ASTM D7668	44.5		44.2	45.9	45.4
DVPE	kPa	ASTM D 5191					
TVP at 25°C	kPa	ASTM D 6378 18a	0.6	0.3	1.5		
TVP at 38°C	kPa	ASTM D 6378 18a	1.4	0.8	2.7		
TVP at 60°C	kPa	ASTM D 6378 18a	3.6	1.9	5.5		
TVP at 80°C	kPa	ASTM D 6378 18a	7.2	3.8	10.6		
TVP at 100°C	kPa	ASTM D 6378 18a	13.9	7.3	19.5		
AIT	°C	ASTM E 659			231		
Thermal conductivity	mW/K*m	ASTM D2717 :1995			120.2		
Thermal diffusivity	mm2/s	ASTM D2717 :1995					
Surface tension at 25°C	mN/m	EN 14370	29.89	30.11	29.9	29.38	29.44

APPENDIX 4 - EXPERIMENTAL METHODS

Derived cetane number (DCN) - ASTM D7668

DCN (derived cetane number) analysis uses a constant-volume combustion chamber that is heated and pre-filled with compressed air. A small fuel sample is injected directly into the chamber at a controlled temperature. This causes an auto-igniting combustion cycle, which is detected by a pressure sensor. Each injection generates a pressure wave (Figure 35) from the combustion of the fuel.

Figure 35 *Pressure wave in the chamber depicting IQT ignition delay time [49]*

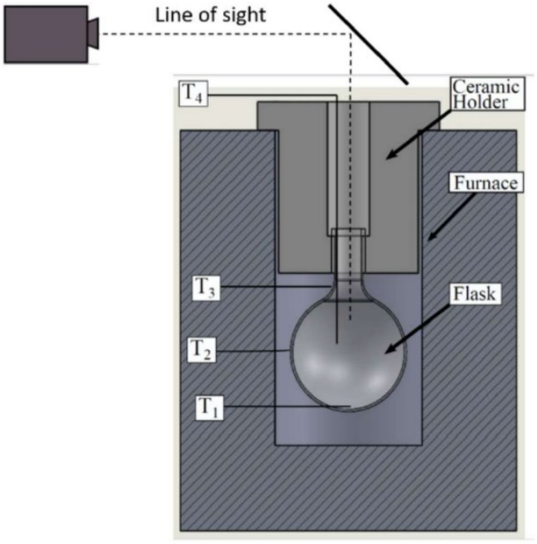


The main parameters measured are ignition delay (ID) and combustion delay (CD). The ID and CD values from 15 auto-ignition cycles are statistically analysed, with outliers eliminated and the remaining results averaged. These averages are then converted into a DCN using an equation dependent on ID and CD, as defined in the ASTM D 7668 standard. The resulting DCN is used to characterize the auto-ignition of a fuel and correlates well with cetane number (CN) measured with the ASTM D 613. This method is applicable to DCNs between 38.45 and 64.35.

Auto-ignition temperature (AIT) - ASTM E659

Analysing the autoignition temperature (AIT) of a chemical product involves determining the minimum temperature at which the product ignites spontaneously upon contact with air without external energy input. To perform this analysis, a 500 mL spherical flask (Figure 36) is heated to a predefined temperature. 0.1 mL of the liquid sample is then introduced into the flask thought the open top. The system in then visually monitored for 10 min to detect any ignition event, indicated by a visible flash of light. If no ignition is detected, the temperature setpoint is increased progressively and the sample injection and observation is repeated. If the ignition occurs the temperature is decreased progressively, and the procedure is repeated until the temperature transitions between ignition and non-ignition.

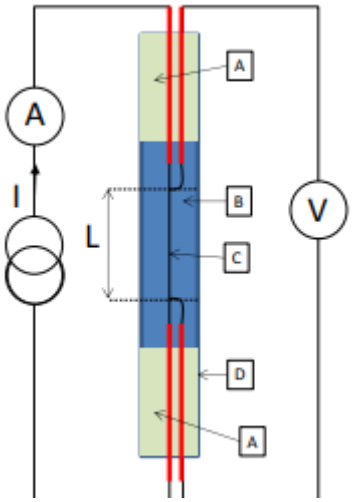
Figure 36 Schematic diagram of AIT measurement [22]



Thermal conductivity – ASTM D2717

During the analysis of the thermal conductivity (ASTM D 2717), a platinum wire (Figure 37) is inserted into a cell containing a liquid sample and is then electrically heated. This heating creates a temperature gradient within the liquid sample. The temperature variation thus generated, linked to the variation in the electrical resistance of the wire, is used to calculate the thermal conductivity of the fluid. The method is based on the assumption of an infinitely long wire with negligible diameter and no thermal capacity, immersed in the fluid to be analysed. The wire acts as a heat source, generating a thermal field in the fluid that causes convective movements. The amplitude and duration of this heat flow directly influence the fluid's thermal response, and thus its conductivity measurement.

Figure 37 Schematic diagram of thermal conductivity measurement [50].

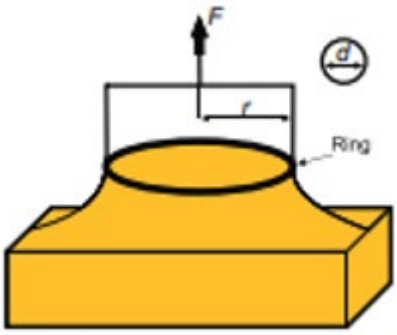


Note on Figure 36: A - cylinders, B - sample, C - Platinum wire, D - glass tube

Surface tension – EN 14370

This method measures the static surface tension of various liquids, including solutions containing surfactants, as well as organic and inorganic compounds. A glass container filled with the liquid sample is placed in a thermostatic bath within the tensiometer. A temperature sensor is immersed in the liquid to precisely control its temperature, and the liquid is left to stand until a stable thermal equilibrium is reached prior to measurement. To measure the interface force, a ring is immersed and pulled multiple times in the sample in order to create a meniscus Figure 38.

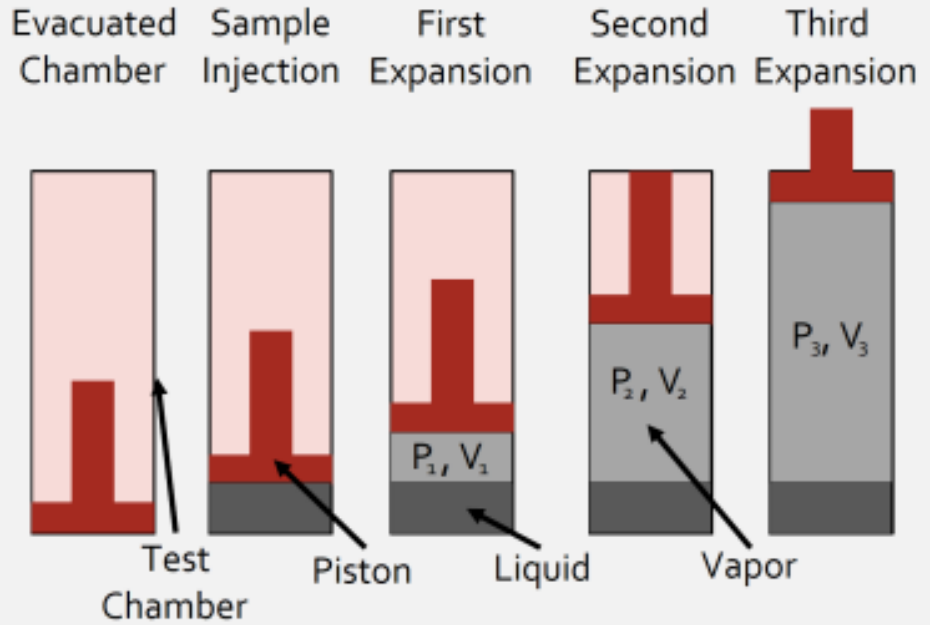
Figure 38 Schematic diagram of surface tension measure [51].



True vapor pressure (TVP) – ASTM D6378

This method applies to liquids with boiling points above 0°C and vapor pressures between 7 kPa (1.0 psi) and 150 kPa (21 psi) at 37.8°C.
The test begins with the introduction of a known volume of the sample into a sealed chamber with piston where the temperature is controlled. Once sealed, the temperature is raised to a specified target while the chamber volume is expanded for the first time (Figure 39). Then, two additional volume expansions are performed until the final volume is equal to (X + 1) times the initial sample volume. At each expansion, the total pressure inside the chamber is measured.

Figure 39 Schematic diagram of the three-expansion method [52]



These three pressure values are then used to calculate the vapor pressure of the sample, according to the following equation:

$$VP = P_3 - \frac{(P_1 - P_3)(P_2 - P_3)}{\frac{V_3 - V_1}{V_2 - V_1}(P_1 - P_2) - (P_1 - P_3)}$$

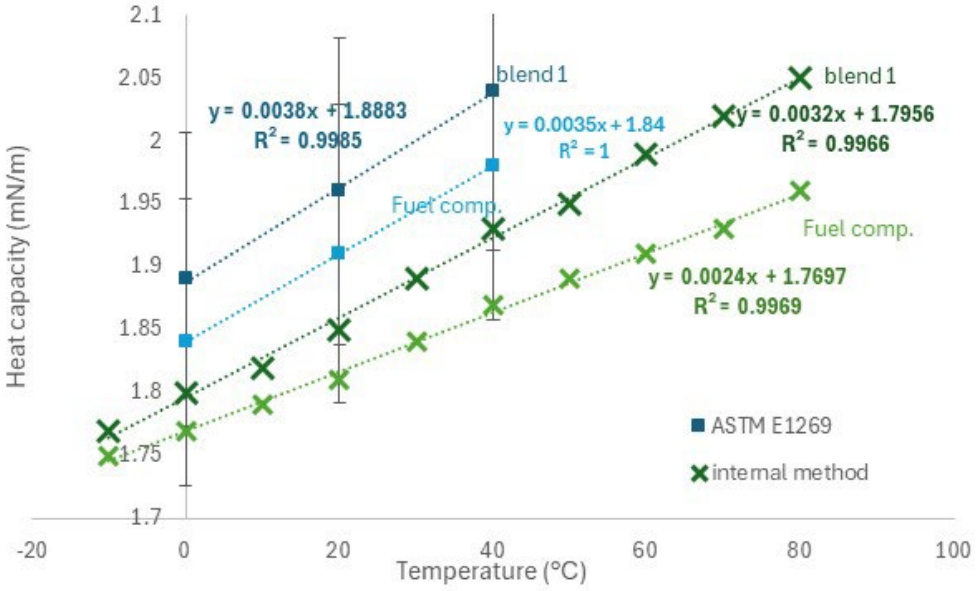
Equation 1 Formula for determining the vapor pressure with the three-expansion method [52]

Heat capacity –ASTM E1269 and IFPEN method

The ASTM E1269 for determining the specific heat capacity using Differential Scanning Calorimetry (DSC) starts by recording a baseline by heating an empty container to account for the thermal inertia of the system. Then, a pure reference material, such as sapphire, is tested under the same conditions and the specific heat values of this reference are used for calibration. Finally, the real sample is measured using the same parameters. The specific heat of the sample can be determined by comparing the reference and sample heat flows.

In this study, the mixtures were analysed using an internal method known as the direct method, with an uncertainty of 10%. This method directly calculates the specific heat capacity (Cp) by dividing the heat flux signal by the heating rate and sample mass.
To assess the reliability of the direct method, it was compared with the standardized method based on ASTM E1269, in which the specific heat (Cp) is measured with a mico DSC device. The results of the blend 1 and another fuel formulated with fuel 1, solvesso 100, 150 and 200 were compared (Figure 40). The results showed small and insignificant differences between the two methods, leading to the conclusion that the internal method can be used with minimal risk of error.
The ASTM E1269 repeatability is used as a reference for the internal results due to significant similarities in the methods.

Figure 40 Comparison of the ASTM E1269 and internal method for heat capacity testing

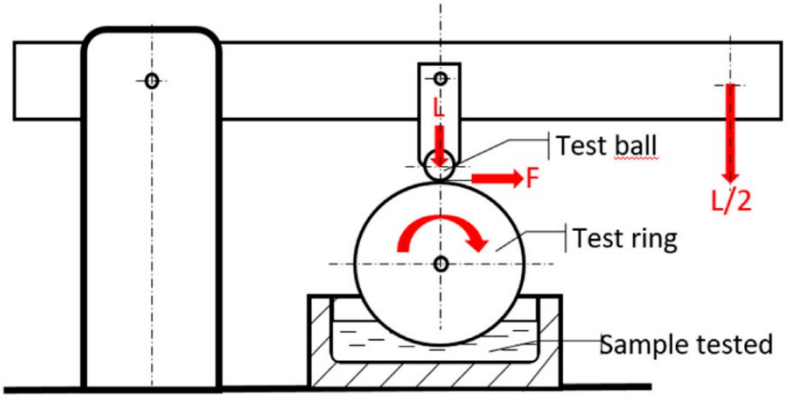


Lubricity – ASTM D5001

The lubricating performance of jet fuel is evaluated using the Ball-on-Cylinder Lubricity Evaluator (BOCLE) (Figure 41) method. In this setup, the test fluid is placed in a temperature and humidity-controlled chamber. A fixed steel ball is pressed against a rotating steel cylinder that is partially immersed in the test fluid and held under constant load.

Contact friction causes wear on the ball's surface. After the test, the diameter of the wear scar on the ball is measured under a microscope, which gives an indication of the lubricating capacity of the fluid. The smaller the wear scar diameter, the better the lubricity of the fluid.

Figure 41 Schematic diagram of BOCLE measurement [53] .



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