FAA Continuous Lower Energy, Emissions, and Noise (CLEEN II) Technologies Program

Rolls-Royce CLEEN II Sustainable Aviation Fuels – Public Version

OTA Number:
DTFAWA-15-A-80012

Engineering Department Report (EDR)

EDNS04000136234/002

APPROVED FOR PUBLIC RELEASE

FAA Continuous Lower Energy, Emissions, and Noise (CLEEN II) Technologies Program

Rolls-Royce CLEEN II Sustainable Aviation Fuels – Public Version

OTA Number:
DTFAWA-15-A-80012

Engineering Department Report (EDR)

EDNS04000136234/002

October 2021

Revision History
EDNS04000136234

Revision	Date	Comments
001	August 2021	Initial issue of Public Technical Report- Brad Wall
002	October 2021	Incorporated FAA comments

Table of Contents

List of Figures

List of Tables

Acronyms and Abbreviations

ASTM	American Society of Testing and Materials
ATJ-SKA	alcohol-to-jet synthetic kerosene with aromatics
a.u.	arbitrary units
BOCLE	Ball-on-Cylinder Lubricity Evaluator
CAAFI	Commercial Aviation Alternative Fuels Initiative
CLEEN	Continuous Lower Energy, Emissions, and Noise
CO	carbon monoxide
CO_2	carbon dioxide
CSD	cross-sectional diameter
cSt	centistoke
EI	emission indices
ERC	Energy Research Consultants
EtOH	ethanol
EU	European Union
f/a	fuel-air ratio
FAA	Federal Aviation Administration
FANN	full annular
FFP	fit for purpose
FSN	fuel spray nozzle
FT	Fischer Tropsch
H_2	hydrogen
HEFA	hydroprocessed esters and free fatty acids
in.	inch
IRHD	International Rubber Hardness Degrees
LBO	lean blow out
M	million
mm	millimeter
NextGen	next-generation
NHC	net heat of combustion
NOx	nitrogen oxide
PDI	phase Doppler interferometry
SAF	sustainable aviation fuel
SH	sulfur-hydrogen
SMD	Sauter mean diameter
SPK	synthetic paraffinic kerosene
UDRI	University of Dayton Research Institute
UHC	unburned hydrocarbon
U.S.	United States
WSD	wear scar diameter

Summary

The Federal Aviation Administration (FAA) Continuous Lower Energy, Emissions, and Noise (CLEEN II) program is a next-generation (NextGen) effort to accelerate development and commercial deployment of environmentally promising aircraft technologies and sustainable alternative fuels. Rolls-Royce, a key partner of this program, is promoting the development and introduction of viable, renewable alternative fuels to achieve the NextGen Air Transportation System goals.

The Rolls-Royce CLEEN II Sustainable Aviation Fuel program has succeeded in promoting the introduction of a viable 100% sustainable aviation fuel as a possible future candidate fuel, thus contributing to the achievement of the FAA's NextGen Air Transportation System goals. This program was designed to push past the current 50% blend wall by determining the feasibility of using fully-synthetic sustainable aviation fuels in aircraft systems. The LanzaTech ATJ-SKA fuel was characterized under engine representative conditions and found to have the potential to be included in national and international aviation fuel specifications. This program advanced the scientific understanding of these fuels and therefore supports the longer-term aim to increase the use of sustainable fuel within the aviation transport sector and thus improve the overall environmental performance relative to current operations. The results and information from this program will contribute to existing industry work streams aimed at enabling increased use of sustainable fuels for aviation. In addition, the outcomes of this program complement current work under the auspices of several organizations, including the Commercial Aviation Alternative Fuels Initiative (CAAFI), ASTM International, and European Union (EU) and the U.S. Government.

This robust evaluation program has characterized a novel fully-synthetic fuel's performance under representative engine conditions. The goal has been accomplished through a series of "back-to-back" rig tests with conventional Jet A fuel assessing the fuel's impact on combustor performance and emissions. Elastomeric seal performance has also been assessed using the innovative Elastocon rig capability developed and demonstrated under CLEEN I.

Rolls-Royce conducted a series of laboratory, material, and rig tests to demonstrate the acceptability of fully-synthetic alcohol-to-jet synthetic kerosene with aromatics (ATJ-SKA). Rolls-Royce teamed with LanzaTech and Swift Fuels to provide the ATJ-SKA fuel for the program.

The test program included:

- Laboratory analysis
- Fuel spray characterization
- Ignition and lean blow out testing
- Emissions testing
- Elastomer material compatibility

This report has been prepared as part of the Rolls-Royce and FAA CLEEN II program to assess future potential sustainable aviation fuels. This document constitutes the Final Public Test Report for the Rolls-Royce Sustainable Aviation Fuel Program.

1. Introduction

This report has been prepared as part of the Rolls-Royce and FAA CLEEN II program to promote the introduction of viable sustainable aviation fuels (SAFs) to achieve the NextGen Air Transportation System goals.

Rolls-Royce Corporation in Indianapolis, Indiana (henceforth referred to here as Rolls-Royce) is dedicated to supporting the development and introduction of sustainable aviation fuels. As a leader in the aerospace industry, Rolls-Royce has long been committed to promoting fuel technologies of the future that will protect our communities and our environment, thus lowering our carbon footprint. This program provides an important next step in the advancement of this technology and supports SAF rapid introduction, satisfying the stated goals of CLEEN II and the NextGen Air Transportation System.

The Rolls-Royce CLEEN II SAF program was designed to push past the current 50% blend wall by determining the feasibility of using sustainable aviation fuels in aircraft systems. A fully-synthetic SAF was tested back-to-back with conventional fuel to assess the fuel's impact on combustion performance, elastomer compatibility and emissions under engine realistic conditions. Rolls-Royce conducted a series of laboratory, material, and rig tests to demonstrate the fuels acceptability.

The testing conducted included:

- Laboratory analysis
- Fuel spray characterization
- Ignition and lean blow out testing
- Emissions testing
- Elastomer material compatibility

This document constitutes the Final Public Test Report for the testing performed under the Rolls-Royce CLEEN II Sustainable Aviation Fuel Program.

2. Glossary of Terms

Aromatics	Unsaturated ring hydrocarbon compounds.
ASTM D1655 (Jet A/A-1)	Internationally recognized specification defining requirement for conventional jet fuel. This specification allows the use of fuel manufactured to ASTM D7566.
ASTM D7566	Specification defining requirements for jet fuel manufactured from blends of conventional fuel and synthetically derived fuels.
ATJ-SKA	Fully-synthetic fuel used in this program known as alcohol-to-jet synthetic kerosene with aromatics.
Conventional Fuel	Mixtures of paraffins and aromatics (nom 8% - 25%) derived wholly from conventional petroleum sources (mainly crude oil) using established processes.
Cycloparaffin	A paraffin that is a saturated cyclic hydrocarbon.
Hydrotreating/Hydroprocessing	Refining method of removing reactive and non-reactive (i.e., sulfur and olefins) compounds by reaction of hydrogen over catalysts. Severe conditions can also change the chain length and produce SPK in the jet fuel range.
Iso-paraffin	Normal paraffins that are open, straight-chain saturated hydrocarbons.
Mesitylene	Mesitylene is a 1,3,5-Trimethylbenzene, which is a benzene ring with three methyl groups attached. This aromatic was blended in the ATJ fuel.
N-paraffin	A paraffinic hydrocarbon of branched-chain structure.
Synthetic	Blends stocks or final product derived from non-petroleum sources.
Synthetic Paraffinic Kerosene (SPK)	Saturated paraffins comprising normal – straight chain, iso – branched chains, and cyclo – saturated ring types. These molecules occur in conventional fuels but SPK refers to products made synthetically.

3. Program Overview

3.1 Overall Program Objectives

The Rolls-Royce CLEEN II SAF program has been designed to push past the current 50% blend wall and determine the feasibility of using 100% sustainable aviation fuels in aircraft systems. The objective of this program is to evaluate sustainable aviation fuels that have the ultimate potential to be included in national and international aviation fuel specifications. This advances the scientific understanding and therefore supports the longer-term aim to increase the use of sustainable fuel within the aviation transport sector and thus improve the overall environmental performance relative to current operations. It also supports the inclusion of increased non-petroleum based products in jet fuel that will provide benefits in terms of fuel price stability, availability and possibly engine performance and emissions.

The following focus was followed during the design and execution of this test program:

- Promotes the development and introduction of viable renewable alternative fuels to achieve NextGen Air Transportation system goals
- A robust evaluation program that characterized a fully-synthetic fuel’s performance under representative engine conditions
- Accomplished through a series of back-to-back rig tests with conventional Jet A fuel
- Fuel chemistry/properties relationship upon fuel spray, combustor performance, operability, and emissions
- Understand elastomeric seal performance due to cyclic fuel switching under more realistic engine conditions
- Data generated can be shared with the ASTM Aviation Fuel Community and aid in fuel certification process

The program consisted of laboratory scale testing of candidate SAF leading to rig scale testing. Testing includes the characterization of key fuel properties that impact engine performance, handling, emissions, system material compatibility and cost of ownership. This technical report provides a way to share the data within the industry to provide the basis for further research and development programs to evaluate, approve, and introduce into the market place SAFs that are considered suitable for use and viable for production at a scale that will make a significant impact on aviation fuel supplies. It is also intended that results and information from this program will contribute to existing industry work streams aimed at enabling increased use of sustainable fuels for aviation. The outcomes of this program complement current work under the auspices of several organizations, including the CAAFI, ASTM International, and EU and the U.S. Government. Particularly for ASTM activity, work is focused on approval of fuels for revenue use.

Rolls-Royce believes this program supports the FAA’s goal to promote the development and introduction of viable renewable alternative fuels in engine systems, thus meeting NextGen Air Transportation system goals. The outcome of this program complements the work being carried out by the CAAFI and ASTM Aviation Fuel groups for the evaluation and qualification of viable sustainable aviation fuels.

3.2 Program Elements

Under the Rolls-Royce CLEEN II SAF program, a fully-synthetic SAF was tested back-to-back with conventional fuel to assess the fuel’s impact on engine systems under engine realistic conditions. This program conducted activities necessary to further understand the relationship between fuel composition and properties (viscosity, density, material compatibility, etc.), combustor performance and operability, gaseous and particulate emissions, and elastomer compatibility. Rolls-Royce used a sequential and methodical test approach to evaluate the performance of an SAF. This evaluation program was conducted in accordance with ASTM D4054 standard practice. The testing conducted included:

- Laboratory analysis
- Fuel spray characterization
- Ignition and lean blow out testing
- Emissions testing
- Elastomer material compatibility

Overall elements of the evaluation program included:

- Candidate fuel down-selection
- Laboratory test program
- Rig test program
- SAF assessment and reporting

Key points to note on the design of the program are:

1) The general progression from specification, through laboratory scale, fit for purpose testing, and then onto rig testing reflects the process used in ASTM D4054 [Ref. 1].
2) This program uses some of the test methods and compares results to limits contained in ASTM D7566 [Ref. 2], ASTM D1655 [Ref. 3], or ASTM D4054, but is nowhere near comprehensive enough to provide approval for use where specific OEM hardware tests may be needed.
3) Each stage of testing provides the basis and support for the next level of testing. For example, detailed laboratory analysis allows interpretation and explanation of how and why candidate fuels behave as they do in subsequent testing.
4) Results will therefore provide an indication of:
    a. The potential for candidate fuel to succeed through the ASTM approval process.
    b. The potential for the current restrictive limits to be relaxed in certain cases.
    c. The potential risks and/or benefits of changing fuel specification limits in terms of engine operation, emissions, performance, etc.

3.2.1 Candidate Fuel Down-selection

Rolls-Royce identified, in cooperation with the FAA, one sustainable jet fuel to be tested. The fuel was down-selected from a broad range of potential fuel suppliers, understanding the fuels potential, information on raw materials, processes, maturity, and potential sustainability. The candidate fuels requirements were set in in terms of suitability, sustainability, and industrial capability. This activity defined and ensured agreement between all parties regarding selection of candidate fuel for further examination and testing within the program. Once identified, the subject SAF was acquired for the test program.

3.2.2 Laboratory Test Program

Laboratory testing included standard specification testing and additional fit for purpose (FFP) testing of candidate fuel. The details of FFP testing were based on a rational review of the candidate fuels' chemical, physical, and performance properties. Aspects where sufficient evidence or experience was already available to predict outcome were not tested. Such testing was carried out in accordance with ASTM D4054 and ASTM D1655/D7566 so data generated would contribute to the assessment of potential approval but would not include the full suite of testing required. Fuel samples for analysis were taken at various stages of the program including initial bulk shipment, both before and after each of the tests, to ensure consistency.

3.2.3 Rig Test Program

3.2.3.1 Fuel Spray Characterization

Because alternative fuel properties relevant to atomization may significantly deviate from those of conventional jet fuels, it is important to assess the spray quality of the fuel to provide better prediction of the combustion characteristics and emissions. Rolls-Royce conducted a series of tests using an atomization spray rig to measure spray Sauter mean diameter (SMD) and drop size distribution. Spray visualization using laser illumination was also performed at different test points to identify any noticeable differences in spray features between the SAF and conventional jet fuels. The test scope included a range of fuel pressure differentials and air pressure drops across the fuel injector simulating the actual operation of the nozzle in the engine.

3.2.3.2 Combustion Operability

Understanding a candidate SAF’s impact upon combustion operability is a key aspect of this test program. A High Pressure Flame Tube was used to assess the suitability of the fuel from a performance, operability and safety perspective. Further understanding into fuel related effects on ignition and lean blow out was gained during the program.

3.2.3.3 Emissions

Fuel composition can have a significant effect on emissions. This testing assessed the potential risks and/or benefits with respect to the impact of fuel compositions outside the current envelope of approved fuels for a range of emissions indicators.

3.2.3.4 Elastomer Material Compatibility

A key limitation in current ASTM D7566 fuels is the exclusion of synthetic aromatics and also the requirement for a minimum of 8% to offset risk of elastomer seal problems. Rolls-Royce has developed a unique capability to measure elastomeric seal performance in real-time under engine representative conditions. The test capability was used to evaluate the relationship between aromatic levels/types in the candidate SAF that is outside the current allowed bounds to elastomer seal performance.

3.2.3.5 SAF Assessment and Reporting

Within the document, Rolls-Royce will report relevant test results and performance data from this test program and make an assessment as to fuel related effects upon engine systems. We will also quantify any effects of the SAF on engine performance. The analyses will include quantification of air emissions relative to conventional jet fuel. This data will be shared with both the FAA and the broader community as needed (e.g., ASTM International).

3.2.4 Program Schedule

Figure 1 presents the overall schedule for the program. The program began in 2016 and completed in 2020. Shaded regions show the period of performance for each element, with chevrons indicating milestones that were achieved.

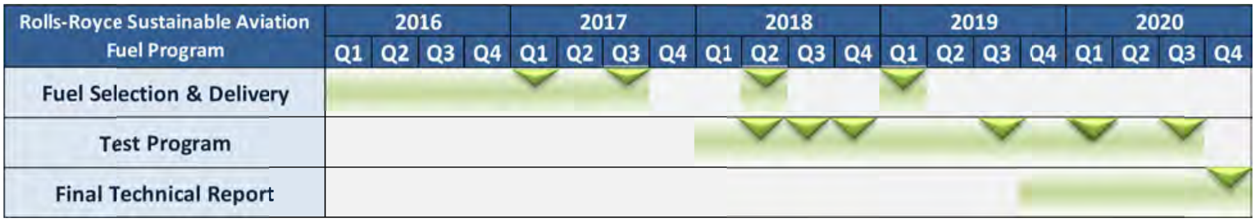


Figure 1. Rolls-Royce Sustainable Aviation Fuel schedule.

4. Test Fuel – Down Selection

As the advancement of alternative fuels development is rapid, it was determined the fuel selection was best suited to be conducted at the time of program launch. To maximize the benefit to the Industry as a whole, Rolls-Royce worked with Industry and the FAA to select an acceptable fuel based on mutually agreed criteria. Acceptable fuels were expected to be “fit for purpose”, and would be anticipated to have no adverse effects on engine performance, operation, reliability, or safety.

Rolls-Royce identified, in cooperation with the FAA, one sustainable jet fuel to be tested and defined as LanzaTech-Swift Fuels ATJ-SKA in the context of this report. Note: This ATJ-SKA is not currently an approved ASTM pathway. The fuel was down selected from a broad range of potential fuel suppliers by understanding the fuel’s potential, information on raw materials, processes, maturity, and potential sustainability. The candidate fuel requirements were set in in terms of suitability, sustainability, and industrial capability. This activity defined and ensured agreement between all parties regarding selection of candidate fuel for further examination and testing within the program. Once identified, the SAF was acquired for the test program.

4.1 Fuel Supplier Screening

For consideration in this program, sustainable aviation fuels with higher blend percentages or fully-synthetic jet fuels were of interest to Rolls-Royce. Synthetic kerosene fuels approved in 2016 (i.e., FT and HEFA) consisted primarily of normal and iso-paraffins but did not contain aromatics. These fuels are blended with conventional jet fuels to maintain an 8% minimum aromatic content. Another area of initial interest was determining the impact of higher concentrations of cyclo-paraffinic content on engine performance. Ultimately, Rolls-Royce focused on fully-synthetic aviation jet fuel containing aromatics. Significant progress has been made in synthetic aromatics that can be blended with synthetic kerosene as well as fully-synthetic aviation jet fuels, and the Industry is interested in pushing past the 50% blend wall.

In 2016, a search for a suitable CLEEN II candidate fuel was initiated early in the program. A survey of a number of newer technologies within the ASTM qualification process was conducted (Table 1). Suitable candidates were adequately positioned within the ASTM framework, with decisions based on a balance of not being too near full qualification but far enough along to have a good understanding of basic properties of the fuel (Step 3) and an understanding that suitable quantities of the fuel could be produced in the required timeframe.

Table 1. Survey results of candidate fuel.

Pathway	Step 3 OEM Review	Step 7 Review	ASTM Ballot Review
ATJ-SPK (Isobutanol)	Complete	Complete	In process
Virent SK	Complete	CY16	CY16
ARA CHJ	CY16	CY16	CY17
Virent SAK	CY16	CY17	CY17
Green Diesel	CY16	TBD	TBD
ATJ-SPK (Ethanol)	TBD	TBD	TBD
ATJ-SKA	TBD	TBD	TBD
HDCJ (KiOR)	On-Hold	TBD	TBD

Based on research of available fuels for the program, Rolls-Royce decided to pursue two suitable options. Initially, Rolls-Royce was interested in investigating the impact of high cyclo-paraffinic content on engine performance. Specifically, Virent/Shell's HDO-SK was of interest as it had a higher than average cyclo-paraffinic content (approximately 80%) when compared to petroleum Jet A/A1. Discussions with Virent to gauge their ability to support the program progressed. Eventually, it was determined that Virent could not support program needs.

As a result, Rolls-Royce decided to pursue a second option and entered into discussions with LanzaTech Inc., to inquire about their interest and ability to supply ATJ for the CLEEN II program. It was decided that a fully-synthetic sustainable aviation fuel with synthetic aromatics (ATJ-SKA) supplied by LanzaTech was to be used in the CLEEN program.

4.2 Test Fuel Selection

Rolls-Royce teamed with LanzaTech Inc., of Skokie, Illinois, to supply a fully-synthetic SAF with aromatics known as ATJ-SKA (alcohol-to-jet synthetic kerosene with aromatics). The 100% SAF was readily available and met ASTM D1655 specification requirements. Specifically, the primary fuel used throughout the CLEEN II program was a fully-synthetic ATJ-SKA fuel; nominally composed of 87% LanzaTech "LT/PNNL ATJ" blended with 13% Swift Fuels synthetic aromatic. The synthetic aromatic was produced using Swift Fuels Technology's conversion process to make nonrenewable mesitylene (1,3,5-Trimethylbenzene). This fuel met CLEEN program goals of promoting higher blend percentages, and has the potential to lower aviation's greenhouse gas footprint. LanzaTech provided a range of support throughout the program, including:

- Technical expertise and assistance
- Manufacturing and procuring identified fuels according to fuel specification ASTM D1655 (see below)
- Mixing two fuel components to required blend percentages (87% LanzaTech ATJ-SPK/13% Swift Fuels synthetic aromatic mesitylene)
- Delivering fuel in required volumes according to schedule (see below)
- Supplying fuel certifications with each shipment
- Providing technical support and participate in conference calls as needed throughout the duration of the program (December 2016 – December 2020).
- Delivering fuel to three separate locations on schedule (Table 2)

Note: LanzaTech's support throughout the program was excellent and their expertise and dedication in accomplishing the program objectives is greatly appreciated.

Table 2. Summary of fuel shipments.

Test	Volume, gallons	Date	Where
Laboratory/FFP	10	November 2017	Rolls-Royce, Plant 8
ERC Fuel Spray	20	December 2017	Irvine, CA
Elastocon	60 (90/10) 20 (96/4)	January 2018	Sheffield University, UK
High Pressure Flame Tube	100	April 2018	Rolls-Royce, Plant 8
FANN	2000	March 2019	Rolls-Royce, Plant 8
	2210 Total		

Figure 2 is a picture of fuel totes containing 2000 gallons of ATJ-SKA delivered to Rolls-Royce for full annular rig testing under the CLEEN II program.

Figure 2. ATJ-SKA fuel totes.

4.3 ATJ-SKA Fuel Overview

The ATJ-SKA fuel used in this program was provided by LanzaTech Inc. The ATJ-SKA (Appendix A) is a fully-synthetic and sustainable aviation fuel composed of 87% LT-PNNL ATJ-SPK and 13% Swift Fuels aromatic (Figure 3). This level of aromatics was required for the CLEEN fuel to meet ASTM D7566 Table 1 and thus ASTM D1655 density requirements. Further information regarding these two synthetic fuels will be described below.

A preliminary review of available fuel properties gained from Tier 1 and 2 ASTM qualifications indicated the CLEEN fuel would provide satisfactory performance in engine systems. This fuel was expected to demonstrate the following positive aspects:

- ✓ Fully-synthetic kerosene fuel
- ✓ Allows for proper atomization and fuel system performance
- ✓ Acceptable combustion performance anticipated
- ✓ Acceptable elastomer seal performance anticipated
- ✓ Meets ASTM D1655 requirements

However, since the aromatic content of the fuel is only C9 hydrocarbon at 13%, there may be slight differences in properties since conventional fossil Jet contains a range of aromatics from C8-C16.

4.3.1 Description of LT-PNNL ATJ-SPK Process

In ASTM D7566, ATJ-SPK is defined as “an SPK produced starting from alcohol and processed through the following steps: dehydration, oligomerization, hydrogenation, and fractionation.” LanzaTech uses a proprietary microbe that produces ethanol via fermentation of compressed CO and CO_2, then converts the ethanol into usable hydrocarbon products. Note much of the information within this section was obtained from the LanzaTech ATJ-SPK research report [Ref. 4].

Figure 3. ATJ-SKA Fuel used in CLEEN Program

> *The LanzaTech technology platform can produce low cost alcohols through bacterial fermentation of carbon monoxide (CO) or a wide range of CO, hydrogen (H_2) and carbon dioxide (CO_2) gas mixtures. Because the proprietary microbes can produce alcohols from CO with or without H_2, and in the presence of contaminants, the process can accommodate a diverse set of input gas streams. CO-containing industrial waste gas streams from steel mills, refineries, and petrochemical plants can be used for fuel production, capturing carbon, as an alternative to flaring or cogeneration. CO or mixed CO + H_2 (syngas) streams can also be derived by gasification or steam reforming of a wide range of abundant, low-value, Jet Fuel ATJ-SPK non-food feedstocks including woody biomass, forest and crop residues, municipal solid waste, biogas as well as commercially available sustainable ethanol. [Ref. 4]*

In the LanzaTech/PNNL ATJ-SPK production process (Figure 4), ethanol (EtOH) from any source is chemically converted to synthetic jet fuel via the four steps defined for ATJ-SPK production: dehydration, oligomerization, hydrogenation and fractionation. The EtOH is first dehydrated to ethylene, a C2 olefin. Ethylene is then oligomerized into longer carbon chain olefins that boil primarily in the jet range. The jet-range olefins are hydrogenated to saturate the molecules and form paraffins. Finally, the paraffins are fractionated to isolate the jet product as stable, wide boiling, paraffinic kerosene.

> *Innovation, scale up, and project execution are core to LanzaTech. Throughout its sixteen-year history the company has consistently developed innovative gas fermentation technology solutions in the laboratory, scaled them, and is now deploying them commercially. LanzaTech has optimized each part of its process including gas treatment, gas conversion, product recovery, and water recycling. Meanwhile, LanzaTech's gas fermentation process has been demonstrated at four sites with 50,000 hours of operation in the field using steel mill waste gases plus another 50,000 hours of operating in the field integrating gasification, gas treatment and gas fermentation. The success of these 100,000 hours of experience at pilot and demonstration scale led to the May 2018 startup of the first operating commercial gas fermentation facility in the world at the Jingtang Steel Mill in Caofeidian in Hebei Province, China. Since startup, over 25 million gallons of ethanol has been produced, and a second facility started up in China with the same partner in April 2021. With co-funding awarded by the U.S. Department of Energy, LanzaTech with LanzaJet is in the procurement phase of a commercial demonstration project that will produce 10 million (US) gallons per annum of sustainable aviation fuel (SAF) and renewable diesel starting from sustainable ethanol sources. Production is expected to start in late 2022. [Ref. 4]*

4.3.2 Description of Swift Fuel Aromatic

The aromatic portion of the ATJ-SKA fuel used in the program was supplied by Swift Fuels LLC, of Lafayette, Indiana. Swift used a synthetic conversion process to make mesitylene (1,3,5-trimethylbenzene), which can be used as an aromatic fuel blend component (Figure 5). The mesitylene compound is a benzene ring with three methyl groups attached.

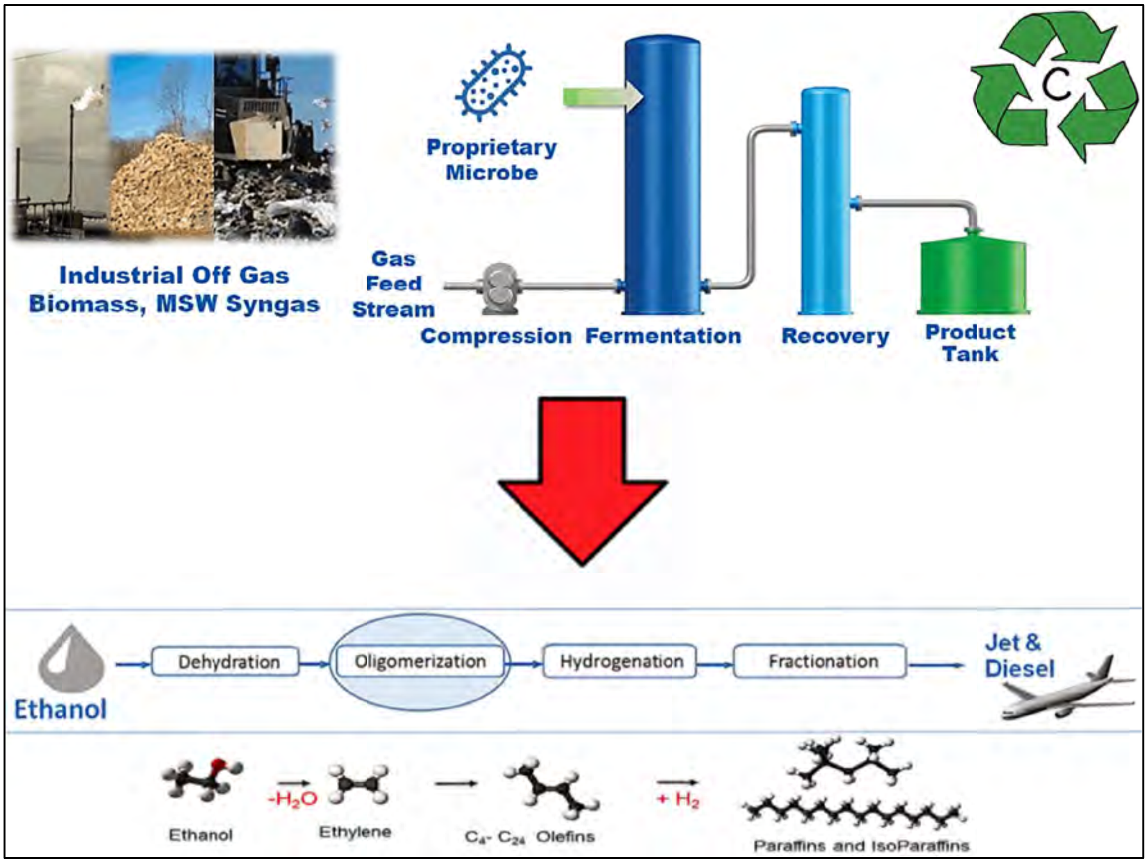


Figure 4. LT-PNNL ATJ-SPK production process.

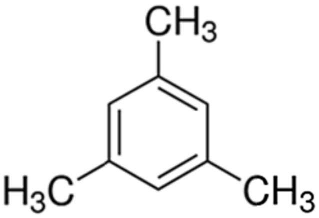


Figure 5. Mesitylene chemical structure.

Mesitylene can be produced from either a renewable route using biomass or via a nonrenewable route from an aromatic rich gasoline stream. The mesitylene molecular structure is expected to be identical regardless of whether produced via renewable or nonrenewable routes. The mesitylene used in this program was via the nonrenewable route due to it low cost and ready availability. This was determined to be acceptable from a technical perspective as it would demonstrate mesitylene's ability to be an acceptable aromatic fuel blend component for use in aviation fuels.

Aromatics are hydrocarbons with a six-carbon ring, with alternating single and double bonds between the carbon atoms. Aromatics are important to elastomeric seals in an engine. Seals swell in the presence of aromatics; therefore controlled seal swell is important.

Initially, the aromatic content in the ATJ-SKA was targeted to be 8%. Due to the density of ATJ-SPK being outside of ASTM D1655 limits of 775 – 840 kg/m^3, additional aromatic was needed to bring the final fuel blend back into jet fuel density range. It was determined that 13% by volume blend of Swift Fuels aromatic was required to obtain a finished fuel density of 776 kg/m^3. The boiling point of C9 hydrocarbon mesitylene is 164.7°C, which is very light for typical aromatics in conventional jet fuel.

Overall, an 87% by volume blend of LanzaTech ATJ-SPK with 13% Swift Fuels aromatic was the final fuel chosen for the CLEEN II program. This test fuel meets program goals of promoting higher synthetic blend percentages, along with offering the potential to reduce carbon footprint of aviation. In addition, the fuel has commercial viability, is readily available and demonstrates suitability in aviation.

5. Laboratory Test Program

As the initial testing phase of the CLEEN II program, a laboratory characterization of the ATJ-SKA test fuel's properties was required to satisfy two purposes. The first was to assess whether the fuel was fit for purpose and suitable for continued testing. The other purpose was to ensure the fuel from different fuel shipments throughout the program was consistent in quality and that its fuel properties did not vary significantly, thus potentially impacting the test results and interpretation during subsequent tests within the evaluation program. This testing was accomplished via laboratory analysis of key chemical and physical fuel properties to the requirements of ASTM D7566 requirements. SPL Incorporated (formerly Alcor Petrolab), of Arlington Texas, was selected as the primary laboratory to perform the analysis. The University of Dayton Research Institute (UDRI) was also used to perform complex compositional analysis.

5.1 Test Methodology

Laboratory testing included standard specification testing and additional FFP testing of candidate fuel. The details of FFP testing were based on a rational review of the candidate fuels' chemical, physical, and performance properties. Aspects where sufficient evidence or experience was already available to predict outcomes were not tested. Such testing was carried out in accordance with ASTM D4054 and ASTM D1655/D7566 so data generated might contribute to the assessment of potential approval but did not include the full suite of testing required. Fuel samples for analysis were taken at various stages of the program, including initial bulk shipment, and both before and after each of the tests to ensure consistency. A laboratory analysis of the ATJ-SKA for the following fuel properties was conducted in accordance with ASTM D7566:

- Chemical
- Bulk physical and performance
- Composition (purity and trace compounds)
- Select fit-for-purpose

5.2 Specification and Fit for Purpose Test Results

The main objective of this effort was to compare the ATJ-SKA against the ASTM D1655/7566 requirements, as well as against experience with other conventional fuels. Two competent and certified laboratories performed the laboratory analysis of the ATJ-SKA fuel. Alcor Petrolab performed the majority of the laboratory analysis in accordance with ASTM methods identified in ASTM D1655/7566. UDRI, in Dayton, Ohio, performed the detailed hydrocarbon analysis of the ATJ-SKA. The laboratory test results will be reviewed along with a conclusion drawn as to the anticipated suitability of the fuel for use in aerospace engines.

Alcor Petrolab characterized the standard specification properties of the ATJ-SKA fuel. A summary of the test results can be found in Table 3. Overall, the ATJ-SKA meets the majority of specification requirements and its properties are comparable to other jet fuels. There were a few minor exceptions related to the T50-T10 distillation, thermal stability, and water content. Further discussion of these test results and FFP properties will be covered below.

Table 3. Summary of specification test results.

Property	ASTM Test Method	Units	ASTM D1655 & D7566 Table 1 Limits	ASTM D7566 Annex A5 Extended Limits	ATJ-SKA
Color, Saybolt	D6045				+30
HYDROCARBON COMPOSITION					
Aromatics, total	D1319	vol %	8 to 25	0.5 mass % max	13.0
Olefins		vol %			2.2
Saturates		vol %			84.8
Aromatics, total	D6379	vol %	26.5 max		11.4
Mono Aromatics, % of total		vol %			11.4
Di-aromatics, % of total		vol %			0.0
Normal & Iso-paraffins	UDRI D2425	wt %			80.72
Cycloparaffins		wt %		15 mass % max	4.95
Aromatics, total		wt %			14.33
Hydrogen Content	D7171	wt %			14.56
Carbon + Hydrogen	D5291	mass %		99.5 min	100.0
Nitrogen		mass %			<0.1
Hydrogen Content		mass %			14.0
Carbon content		mass %			86.0
NON-HYDROCARBON COMPOSITION					
Acidity	D3242	mg KOH/g	0.10 max	0.015 max	0.004
Mercaptan Sulfur	D3227	mass %	0.003 max		< 0.0001
Sulfur, Total	D2622	mass %	0.30 max	0.0015 max	< 0.0001
Metals (Al, Ca, Co, Cr, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Pd, Pt, Sn, Sr, Si, Ti, V, Zn)	D7111	mg/kg		0.1 max per metal	see below*
Total Halogens	D7359	ppm		1 max	<0.2
Fluorine		ppm			<0.1
Chlorine		ppm			<0.1
VOLATILITY					
Distillation Temperature	D86				
IBP		℃			154.9
5%		℃			
10%		℃	205 max	205 max	165.6
15%		℃			
20%		℃			
30%		℃			
40%		℃			
50%		℃	Report	Report	179.7
60%		℃			
70%		℃			
80%		℃			
90%		℃	Report	Report	221.3
95%		℃			240.3
Final Boiling Point		℃	300 max	300 max	257.9
Distillation Residue		vol %	1.5 max	1.5 max	1.3
Distillation Loss		vol %	1.5 max	1.5 max	1.0
T50 - T10		℃	15 min		14.1[1]
T90 - T10		℃	40 min	21 min	55.7
Flash Point	D93/D56	°C	38 min	38 min	45
Density at 60°C	D4052	kg/m^3			742.3
Density at 40°C					757.3
Density at 15°C			775 - 840	730 to 770	775.9
Density at -20°C					805.5
Density at -40°C					819.6
FLUIDITY					
Freeze Point	D2386/D5972	°C	-40 max	-40 max	-59
Kinematic Viscosity	D445	mm^2/s			
-40			12 max		5.681
-20			8.0 max		3.035
0ºC					1.939
20ºC					1.370
40ºC					1.045
COMBUSTION					
Net Heat of Combustion	D4809	MJ/kg	42.8 min		43.691
Napthelenes	D1840	vol %	3.0 vol% max		<0.08
Smoke Point	D1322	mm	25.0 min or 18.0 min and 3% max nap		18.5
CORROSION					
Copper Strip Corrosion 2 hrs @ 100 °C	D130		No. 1 max		1B
THERMAL STABILITY					
Thermal Stability, Breakpoint	D3241	℃	260°C	325°C	300[2]
max Delta P		mmHg	25 max	25 max	1
visual tube rating		VTR	<3	<3	0
CONTAMINANTS					
Existant Gum	D381	mg/100ml	7 max		<1
Microseparometer Rating	D3948				
Without electrical conductivity additive			85 min		100
With electrical conductivity additive			70 min		NA
Particulate Contamination	D5452	mg/L			<0.38
Water Content	D6304	mg/kg		75 max	80[3]
LUBRICITY					
Lubricity, BOCLE (WSD)	D5001	mm	0.85 max		0.77

Note 1: The fuel has only C9 aromatics (13%) which has a very light boiling point when compared to conventional Jet of C8-C16 aromatics, so the blend does not quite meet the T50-T10 specification requirements of 15.

Note 2: The Swift Fuels Mesitylene passes the thermal stability requirement at 260°C, so the actual breakpoint of 300°C easily meets the requirement.

Note 3: The water content of the Swift Fuels Mesitylene as received by LanzaTech was 155 ppm, so the water content of the blend was slightly higher than the specification limits.

5.2.1 ATJ-SKA Composition

5.2.1.1 Hydrocarbon Composition

Hydrocarbon chemistry is an important fuel property describing the chemical makeup, distribution, and ratio of various hydrocarbons present in jet fuel. Typical petroleum derived aviation fuel is composed of a mixture of normal paraffins (n-paraffins), isoparaffins, cycloparaffins, and aromatics. Hydrocarbon composition was determined using a UDRI GCxGC method (UDR FC-M-101) that provides hydrocarbon composition as a function of carbon number. Figure 6 shows the GCxGC contour plot from the analysis.

A summary of the GCxGC analysis of the ATJ-SKA fuel is provided in Table 4, which shows the fuel is comprised of isoparaffins, n-paraffins, cycloparaffins and aromatics which are also the primary constituents in petroleum derived Jet A fuel. The composition breakdown by weight percent is shown in Table 4.

As can be seen from the data, the ATJ-SKA fuel is predominately iso-paraffinic in nature, with lower levels of normal and cycloparaffins than typical petroleum derived fuels. The aromatic content of the ATJ-SKA was determined to be 14.33% by weight and shown to be primarily composed of alkylbenzenes (mesitylene). Aromatics are hydrocarbons with a six-carbon ring, with alternating single and double bonds between the carbon atoms. Aromatics are important to elastomeric seals in an engine. Seals swell in the presence of aromatics; therefore controlled seal swell is important.

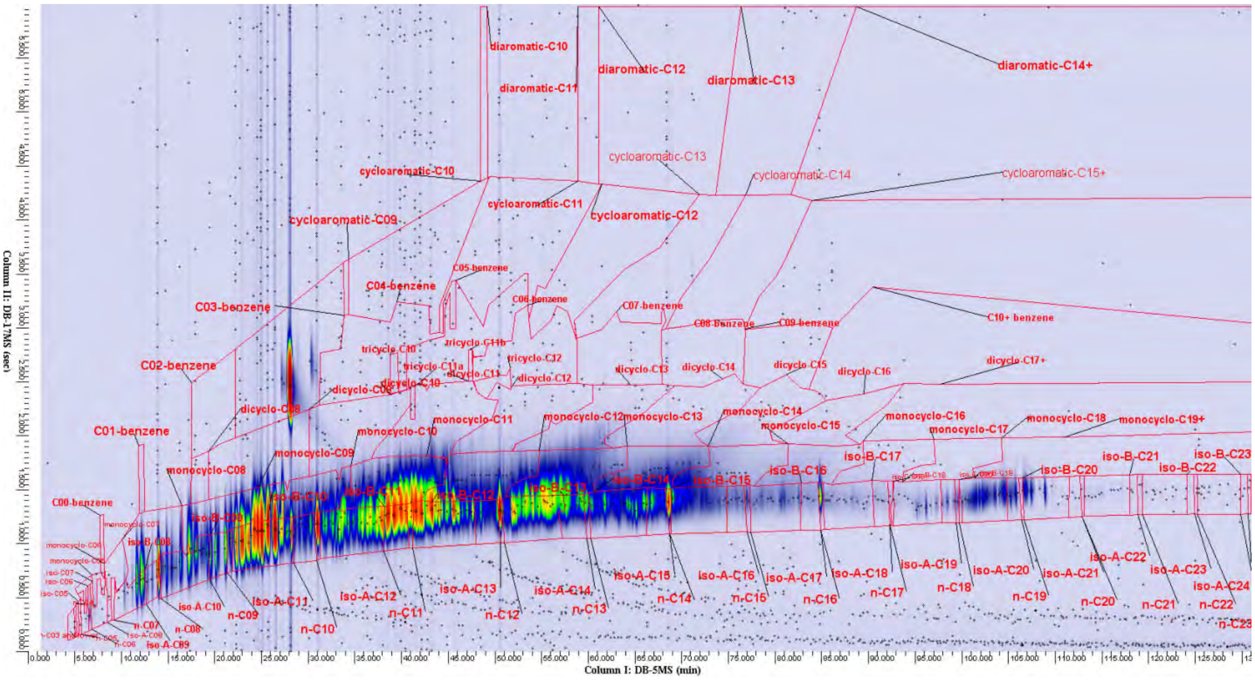


Figure 6. GCxGC contour plot for ATJ-SKA.

Table 4. Hydrocarbon composition by weight percent.

	Weight %	
	ATJ-SKA	**Typical Jet A-1**
Total Aromatics	14.33	17.66
Diaromatic	<0.01	3.72
Cycloaromatic	<0.01	0
Alkylbenzenes	14.32	13.94
Total Cycloparaffins	4.95	27.32
Monocyloparaffin	4.89	18.8
Dicycloparaffin	0.06	8.07
Tricycloparaffin	<0.01	0.45
iso-Paraffin	71.04	30.2
n-Paraffin	9.68	19.6
Indanes and Tetralins	0	5.41

Figure 7 and Figure 8 contrast the hydrocarbon types between ATJ-SKA and typical Jet A-1. As can be seen in the figures, petroleum derived Jet A-1 typically has evenly distributed amounts of aromatics, cycloparaffins, n-paraffins and isoparaffins. In contrast, ATJ-SKA is predominately isoparaffinic. This is a design of the alcohol to paraffinic jet conversion process.

Figure 9 shows the ATJ-SKA fuel is distributed across carbon numbers from C8 to C16. Also of note is the fuel contains minimal carbon numbers (over C16) that could degrade low temperature properties. This wide distribution is considered within experience of other approved fuels. The distribution of hydrocarbons across a range of molecular weights can be further characterized by the distillation or “boiling range” characteristics of the fuel, which will be discussed below.

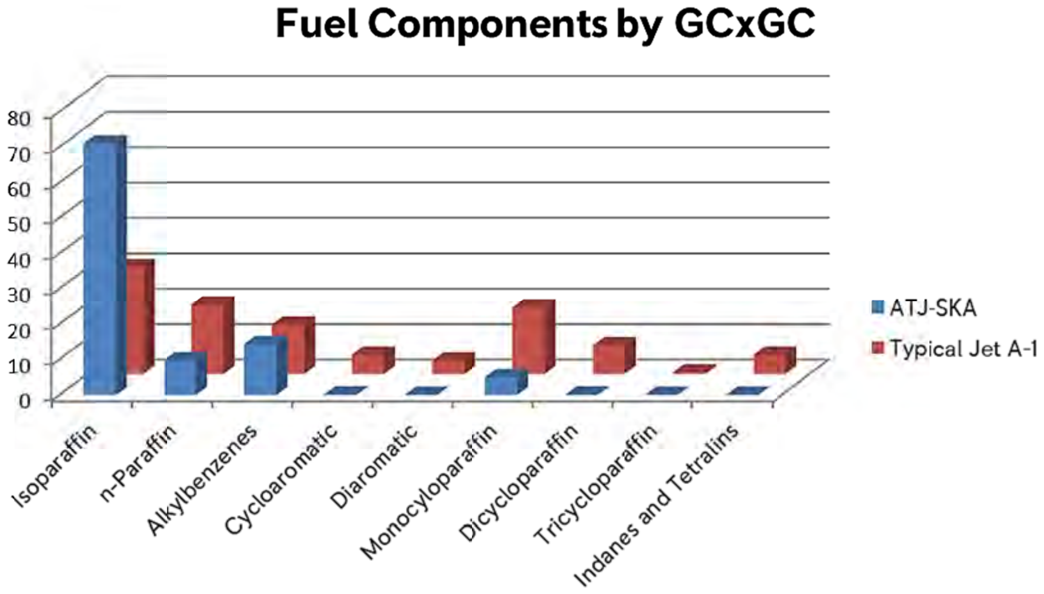


Figure 7. Typical Jet A-1 Comparison to ATJ-SKA.

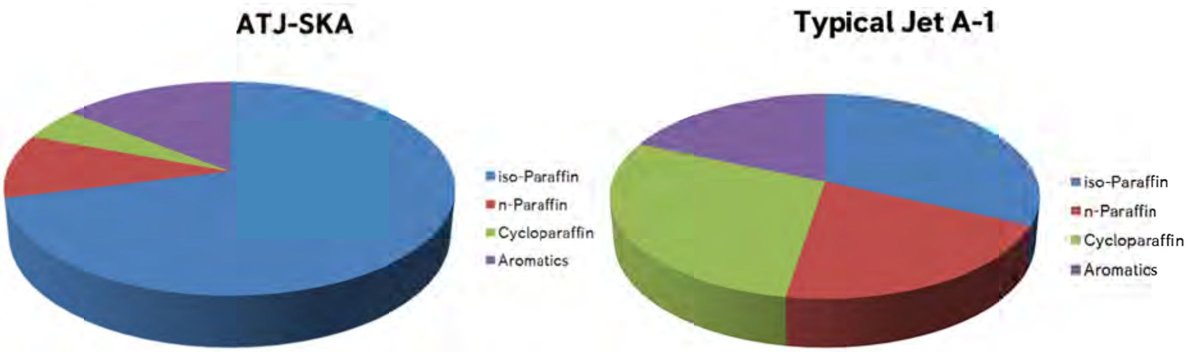


Figure 8. Hydrocarbon composition pie chart.

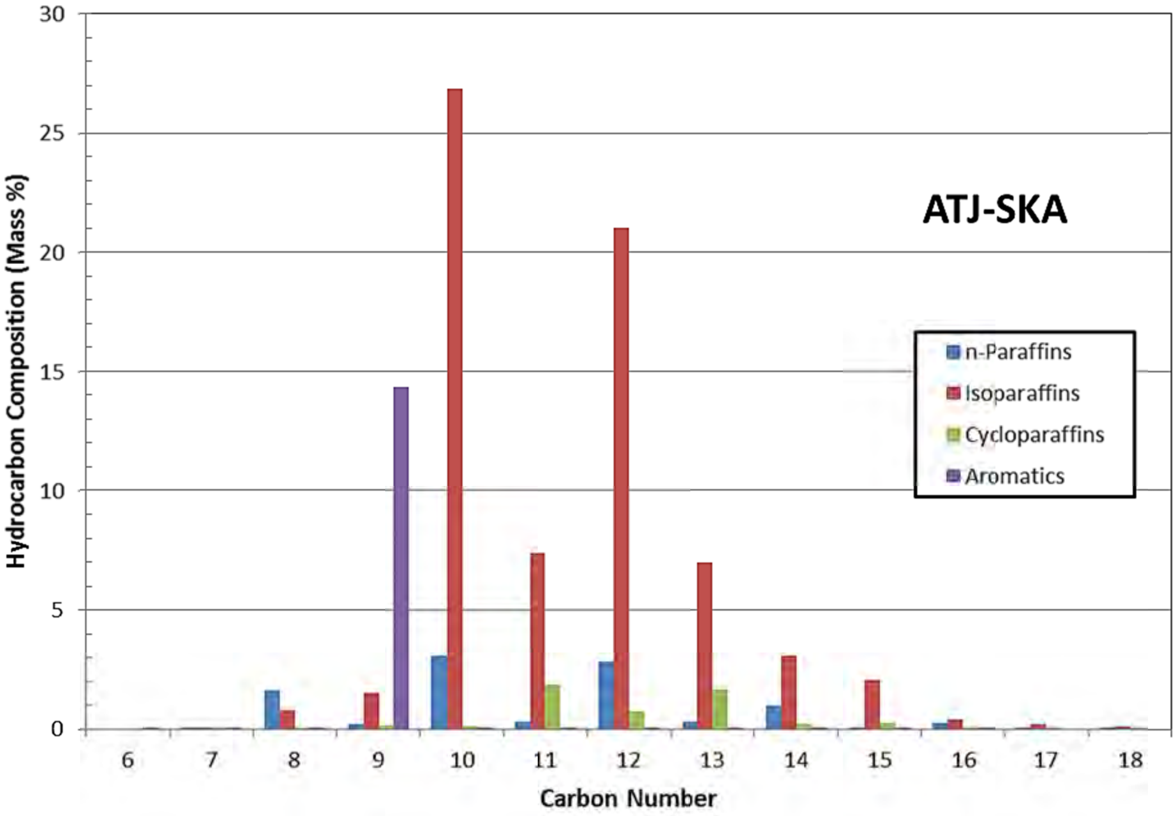


Figure 9. Histogram of carbon chain distribution.

The hydrogen content of ATJ-SKA was measured using ASTM D7171 [Ref. 5] and found to be 14.56 weight percentage, which is greater than typical Jet A fuel of around 13.9% w/w. The carbon plus hydrogen content of the fuel was found to be 100% in accordance with ASTM D5291 [Ref. 6]. These results confirmed there were no unknown constituents or contaminates in the composition.

5.2.1.2 Organics, Trace Metals, Oxygenates

Aviation fuels often contain a class of organic compounds that consist of a sulfur-hydrogen group (SH) bounded to a hydrocarbon chain R, to form R-SH. These sulfur groups in mercaptans increase the reactivity of the compound, which can lead to a corrosive attack on fuel-wetted metallic components within the fuel system. Therefore, mercaptan sulfur is tightly controlled. ATJ-SKA fuel contained less than 0.0001 mass percentage of mercaptan sulfur and total sulfur. This was well within ASTM D7566 specification limits.

Organic trace materials (alcohols and carbonyls) and trace metals (copper, zinc, etc.) levels were evaluated and found to be below the maximum allowable concentration. The ATJ-SKA fuel contained ultra-low levels of sulfur, low levels of inorganics, and organics. The ATJ-SKA fuel demonstrated lower levels of these trace materials when compared to conventional Jet A fuel, which is due to the severity of hydroprocessing. A summary of the ATJ-SKA trace material composition is presented in Table 5.

Table 5. ATJ-SKA fuel composition summary.

Non-hydrocarbon composition				
Property	**ASTM test method**	**Units**	**ATJ-SKA**	**Jet A baseline**
Acidity	D3242	mg KOH/g	0.004	0.004
Mercaptan sulfur	D3227	mass %	< 0.0001	<0.0001
Sulfur, total	D2622	mass %	< 0.0001	0.037
Metals (Al, Ca, Co, Cr, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Pd, Pt, Sn,	D7111	mg/kg	<0.1*	<0.1*
Total halogens	D7359	ppm	<0.2	<0.2
Fluorine		ppm	<0.1	<0.1
Chlorine		ppm	<0.1	<0.1

* Noted elevated levels of sodium and silicon due to contamination from glassware during lab analysis (sodium borosilicate)

5.2.2 Volatility

The volatility of a fuel is an important characteristic to understand as it relates to altitude relight, fluid dynamics, atomization, fire safety, and calculating energy content. Volatility characteristics that will be discussed in the following subsections include boiling point distribution, density, and flash point.

5.2.2.1 Boiling Point Distribution

The distillation profile of aviation fuel indicates the range of temperatures over which the fuel boils at a pressure of 1 bar. Typically, jet fuels are composed of a mixture of varying lengths of hydrocarbon chains, causing a particular range of boiling temperatures. Lighter compounds (i.e., shorter hydrocarbon chains) boil initially, and heavier compounds (i.e., longer hydrocarbon chains) boil later in the process. The distillation profile is important to altitude relight. The neat ATJ-SKA fuel is primarily composed of C10, C12 and C14 isoparaffins, and easily meets T90-T10 slope requirements of 40°C with a slope of 55.7°C.

The boiling point distribution of the ATJ-SKA fuel was determined using ASTM D86 [Ref. 7] test method. Figure 10 illustrates the boiling point distribution of the fuel in comparison to other fuels.

Results indicated the ATJ-SKA fuel falls within the limits of Jet A specification, with a relatively flat distribution slope between 10-40% recovered, becoming more pronounced above 50%. This was likely due to the light Mesitylene C9 aromatic.

The slope of these boiling point distributions can further quantify the rate of volatility of the fuel by determining the T50-T10 and T90-T10 values. ASTM D7566 requires a T90-T10 value of

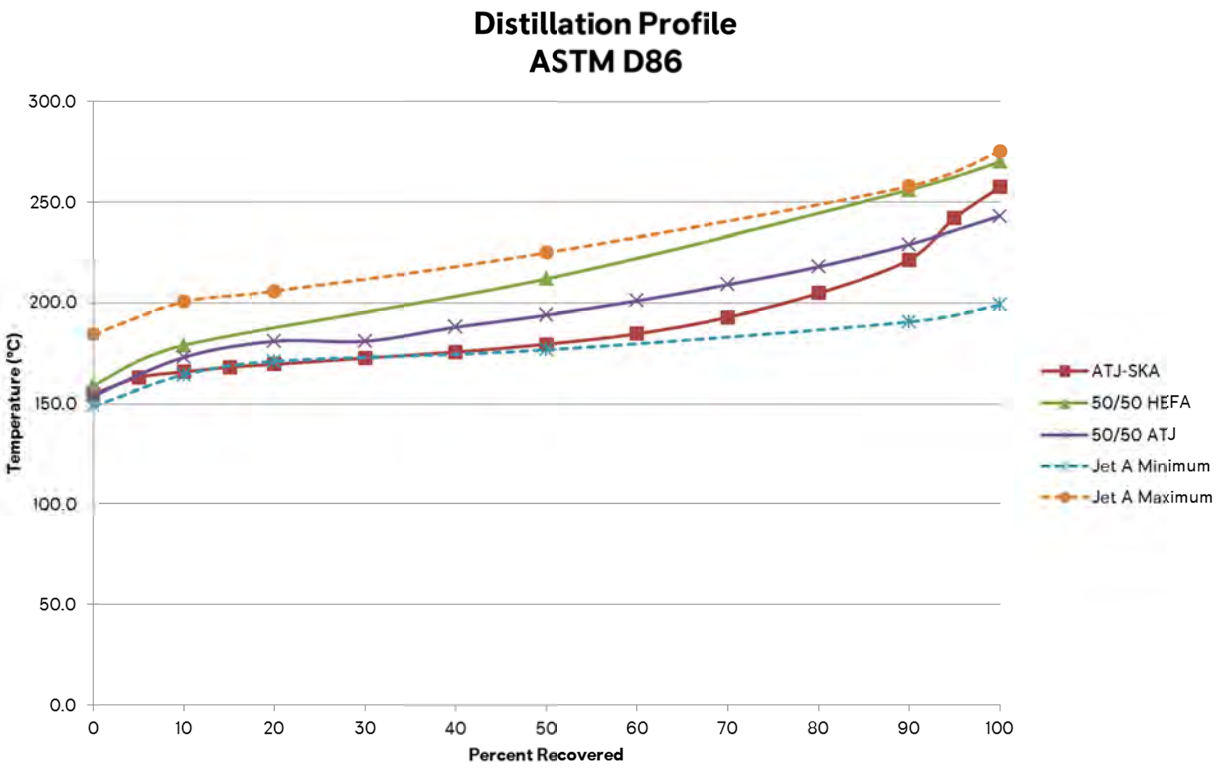


Figure 10. Boiling point distribution.

40°C minimum, and a T50-T10 value of 15°C minimum. The ATJ-SKA slope was evaluated and found to be: 55.7°C (T90-T10) and 14.1°C (T50-T10), which met specification requirements for the T90-T10 but not the T50-T10. This indicated a flatter initial slope indicative of larger amounts of light front end material. These results were expected, as the fuel aromatic was only a C9.

5.2.2.2 Flash Point

The flash point of jet fuels is evaluated to determine the lowest temperature at which fuel vapors evolving from liquid fuel can mix with air to form an ignitable vapor mixture. Flash point affects combustibility, and is also a factor used to determine fire safety in fuel handling. Figure 11 shows the results from flash point testing in accordance with ASTM D56 [Ref. 8]. As can be seen, the flash point of ATJ-SKA was 45°C well above the specification minimum of 38°C, slightly above a 50/50 blend of ATJ-SKA with conventional petroleum jet.

5.2.2.3 Density

Density of fuel influences the energy delivered to the combustor. The density of ATJ-SKA samples was measured using ASTM D4052 [Ref. 9] test method. Figure 12 illustrates the density of fuels over a range of temperatures. The ATJ-SKA density profile is similar to other fuels and meets ASTM D1655 specification requirements. It can also be seen that the density of the fuel is on the lower end of the specification range. This is due to the nature of ATJ type fuels having low densities. The mesitylene aromatic was added to the blend to bring the density up within specification limits.

In summary, the volatility of ATJ-SKA is expected to be within experience and not anticipated to negatively impact altitude relight, fluid dynamics, atomization, fire safety or energy content. Further combustion testing will be required to confirm performance.

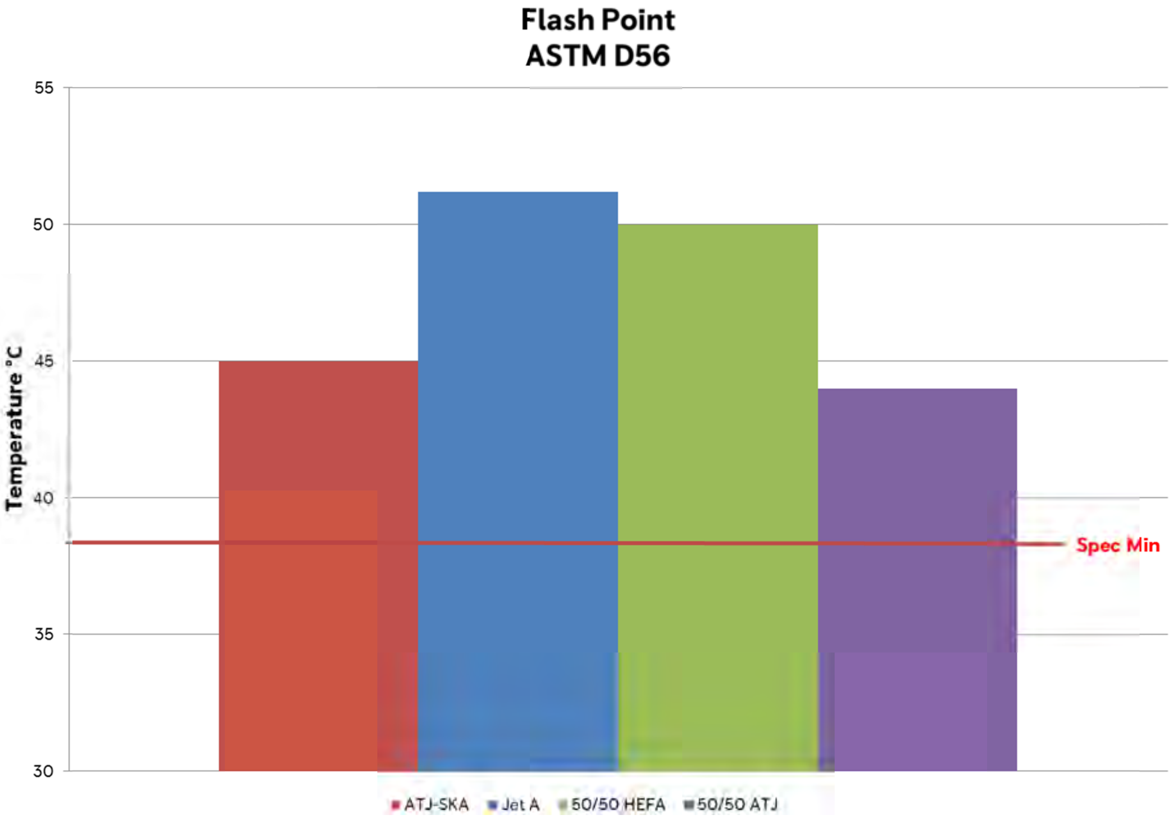


Figure 11. Flash point test results.

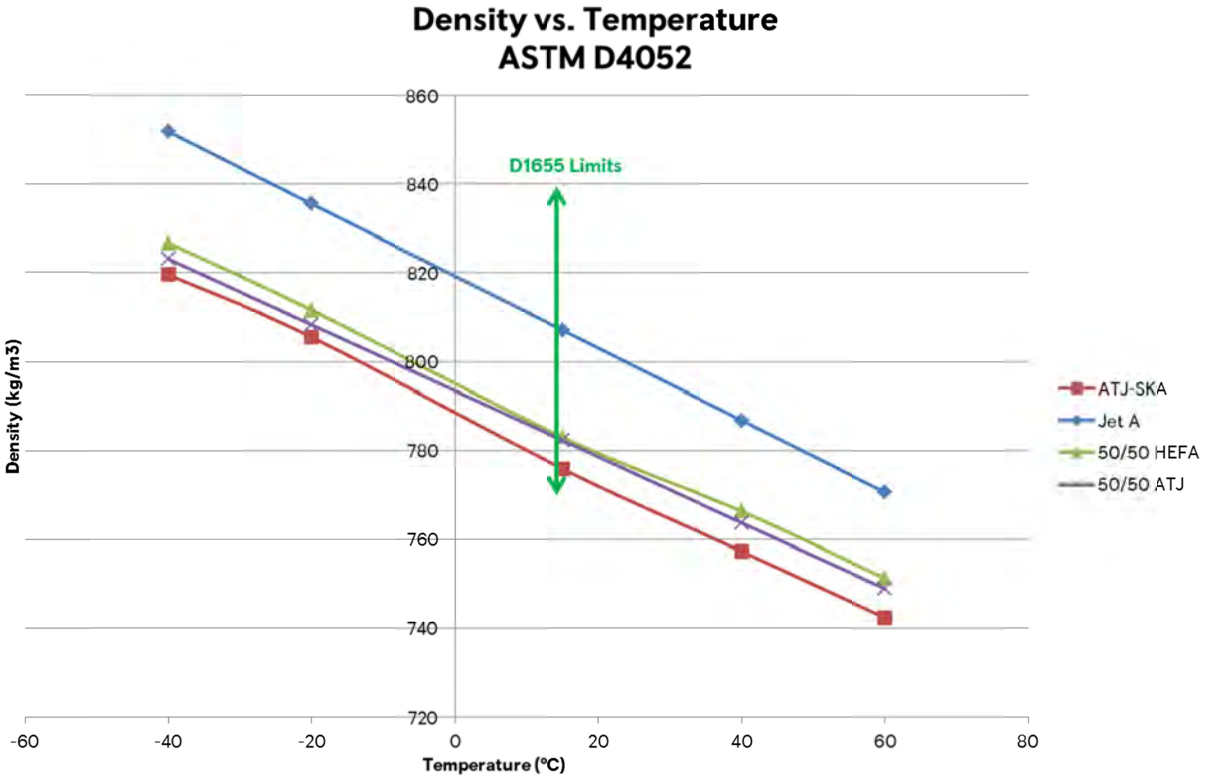


Figure 12. Density versus temperature.

5.2.3 Fluidity

5.2.3.1 Freeze Point

Multicomponent fuels do not freeze (become solid) at a single temperature. The freeze point is the temperature at which the last fuel wax (n-paraffins) crystal melts when warmed. This property is important because unacceptable freeze point values affect low temperature fuel behavior. A poor freeze point can cause issues with pumps and nozzle operations. The freeze point of ATJ-SKA samples was evaluated using ASTM D5972 [Ref. 10] test method. Typical Jet A fuels have a freeze point around -52°C and neat ATJ fuel (without synthetic aromatics) can have a very low freeze point of <-89°C if desired. The ATJ-SKA was found to have a freeze point of -59°C, easily meeting the -40°C specification maximum. The higher temperature freeze point of ATJ-SKA when compared to neat ATJ is likely due to the 13% by volume of mesitylene added to the fuel which has a freeze point of -50°C. The ATJ-SKA fuel had an acceptable freeze point when compared to traditional petroleum jet fuel.

5.2.3.2 Kinematic Viscosity

Viscosity is a measure of a fluid's internal resistance to motion caused by cohesive forces among the fluid molecules. Kinematic viscosity of fuel varies inversely with temperature, with decreasing temperature causing the fuel to increase in viscosity. This relationship is important for fuel system designers, and is used in pressure drop calculations. Viscosity affects pump ability over the operating range of an aircraft mission and can influence fuel delivery capacity of the fuel system. It also relates to droplet size in sprays produced by burner nozzles, and has a large influence on atomization at low temperatures. Petroleum-derived fuels have historically had large variation to the specification limit at -20°C and -40°C, which necessitates a clear understanding of ATJ-SKA performance. Therefore it is necessary to ensure the viscosity behavior of ATJ-SKA is of acceptable behavior to not negatively impact the performance of gas turbines.

The kinematic viscosity of ATJ-SKA was measured in accordance with ASTM D445 [Ref. 11]. Figure 13 shows the kinematic viscosity of test fuel, baseline Jet A and other synthetic fuels. As Figure 13 illustrates, all fuels display a similar slope and fell within the requirement of 8 centistokes (cSt) maximum at -20°C and 12 cSt at -40°C as required in ASTM D1655. The viscosity test results of the ATJ-SKA were found acceptable and within experience, with similar behavior when compared to other fuels. Based on these test results, the ATJ-SKA is expected to have acceptable performance and fluidity with respect to droplet size in sprays, proper atomization, and offer good low temperature performance.

5.2.4 Combustion and Stability

Combustion characteristics and stability of a candidate fuel in engine systems is an important aspect to understand prior to performing combustion rig tests. The net heat of combustion and thermal oxidative stability of the ATJ-SKA can influence engine performance, range of flight, and fuel system deposits. Table 6 reports the combustion and thermal stability data of the ATJ-SKA as compared to other fuels.

5.2.4.1 Net Heat of Combustion

The amount of energy content in fuel is of importance and affects the performance and range of gas turbine engines. Specific energy or net heat of combustion (NHC), in concert with density, influences fuel tank loading requirements for a given range or tank range capacity for an unlimited range request. NHC is the net amount of heat energy released per unit mass in MJ/kg when fuel is ignited. The NHC of ATJ-SKA was determined using ASTM D4809 [Ref. 12] test method. Fuel density is used to calculate the NHC by volume in MJ/l.

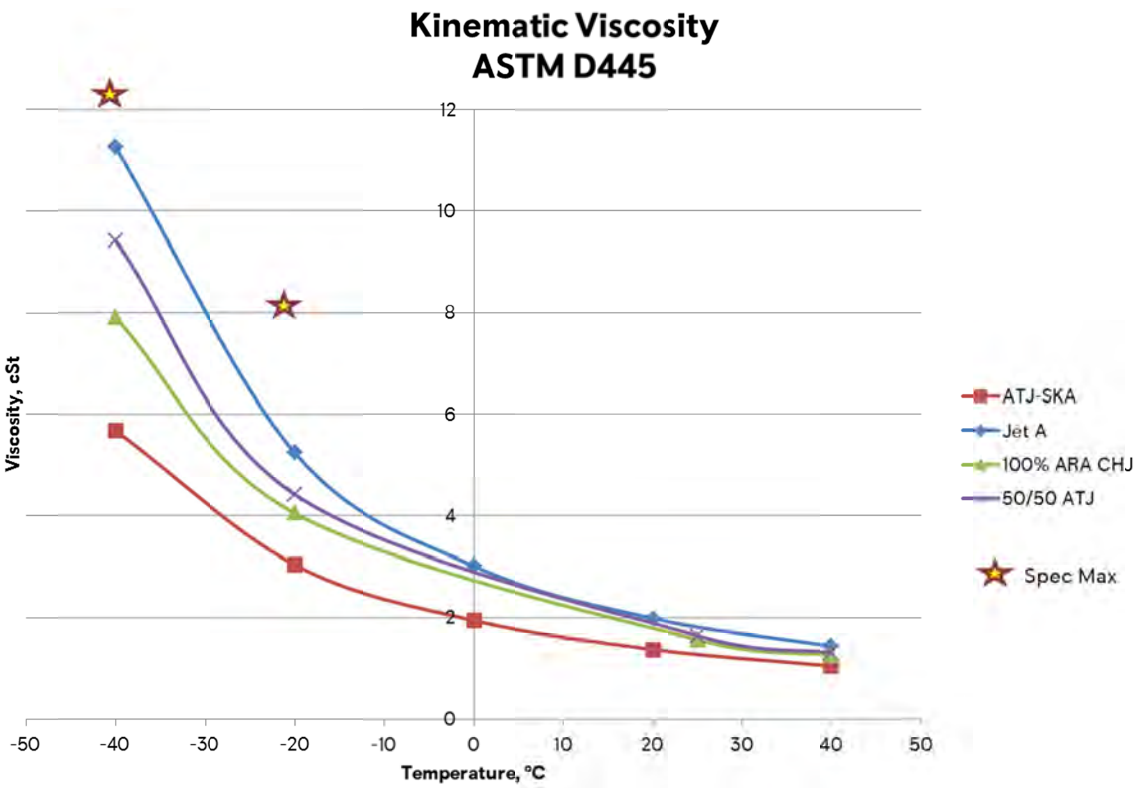


Figure 13. Kinematic viscosity of jet fuels.

Table 6. Net heat of combustion data.

Combustion and Thermal Stability							
Property	**ASTM test method**	**Units**	**ASTM D1655-18a limits**	**ATJ-SKA**	**Jet A**	**100% ARA CHJ**	**50/50 ATJ**
Net heat of combustion by mass	D4809	MJ/kg	42.8 min	43.7	43.2	43.1	43.3
NHC by volume		MJ/l	calculated	33.9	35.1	34.7	33.9
Naphthalenes	D1840	vol %	3% max	<0.08	0.5		1.0
Smoke point	D1322	mm	18.0 min	18.5	21.6	25.0	31.4
Density @15°C	D4052	kg/m^3	report	775.9	812.3	805	782
Thermal stability, breakpoint	D3241	°C	260 min	300	260	260	325
max Delta P		mmHg	25 max	0	0	0	1
visual tube rating		VTR	<3	0	0	2	1

The ATJ-SKA fuel exhibited slightly higher NHC by mass and slightly lower NHC by volume than conventional Jet A. This is expected due to the lower density of the ATJ-SPK blend stock, but meets specification requirements and is within the expected range of conventional fuels. Therefore, the energy release behavior of ATJ-SKA fuel will be within current service experience, with no expected negative impact on operation or performance of the engine.

5.2.4.2 *Thermal Oxidative Stability*

Thermal oxidative stability is another important characteristic in a candidate jet fuel that must be evaluated due to its significant influence on engine design. This property relates to the ability of the fuel to operate at high temperatures and handle increased temperatures within an engine without compromising the substance‘s chemical integrity. Poor thermal stability leads to undesirable oxidation products such as sediments and/or surface deposits in fuel systems, nozzles and on engine hardware thereby reducing performance.

The ASTM D3241 [Ref. 13] JFTOT test was used to determine if the ATJ-SKA fuel had good thermal stability qualities. The thermal oxidative stability of the ATJ-SKA blend was found to meet specification requirements. Table 6 shows the results from testing. The ATJ-SKA had a breakpoint surpassing 300°C, thus easily meeting specification minimum of 260°C. The fuel exhibited good stability, exceeding typical conventional Jet A fuel.

5.2.4.3 *Naphthalenes*

Naphthalenes are aromatics that are unsaturated, cyclic hydrocarbons containing one or more carbon rings, each with six carbon atoms. Double ring aromatics or naphthalenes are separately limited at 3.0% because of their adverse effect on combustion. The naphthalene content of the ATJ-SKA fuel was found to be less than 0.08 volume percent, which is lower than conventional Jet A fuel, thus being considered acceptable.

In summary, the combustion and thermal stability aspects of the ATJ-SKA fuel were evaluated and found suitable and within experience, indicating minimal impact to aircraft range and good deposit resistance.

5.2.5 Other Properties

A listing of other properties is provided in Table 7.

Table 7. Other properties.

Property	ASTM method	Units	ASTM D1655-18a limits	ATJ-SKA
Existent gum	D381	mg/100ml	7 max	<1
Microseparometer rating	D3948			
Without electrical conductivity additive			85 min	100
With electrical conductivity additive			70 min	not measured
Particulate contamination	D5452	mg/L		<0.38
Water content	D6304	mg/kg		80

5.2.5.1 *Trace Materials*

Trace materials found in jet fuel can negatively impact a fuel’s thermal stability and/or affect other properties such as storage stability or gum formation. These contaminants are limited by ASTM D1655/7566 to control adverse impacts.

The ATJ-SKA fuel exhibited low existent gum of less than 1 mg/100ml, low particulate content of less than 0.38 g/L and 80 ppm of water content. The water content of the Swift Fuels Mesitylene as received by LanzaTech was 155 ppm, so the water content of the blend was slightly higher than the specification limits. These results are found to be acceptable.

5.2.5.2 Lubricity

Aviation turbine fuel serves as a lubricant in fuel pumps, engine controls, and servo valves. The hydrocracking process used in synthetic fuel production can remove natural lubricants from the fuel that contributes to lubrication in an engines fuel system. For example, polar compounds, which are hydrocarbons containing other elements such as sulfur, oxygen and nitrogen, act as natural boundary lubricants. These are present in crude oil and straight jet fuel. They act as lubricity improvers by forming thin films on metals surfaces and protecting them from wear. These natural boundary lubricants are often reduced or removed in synthetic fuels due to the severe hydrotreating process. Therefore, synthetic fuels often exhibit a lower lubricity behavior. Assuring the lubricity of a candidate fuel is acceptable is of importance.

The lubricity of ATJ-SKA fuel was tested using the ASTM D5001 [Ref. 14] (BOCLE) method. The lubricity is reported as a function of wear scar diameter (WSD) formed on the test specimen. The ATJ-SKA fuel was found to have a WSD of 0.77 mm, meeting specification maximum of 0.85 mm. Typical petroleum derived fuels have WSD’s ranging from 0.50 mm to 0.75 mm. While the ATJ-SKA had an acceptable score, it should be noted that further research is needed to determine the impact of synthetic fuels and fuel blends on durability of fuel system components.

5.3 Laboratory Evaluation Summary

A full laboratory evaluation of the ATJ-SKA was conducted including standard specification testing and additional fit for purpose testing. The main objective of this effort was to compare the ATJ-SKA against the ASTM D1655/7566 requirements, as well as against experience with other conventional fuels. The FFP testing was based on a rational review of the candidate fuels chemical, physical and performance properties. Such testing was carried out in accordance with ASTM D4054 and ASTM D1655/D7566 so that data generated may contribute to the assessment of potential approval but will not include the full suite of testing required. A detailed laboratory analysis of the ATJ-SKA for the following fuel properties was conducted in accordance with ASTM D7566:

- Chemical
- Bulk physical and performance
- Composition (purity and trace compounds)
- Select fit-for-purpose

The results of the testing were discussed above and a determination on the suitability of ATJ-SKA to be further tested in rig tests of this program was concluded. The results of the evaluation found the fuel exhibited the following characteristics:

- Composition – As compared to conventional Jet A, similar hydrocarbons, different distribution, predominantly iso-paraffinic
- Acceptable volatility and fluidity characteristics
- Fluidity – Similar viscosity profile and good low temperature performance
- Good thermally stability, thus anticipated low risk to fuel system deposits
- Acceptable energy content with minimal impact anticipated to aircraft range due to fuel’s slightly lower energy content on a volume basis
- Combustion and thermal stability-suitable and within experience, indicating minimal impact to aircraft range and good deposit resistance.

The data presented above demonstrates that, with the appropriate controls in ASTM D7566, the ATJ-SKA fuel meets specification requirements, is fit for purpose and expected to perform in a similar manner as conventional jet fuel. Due to ATJ-SKA's predominately iso-paraffinic nature additional combustion rig testing was conducted to further investigate the compositional effect of the fuel on combustion performance.

6. Rig Test Program

Under the Rolls-Royce CLEEN II Sustainable Aviation Fuel program, the ATJ-SKA fuel was tested back-to-back with conventional fuel to assess the fuel's impact on engine systems under engine realistic conditions. The rig test program conducted activities necessary to further understand the relationship between fuel composition and properties (viscosity, density, material compatibility, etc.), combustor performance and operability, gaseous and particulate emissions, and elastomer compatibility. Rolls-Royce used a sequential and methodical rig test program to evaluate the performance of the ATJ-SKA fuel. The rig test program consisted of the following elements:

- Fuel spray characterization
- Ignition and lean blow out testing
- Emissions testing
- Elastomer material compatibility

Fuel Spray Characterization: Because alternative fuel properties relevant to atomization may significantly deviate from those of conventional jet fuels, it is important to assess the spray quality of the fuel to provide better prediction of the combustion characteristics and emissions. Rolls-Royce conducted a series of tests using an atomization spray rig to measure spray SMD and drop size distribution. Spray visualization using laser illumination was also performed at different test points to identify any noticeable differences in spray features between the ATJ-SKA and conventional jet fuels. The test scope included a range of fuel pressure differentials and air pressure drops across the fuel injector simulating the actual operation of the nozzle in the engine.

Combustion Operability: Understanding the ATJ-SKA's impact upon combustion operability is a key aspect of this rig test program. The High Pressure Flame Tube combustion rig was used to assess the suitability of the fuel from a performance, operability and safety perspective. Further understanding into fuel related effects on ignition and lean blow out was gained during the program.

Emissions: Fuel composition can have a significant effect on emissions. This testing assessed the potential risks and/or benefits with respect to the impact of fuel compositions outside the current envelope of approved fuels for a range of emissions indicators.

Elastomer Material Compatibility: Historically a key limitation in current ASTM D7566 fuels is the exclusion of synthetic aromatics and also the requirement for a minimum of 8% petroleum aromatics to offset risk of elastomer seal problems. Rolls-Royce has developed a unique capability to measure elastomeric seal performance in real-time under engine representative conditions using the Elastocon rig. This test capability was used to evaluate the relationship between aromatic levels/types in the ATJ-SKA fuel that is outside the current allowed bounds to elastomer seal performance.

6.1 Fuel Spray Characterization

As a part of the CLEEN II program, the ATJ-SKA fuel was investigated to determine its suitability for use in commercial aircraft applications. To assess the characteristics of the fuel, comparative spray testing was completed to determine fuel dispersion performance. Droplet size is one of the most important performance parameter of fuel spray nozzles. Large drops are slow to vaporize and can lead to local fuel-rich pockets that adversely affect combustion performance. The objective of this effort was to compare the fuel spray nozzle (FSN) performances of the ATJ-SKA fuel to conventional fuels and MIL-PRF-7024 test fluid, and to note any potential issues with the ATJ-SKA fuel in the upcoming combustion tests.

The potential impact of using the ATJ-SKA fuel on combustion quality involves effects of the fuels physical properties on atomization and spray formation processes. The primary properties having a direct impact on fuel injector spray characteristics are viscosity, surface tension, and density. Because the ATJ-SKA properties relevant to atomization slightly deviate from those of conventional jet fuels, it is important to assess the spray quality of the ATJ-SKA against petroleum-based Jet A fuel. This provides a better understanding of the combustion characteristics and emissions resulting from using the ATJ-SKA fuel. Results from this testing will be discussed in the following subsections as reported in Rolls-Royce technical report “Fuel Spray Evaluation of Jet A, ATJ synthetic fuel, and test fluid Mil-PRF-7024” [Ref. 15].

6.1.1 Spray Test Methodology

Spray measurements were performed at atmospheric conditions using a laboratory specializing in high fidelity spray diagnostics. The test set up was configured to permit diagnostics to capture images of the fuel spray flow field, determine the spray patternation characteristics, and measure the spray droplet size and velocity. Since the purpose of the test was to assess fuel-driven effects, the test hardware remained fixed and intact during the duration of the testing, and the testing was conducted in a back-to-back sequence to minimize the risk that some unforeseen time-related factor with the facility or instrumentation would impact the results. The spray study focused on nonreacting diagnostics, and as such, the testing does not quantify any variations due to differing evaporative properties of the fuels.

Three fluids were used to characterize the spray from a pure airblast fuel injector:

- ASTM D1655 Jet A
- ATJ-SKA an ATJ fuel blend using LanzaTech’s ethanol-based ATJ blended with a synthetic aromatic produced by Swift Fuels. Blend proportions were 87% by volume LanzaTech ATJ and 13% Swift aromatic.
- MIL-PRF-7024 Type II, the industry standard calibration fluid for fuel systems.

Fuel injector spray was measured at the laboratory, characterizing the fuel spray using the following diagnostic techniques:

1. *Spray Imaging via photographs with lighting from the camera flash and with lighting from a vertical planar laser sheet.* The spray images provide a qualitative indication of spray quality and spray trajectory.
2. *Spray uniformity and radial fuel mass distribution via optical patternation.* The optical patternation provides details to compare the radial placement of spray. The technique employs a laser sheet that cuts through an axial plane 1.5 in. downstream of the injector exit face. The laser light is scattered by the droplets, and the spray field density is determined from the scattered light intensity. The technique maps out the fuel mass concentrated as a function of the fuel spray’s half angle.
3. *Droplet size via Malvern laser diffraction.* Line ensemble measurement that is widely used in the industry to characterize average spray droplet size.
4. *Pointwise droplet size distribution and velocity via Phase Doppler Interferometry.* Fuel droplets passing through the measurement space scatter the laser light and detectors sense the Doppler frequency and phase shifting to yields spray droplet diameter distribution, axial, and either radial or swirl velocity components.

Fuel sprays are typically characterized at atmospheric conditions where optical access is simplified, and the spray metrics can be quantified using laser based diagnostics. The test conditions, measurement location, and fuel type for the spray test evaluations are defined in Table 8. The table shows the axial position of the measurement with the z-plane location, and the test conditions by percentage pressure drop and fuel-air ratio fraction.

Table 8. Fuel spray evaluation measurements, conditions, and fuel types.

Measurement	Diagnostic	Axial locations and conditions	Fuel
Spray imaging	Flash and vertical laser sheet	4% @ 0.03, 0.05 2% @ 0.015, 0.03	Jet A, ATJ-SKA, 7024
Spray patternation	Optical patternation	Z=1.5", 4% @ 0.03, 0.05	Jet A, ATJ-SKA, 7024
Droplet size, line integrated	Laser diffraction (Malvern)	Z=1.5 in., 4% @ 0.03, 0.05 Z=1.0 in., 4% @ 0.03, 0.05 Z=1.0 in., 2% @ 0.015, 0.03	Jet A, ATJ-SKA, 7024
Droplet size and velocity, point measurement	Phase Doppler interferometry	Z=1.0 in., 4% @ 0.03, 0.05 Z=1.0 in., 2% @ 0.03 (11 pts X, 11 pts Y)	Jet A, ATJ-SKA
Droplet size and velocity, point measurement	Phase Doppler interferometry	Z=0.5 in., 4% @ 0.03 Z=1.5 in., 4% @ 0.03 Z=2.0 in., 4% @ 0.03 (11 pts X, 11 pts Y)	Jet A, ATJ-SKA
Droplet size and velocity, point measurement	Phase Doppler interferometry	Z=1.0 in., 4% @ 0.03 (11 pts X, 11 pts Y)	7024

6.1.2 Spray Test Results

6.1.2.1 Spray Imaging

To obtain an overall picture of the spray, a spray visualization technique using flash photography and laser illumination was conducted using the ERC spray rig. The purpose of this test was to compare the general features of the ATJ-SKA fuel to those of baseline Jet A and 7024 calibration fluid. The spray cone angle, spray streaking tendency, and spray concentration are some of the important parameters that can reveal any special behavior in fuel sprays.

Spray imaging results as outlined in Table 8 are presented in Appendix B**.** The images in Appendix B are a compilation of images taken in three ways for each test condition. The first grouping of images is a flash photograph of the spray. The second group of images is from a photograph illuminated by both a flash and sheet laser pulse directed through a plane normal to the camera view. The third image grouping is a photograph of laser pulse images with light filtered to the frequency of the laser. These laser sheet illuminated images provide a visualization of the spray inside the spray cone. Each laser pulse is of short duration and captures a frame of the turbulent, fluctuating flow field. For the high fuel-air ratio condition (f/a=0.050), different pulse durations (1/50, 1/100, 1/200) were recorded. The spray cones at each condition were generally stable in time and the spray images show that the visual nature of the spray from the fuel injector was not altered by fuel type.

6.1.2.2 *Spray Patternation*

Spray patternation is determined optically by post-processing an image of scattered light from droplets illuminated by a laser sheet directed across the spray normal to the spray's centerline 1½ inches aft of the nozzle face. The data processing reduces the 360-degree spray image to characterize the spray's radial fuel placement via a spray half angle plot as shown in Figure 14 and Figure 15. The processing technique normalizes the image and presents the fuel spray density in arbitrary units (a.u.) on the figures. The "Alt Fuel" in Figure 14 and Figure 15 is the ATJ-SKA fuel of interest.

Figure 14 isolates the two fuels, presenting Jet A and ATJ-SKA for comparison of the differences in spray dispersion and cone angle. At the 0.030 f/a ratio condition, there is no difference in spray angle between the two fuels. Some minor differences in spray angle are noted for the 0.050 f/a ratio condition. The ATJ-SKA fuel shows a slightly lower fuel spray density at the outer portion of the spray (spray half angles towards the right of the scale).

Figure 15 includes the 7024 calibrating fluid along with the Jet A and ATJ-SKA fuels. The calibrating fluid shows a narrower cone angle at both operating conditions (0.030 and 0.050 f/a ratios) as the spray density shows the outer spray wall falling off more rapidly with the 7024 calibration fluid.

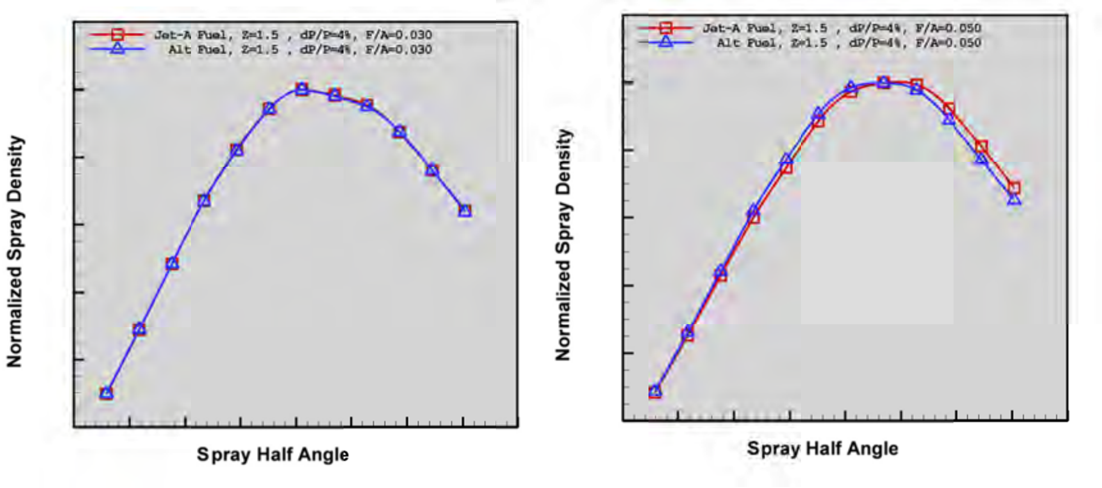


Figure 14. Half angles for Jet A and ATJ-SKA for F/A = 0.030 and 0.050.

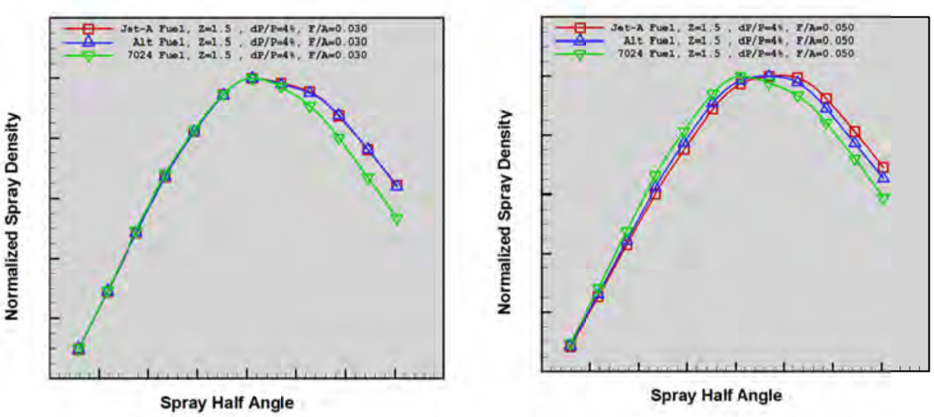


Figure 15. Half angles for Jet A, ATJ-SKA, and 7024 for F/A = 0.030 and 0.050.

6.1.2.3 *Line Integrated Droplet Size (Malvern)*

Malvern laser diffraction determines an ensemble spray particle size by analysis of the laser diffracted light along a line perpendicular to the axis of the spray. This technique is widely used to characterize the spray from a fuel injector. The spray's average droplet size is determined by fitting the spray data to a Rosin Rammler distribution and then reported out as a SMD (or D32).

The SMD results for the three fluids are plotted in Figure 16 where six conditions (A through F) are presented.

The spray results show the following:

- The droplet size as measured by the Malvern is independent of fluid type for a specific test condition over the range of measured conditions. The Malvern results show there is less than a micron difference in spray drop size between the fluids for a specific test condition.
- Droplet size (SMD or D32) is pretty much independent of f/a ratio. This is illustrated repeatedly in Figure 16. The difference in SMD is less than 1 micron between operating conditions A and B with the higher f/a condition showing the slight increase in drop size. A similar pattern is shown between conditions C and D, as well as between conditions E and F.
- Droplet size increases as the spray evolves from z = 1.0 to 1.5 inches. This is seen when comparing measurements A/B to measurements C/D. Closer to the injector (z = 1.0 in.) the droplet size is on the order of 15 micron. Further downstream (z = 1.5 in.), the droplet size is on the order of 18 microns.
- The pressure drop across the fuel injector impacts the spray droplet size. Pressure drop is halved from 4 to 2% when comparing conditions C and F, and the droplet size increases. This tendency would be expected with a pure airblast nozzle, which relies upon air energy to atomize the filming fluid.

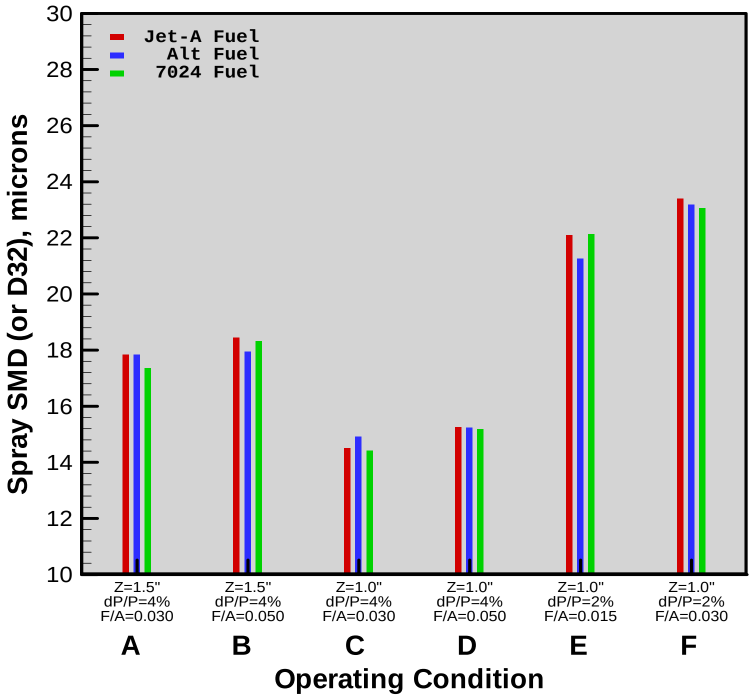


Figure 16. Malvern droplet size measurements for Jet A, ATJ-SKA, and 7024.

It is worth noting that droplet sizes are small, an indication of the atomization effectiveness and the quality of the fuel nozzle design. As can be seen from Figure 16, the fuel nozzle designed for the CLEEN II combustor is quite good as it produces a very fine, small droplet spray. With a good performing fuel nozzle, very minor differences are noted in fuel droplet size. It could be that the high performance nozzle masks a fuel-driven spray droplet size difference that could emerge with a less effective nozzle design.

6.1.2.4 Pointwise Droplet Size Distribution and Velocity via Phase Doppler Interferometry

Phase Doppler interferometry (PDI) employs two pairs of crossing laser beams within the spray, creating a small measurement volume that can resolve point-wise spray details. This optical technique collects multiple samples from each point, which are statistically analyzed to determine velocity and droplet size. As with the Malvern ensemble measurement, the PDI droplet size results are presented as SMD (or D32). The PDI measurements for the three fluids are presented in Figure 17 through Figure 22.

All three velocity components were captured using PDI. The PDI technique resolves two velocity components via the fringe pattern set up by the two crossing laser beams. To capture all 3 velocity components, the nozzle is rotated 90 degrees. An initial traverse is made to collect information to yield the axial (u) and azimuthal (w) velocities. Then the nozzle is rotated 90 degrees and a second traverse is made to collect the axial (u) and radial (v) velocities. As such, repeat measurements of the droplet size and axial velocity are captured and this is shown in Figure 17 through Figure 22.

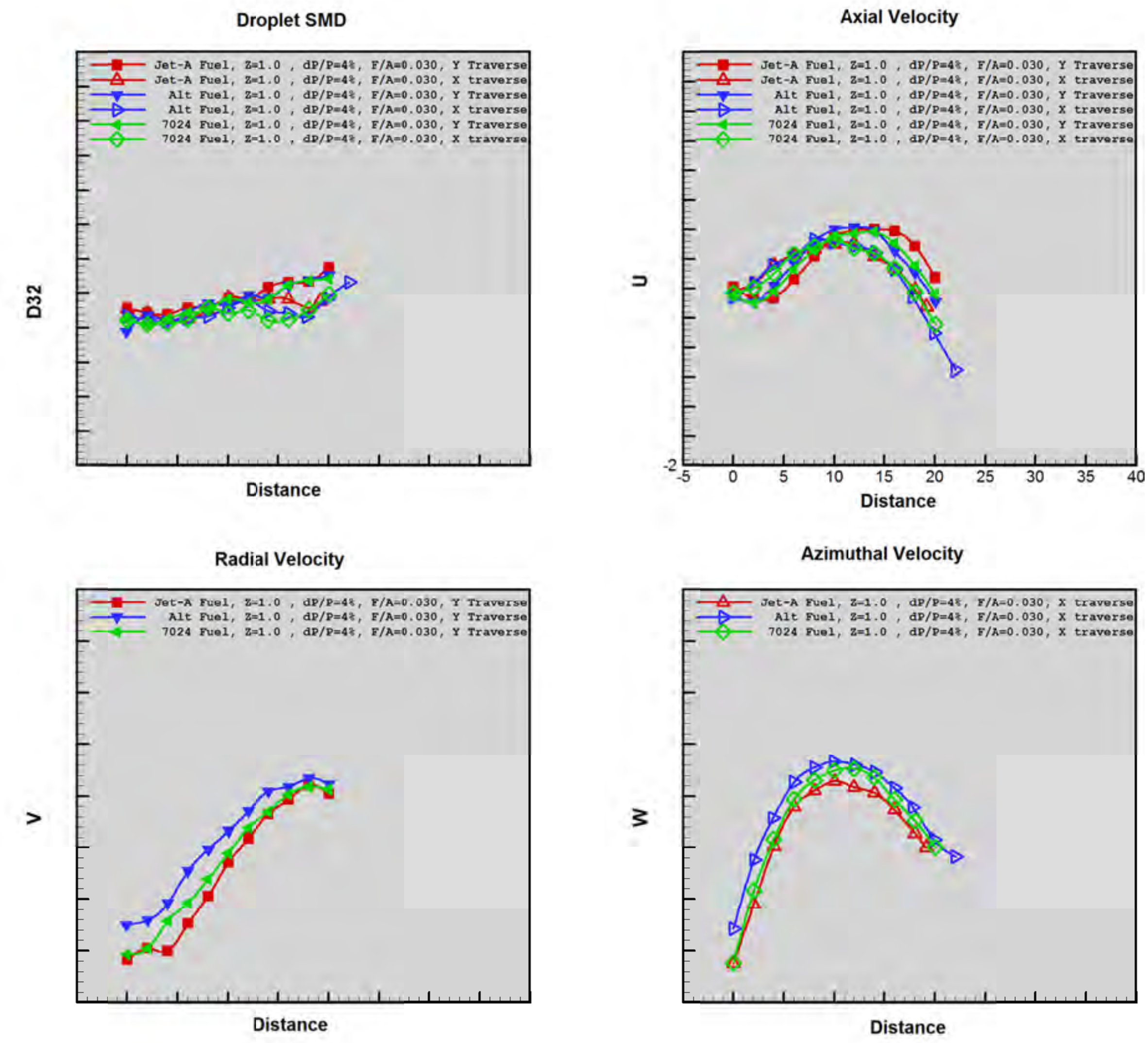


Figure 17. PDI results for D32, U, V, and W for Z=1.0inch, dP/P=4%, f/a=0.030.

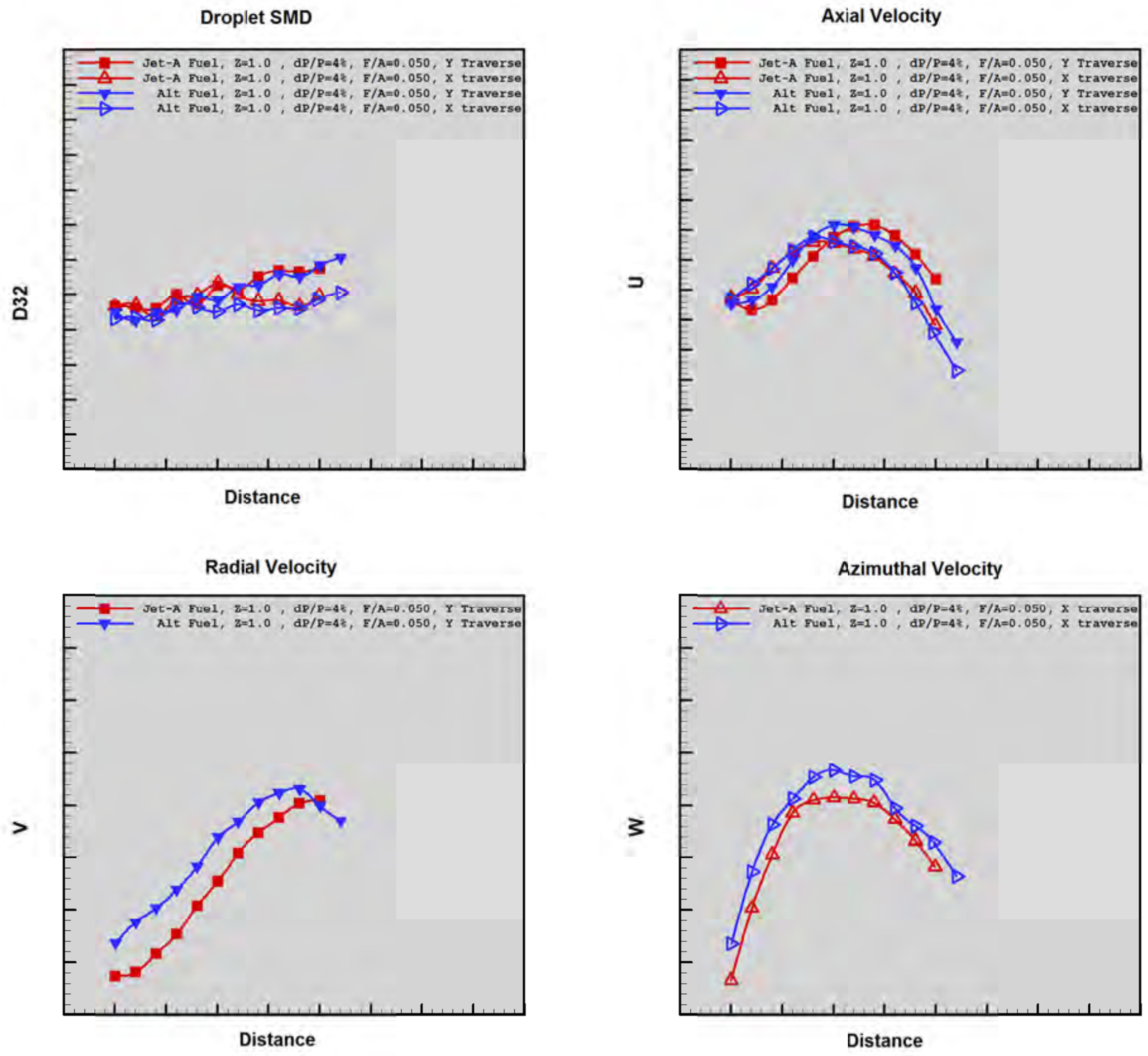


Figure 18. PDI results for D32, U, V, and W for Z=1.0inch, dP/P=4%, f/a=0.050.

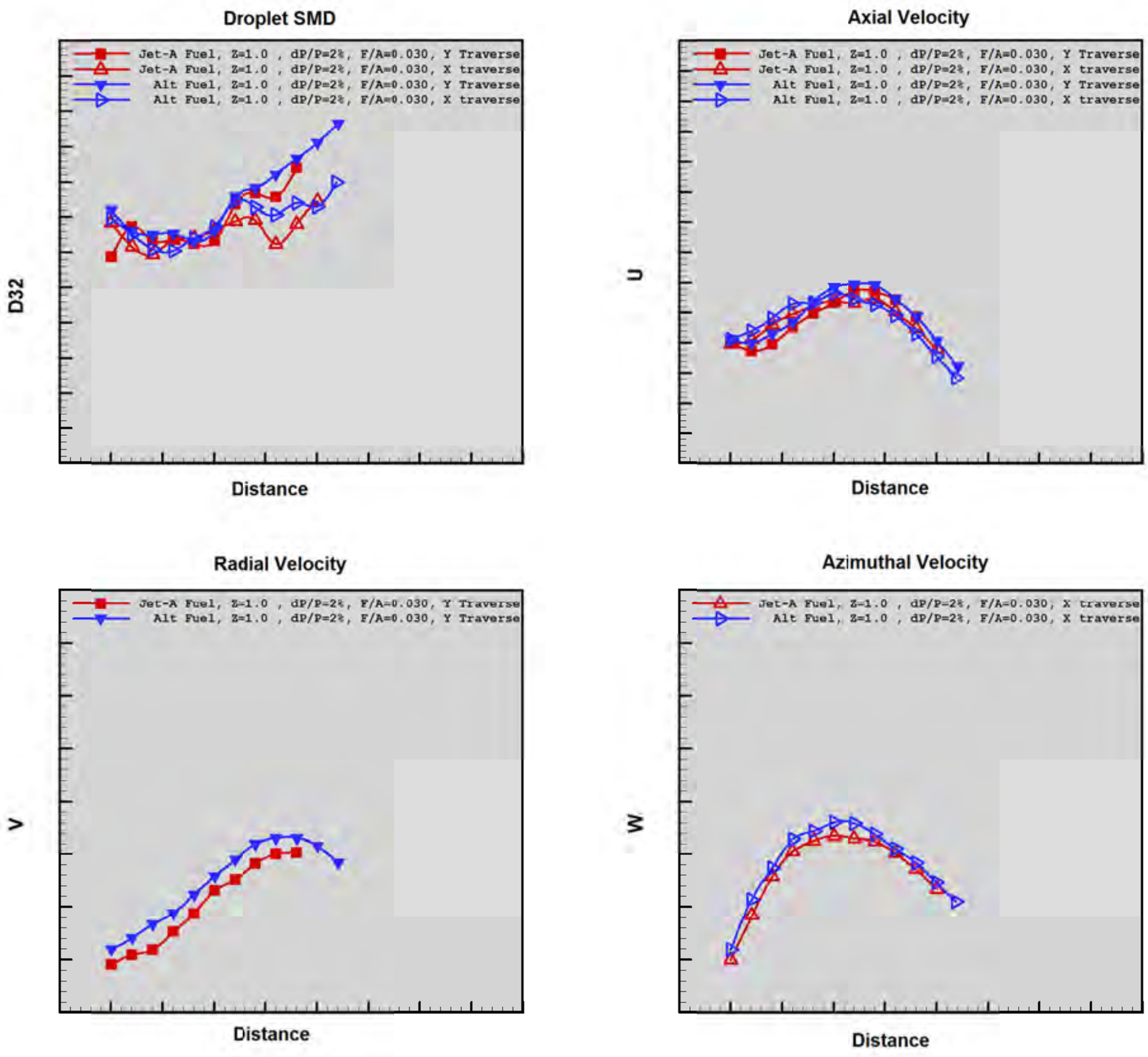


Figure 19. PDI results for D32, U, V, and W for Z=1.0 inch, dP/P=2%, f/a=0.030.

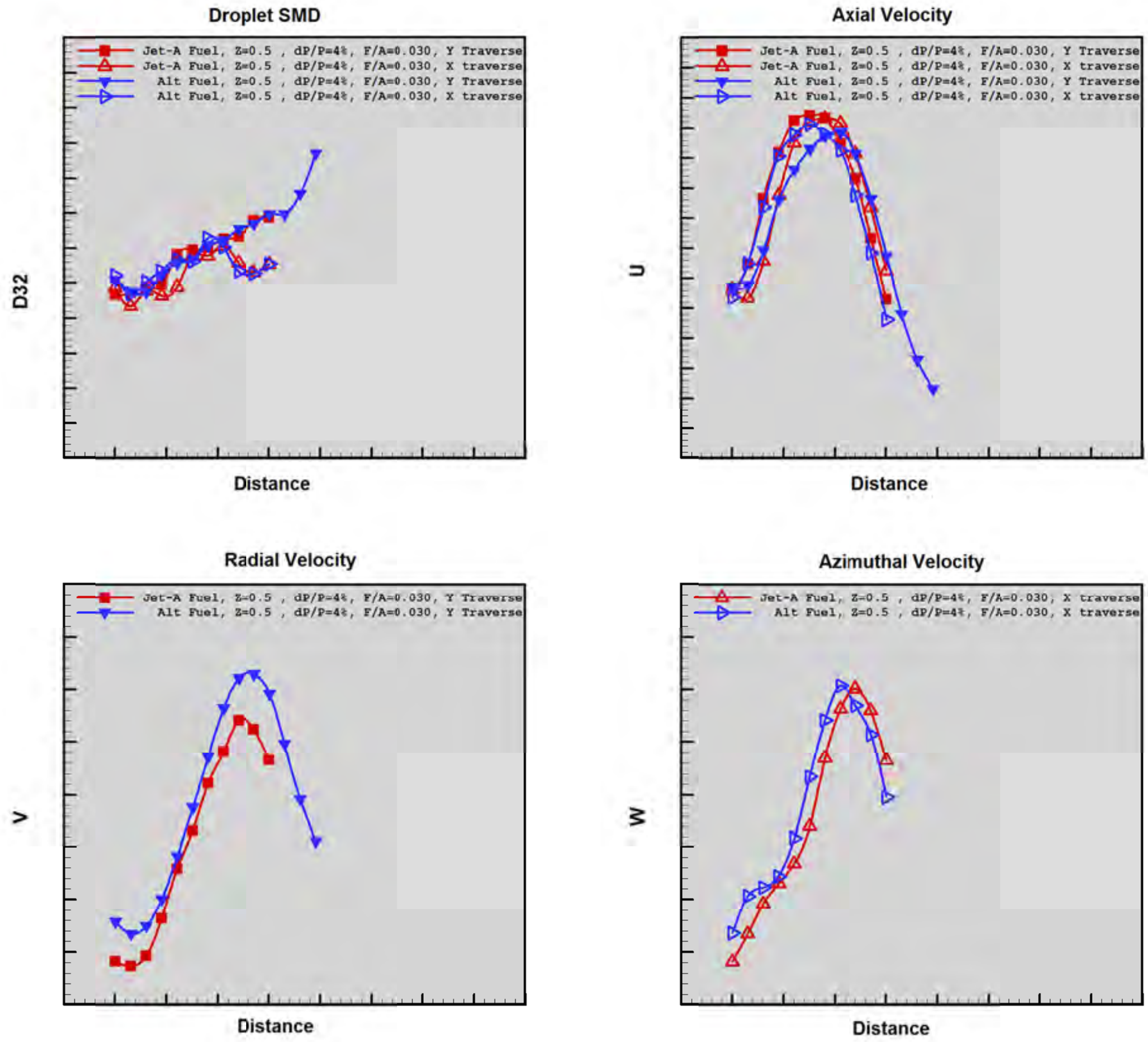


Figure 20. PDI results for D32, U, V, and W for Z=0.5 inch, dP/P=4%, f/a=0.030

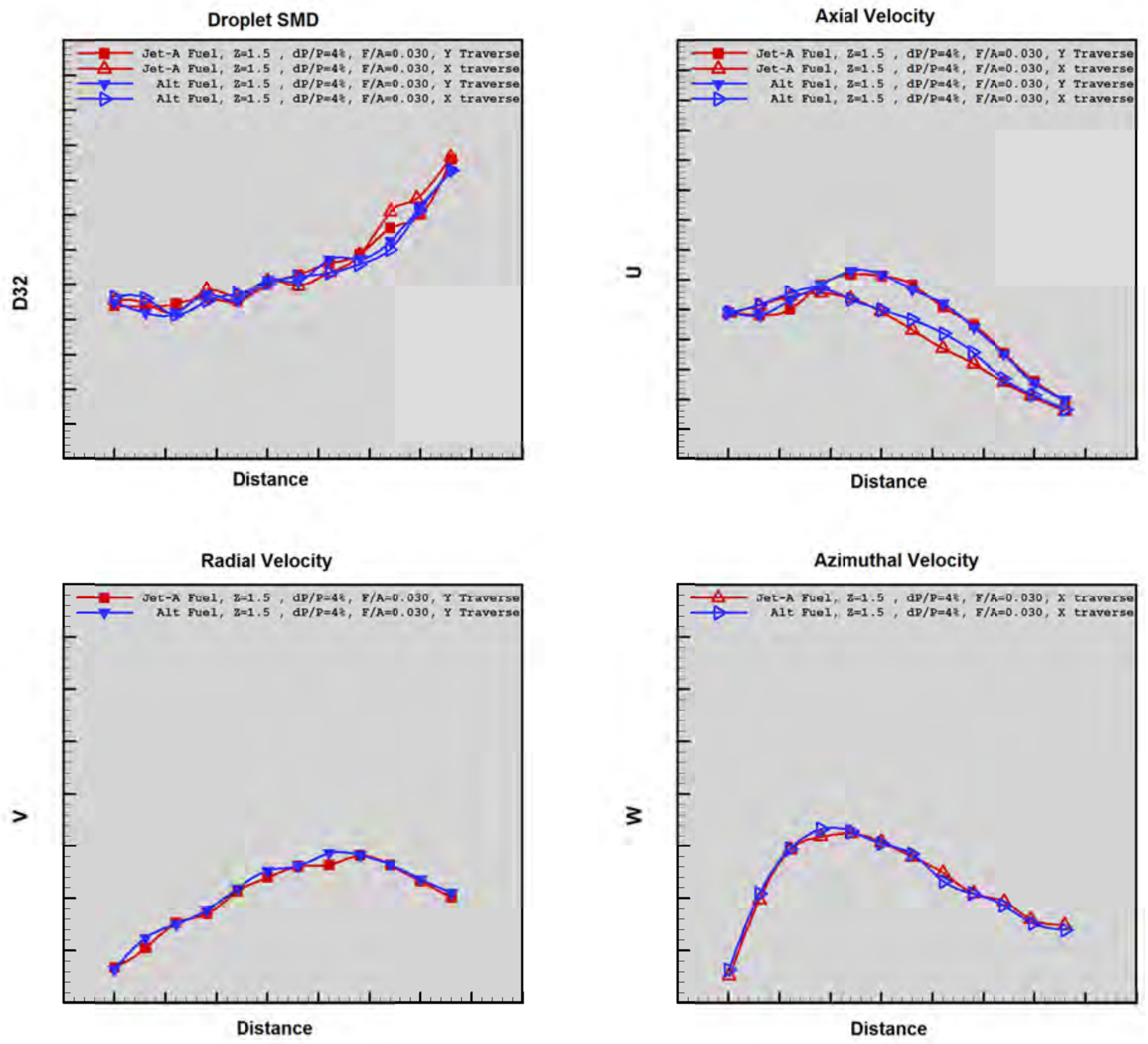


Figure 21. PDI results for D32, U, V, and W for Z=1.5 inch, dP/P=4%, f/a=0.030.

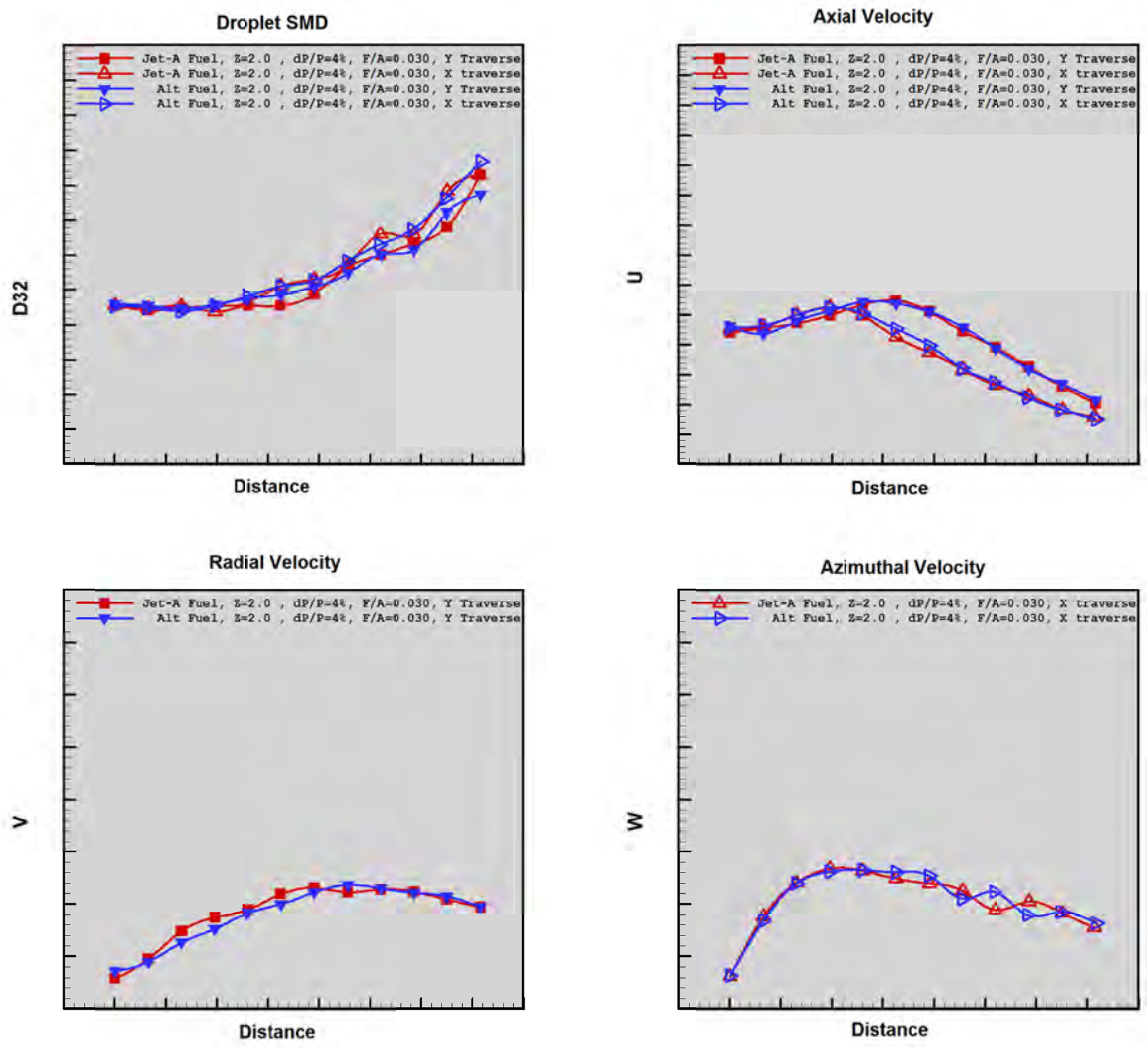


Figure 22. PDI results for D32, U, V, and W for Z=2.0 inch, dP/P=4%, f/a=0.030.

Figure 17 shows droplet SMD and velocity field for three test fluids: the Jet A, ATJ-SKA, and 7024 calibration fluid. There is some droplet size variability due to nozzle rotation near the tip. There is less variability between fluids. Beyond 13 mm, some divergence is observed between droplet sizes of the 3 fluids tested. Jet A is about 1 micron larger droplet at some radial positions. There are some subtle differences in the velocity fields between the fluids. The axial velocity (u) Y-traverse shows greater differences than the X-traverse. The axial velocity of the ATJ-SKA and 7024 at the outer quarter of the spray cone is lower than that measured for the Jet A. Near the central part of the spray, the axial velocity is higher for the ATJ-SKA and 7024. The other velocity components (radial and azimuthal) of the ATJ-SKA are higher than recorded for the Jet A across the entire spray cone. In the case of the radial velocity, the discrepancy becomes progressively higher with movement inwards toward the centerline of the spray.

Pointwise measurements were captured for all 3 fluids at an axial location 1 inch from the nozzle face with airflow set for 4% pressure drop and a 0.030 f/a. This permits a back-to-back assessment of all three fluids. Given the objective was to evaluate the differences between Jet-A and ATJ-SKA, the balance of the PDI testing was confined to Jet A and ATJ-SKA so more conditions could be captured.

The conditions were altered to assess the performance with substantially greater fuel flow and the f/a ratio was set to 0.050 for the results presented in Figure 18. The droplet size for the ATJ-SKA is 1 or 2 micron greater, but the velocity field is very similar to that shown in Figure 17 with the same basic trends and differences noted for that for 0.030 f/a.

The air velocity is reduced by lowering the pressure drop to 2% for the results plotted in Figure 19. As expected, droplet size increases as compared to Figure 17 results. The droplet size difference between ATJ-SKA and Jet A is more pronounced with the ATJ-SKA having larger droplets on the outer half of the spray cone. The velocity field is similar for either fuel. There is a steady trend of having larger radial and azimuthal velocities for the ATJ-SKA fuel.

Figure 18, Figure 20, Figure 21, and Figure 22 show drop size and velocities as the spray develops by taking measurements at different axial distances from the nozzle face. Comparison of these figures shows the spray developing and broadening as the distance from the nozzle tip increases.

Near the nozzle, Figure 17 and Figure 20 show greater drop size variability due to nozzle rotation. As the spray develops and broadens (Figure 21 and Figure 22) downstream, there is minimal effect of nozzle rotation upon the droplet size. The figures also show that the rotational sensitivity is less apparent in the plots of the velocity fields.

As in the Malvern data, there are small difference in the droplet size measured between the Jet A and ATJ-SKA fuels.

With regards to the velocity field, the figures show the axial velocity decays with increasing axial distance as anticipated. The radial extension of the spray shows a general broadening of the velocity field with greater spray half-angles as measurements are taken further downstream.

Overall the PDI results show similarities for droplet size and velocities between the fluids. The spray cone size as measured by the spray width is narrower for the 7024 calibration fluid. Spray widths are comparable for the Jet A and ATJ-SKA. Near the periphery of the spray cone, the ATJ-SKA fuel produced larger droplets.

6.1.3 Spray Test Conclusions

Spray testing was carried out at several conditions and positions within the spray with three different fluids: Jet A as a reference fuel, the ATJ-SKA and the 7024 calibration fluid. For the detailed pointwise measurements, the emphasis was on collecting data for the Jet A and ATJ-SKA fuels. Testing was conducted with a common fuel injector of a pure airblast design.

In general, spray performance of the ATJ-SKA fuel was similar to the Jet A fuel, with only minor differences noted. An overview of the results is presented in the following:

- The visual spray recordings show similar sprays for all test fluids whether illuminated by natural light or by flash laser illumination. No divergence in visual spray behavior was noted for atmospheric test conditions evaluated.
- The spray's density, uniformity, and liquid radial distribution as characterized through the optical patternation measurement, showed only minor differences between Jet A and ATJ-SKA fuels, with slightly lower ATJ-SKA spray density near outer spray at 0.05 F/A. The 7024 calibration fluid produced a slightly narrower spray cone.
- For ambient temperature conditions, droplet sizes were quite similar between the Jet A and ATJ-SKA fuels as the line ensemble droplet size measured with the Malvern showed drop sizes within 1 µm with effective atomization independent of fuel type.

- The pointwise PDI measurements confirmed the droplet sizes were similar with differences in droplet size occurring at the periphery of the spray where larger droplets were recorded for the ATJ-SKA fuel. Axial droplet velocity falls off a bit faster with the ATJ-SKA fuel at the outer portions of the spray cone. For the ATJ-SKA fuel, the accompanying radial and swirl velocities are slightly higher toward the central part of the spray as compared to the Jet A fuel spray.

6.2 High Pressure Flame Tube Rig Test

A rig test was conducted to evaluate the combustion performance of the LanzaTech ATJ-SKA fuel against a reference Jet A fuel. Since the purpose of the test was to assess fuel-driven effects, the test hardware remained fixed and intact during the duration of the testing, and the testing was conducted in a back-to-back sequence to minimize the risk that some unforeseen time-related factor with the facility or instrumentation would impact the results. This back-to-back test allowed a preliminary understanding of the ATJ-SKA fuel-related effects on combustion behavior, operability, and gaseous emissions as compared to baseline Jet A. Results from testing will be discussed in the following subsections as reported in Rolls-Royce technical report “High Pressure Flame Tube Rig Test Results” [Ref. 16].

6.2.1 Flame Tube Test Methodology

The objective of the high pressure testing was to validate fuel nozzle performance and fuel driven effects in a representative primary combustion zone environment. A high pressure rig fitted with a flame tube test vehicle was used for the fuel evaluation (Figure 23). This experimental setup provides a means to assess performance over a range of operating conditions, including elevated pressure and high temperature as shown in Table 9. Key features of this rig include a single sector combustion chamber for testing at high temperatures and pressures. In addition, gas sampling of the combustion products was taken and analyzed for emissions.

Table 9. Test point operating conditions.

Index	Condition
1	Sub idle
2	Idle
3	Approach
4	Climb
5	Climb +

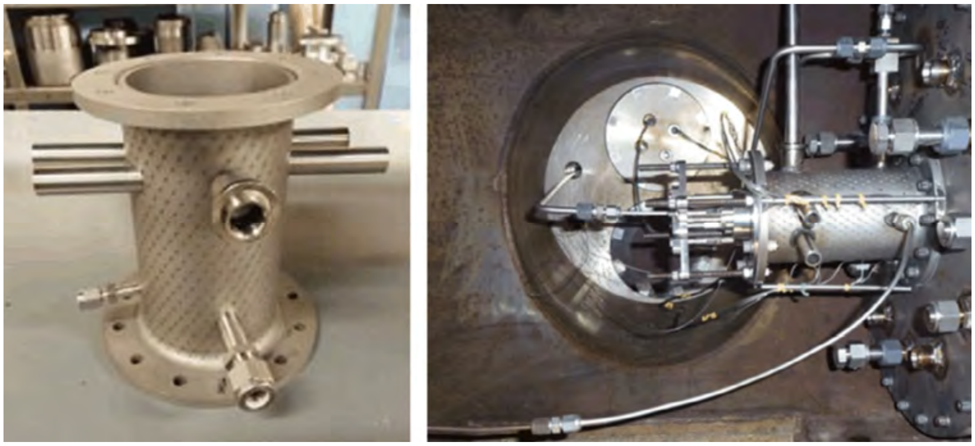


Figure 23. Flame tube (left) and installed in high pressure rig (right).

The test rig and facility was fully instrumented to monitor and control all parameters related to maintaining stable operating conditions. The flame tube was instrumented with thermocouples to monitor metal wall temperatures and a multi-hole gas sampling probe was mounted near the aft flange to capture exhaust gas emission levels. Testing included the following elements:

- Lean stability
- Combustion efficiency
- Gaseous emissions
- Smoke emissions
- Liner metal wall temperature assessment

6.2.2 Lean Stability Test Results

Lean stability is determined by establishing steady state operating conditions at a fuel-air ratio which produces a strong stable flame. Then the fuel flow is slowly reduced until the flame is extinguished. The resultant lean blow out (LBO) fuel flow and fuel-air ratio are recorded. This process is repeated and LBO fuel-air ratio recorded a second time.

The stability testing shows the average LBO f/a ratio is 7% higher for the ATJ-SKA synthetic fuel, showing the flame stability is impaired with the ATJ-SKA fuel.

6.2.3 Gaseous Emissions, Smoke, and Combustion Efficiency Test Results

The impact of the ATJ-SKA fuel on emissions and combustion efficiency was also evaluated in the High Pressure Flame Tube at key points within the flight envelope. It is understood that the fuel properties involved in pollutant formation include those impacting spray characteristics, spray evaporation, and combustion processes within the combustor. Such properties include fuel viscosity, surface tension, density, distillation profile, vapor pressure, aromatic content, and heat of combustion. To further understand the degree of impact the ATJ-SKA fuel properties have, a determination of emissions and combustion efficiency performance was assessed. Tests were conducted at key operating points within the flight envelope.

Figure 24 through Figure 28 presents the experimental results of NOx, CO, UHC, combustion efficiency and smoke. NOx is nitrogen oxide, CO is carbon monoxide, and UHC is unburned hydrocarbon, which are emissions from the combustion of fuel. The results of the ATJ-SKA blend are compared to the baseline Jet-A and other alternative fuels previously tested.

6.2.3.1 NOx Emissions

The flame tube exhaust gas was extracted via the gas sampling probe for four test conditions (Test Conditions 2 through 5 in Table 9) and processed via a NOx analyzer. Figure 24 shows the measured NOx emission indices (EI) for the four operating conditions over a range of fuel-air ratios.

The NOx EI are similar for most test conditions and fuel-air ratios. At idle condition, no difference is observed in NOx EI between ATJ-SKA and Jet A. At approach condition, NOx EI are the same except for a window between certain f/a ratios, where the ATJ-SKA produces lower NOx. A similar dip in NOx EI is seen at climb test condition between certain fuel-air ratios. The trend is reversed at climb+ condition, where NOx EI for ATJ-SKA is consistently higher across the entire fuel-air ratio sweep.

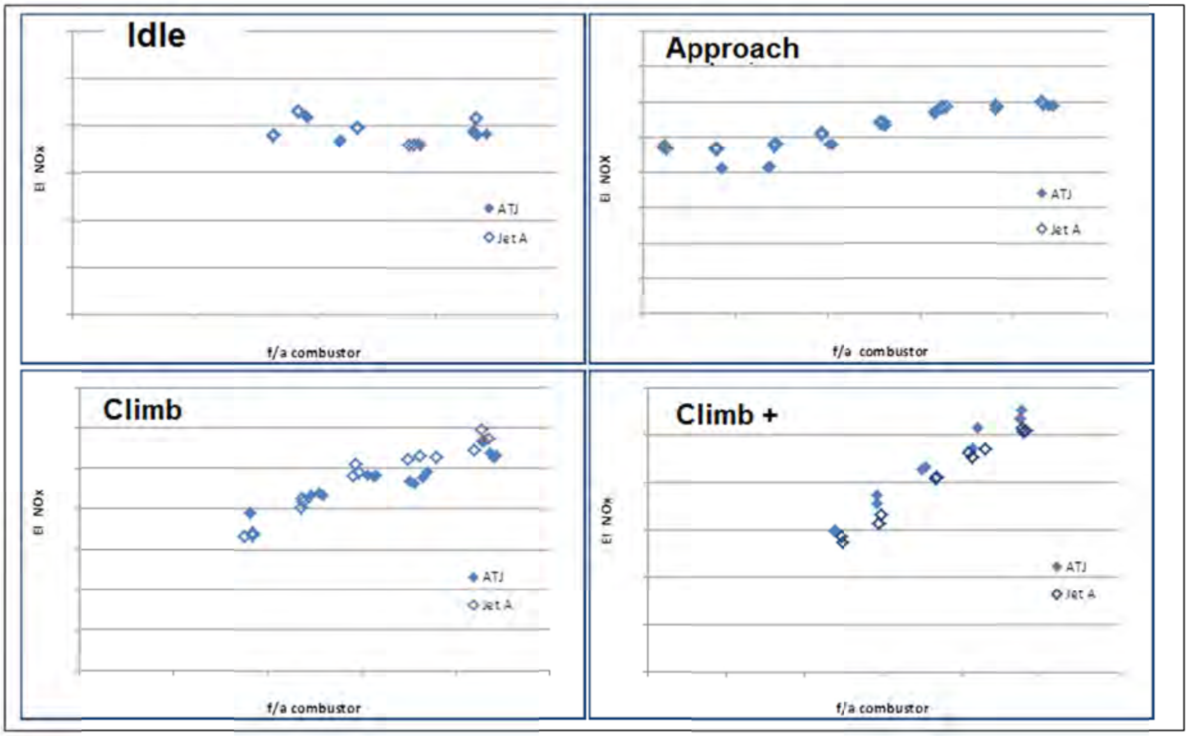


Figure 24. NOx emission indices for four operating conditions.

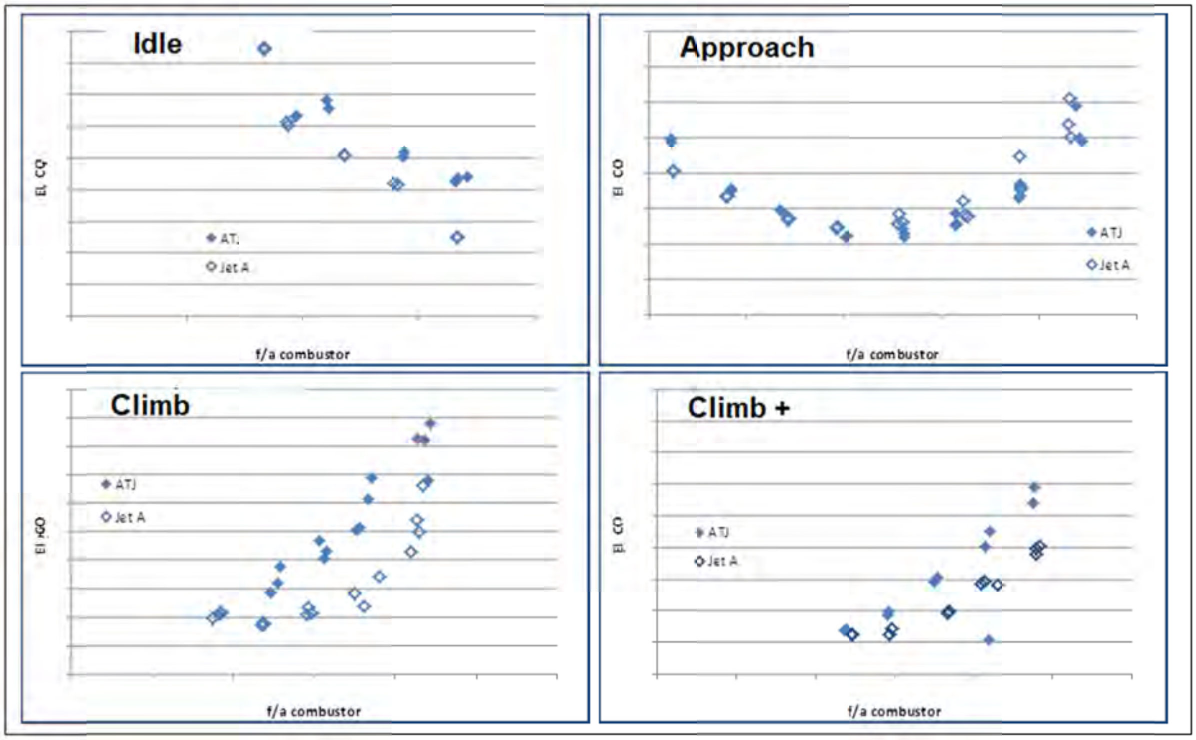


Figure 25. CO emission indices for four operating conditions.

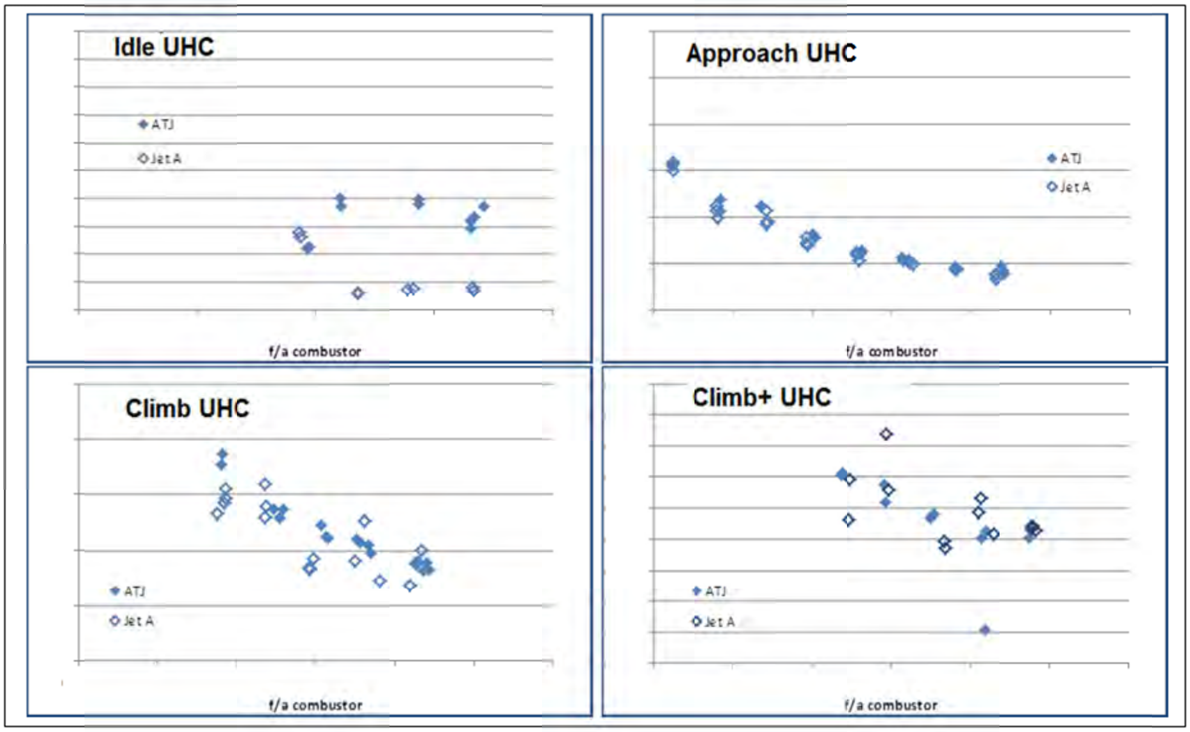


Figure 26. UHC emission indices for four operating conditions.

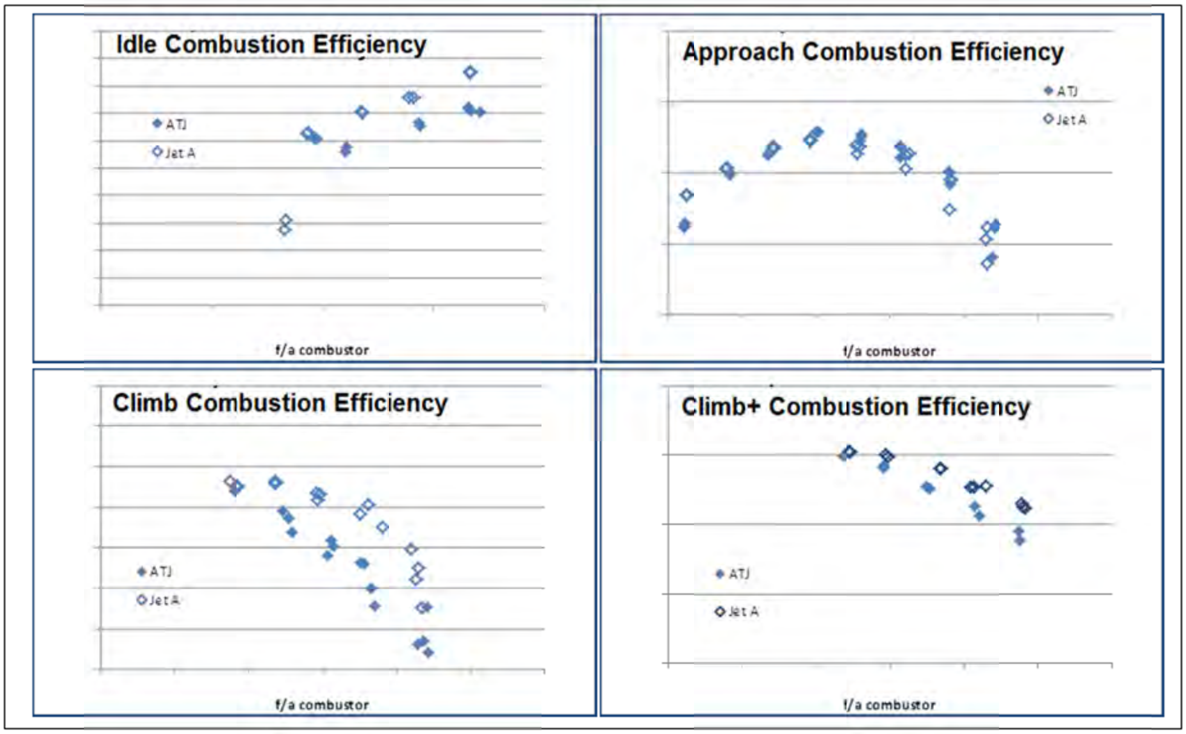


Figure 27. Combustion efficiency for four operating conditions.

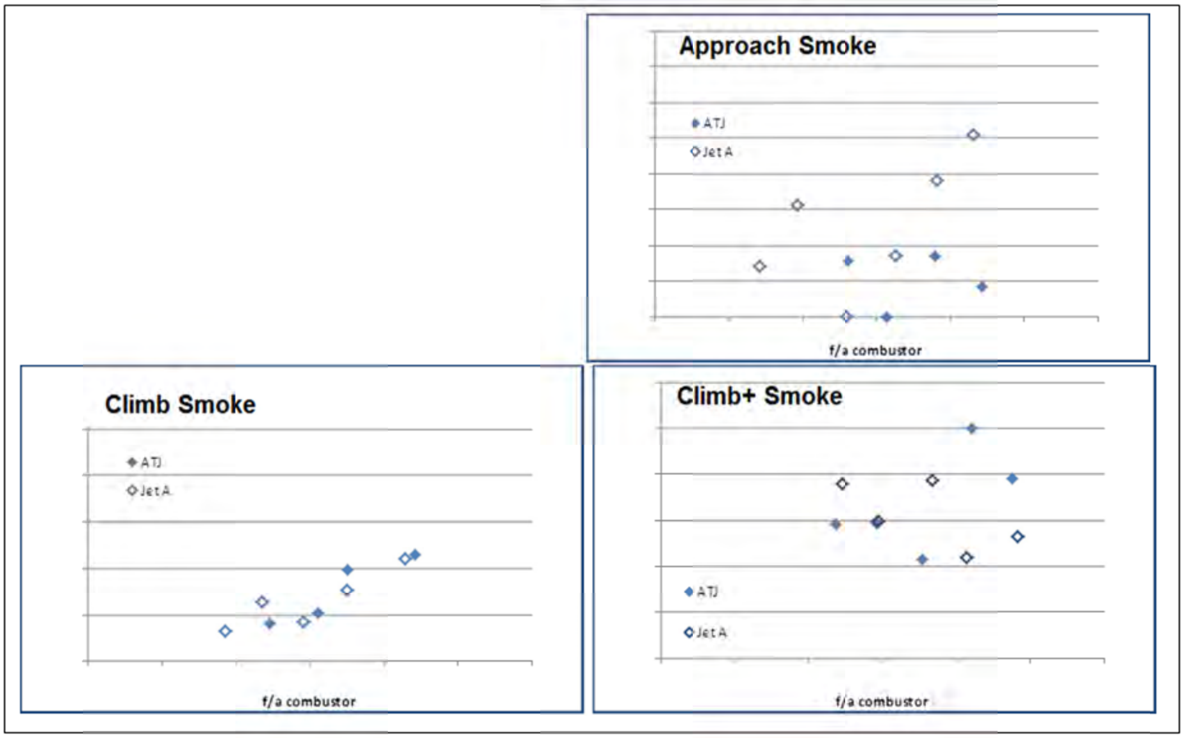


Figure 28. Smoke number for three operating conditions.

6.2.3.2 CO Emissions

The flame tube exhaust gas was extracted via the gas sampling probe for four test conditions (Test Conditions 2 through 5 in Table 9) and processed via a CO analyzer. Figure 25 shows the measured CO EI for the four operating conditions over a range of fuel-air ratios.

In general, the CO EI for the ATJ-SKA fuel are higher than the Jet A fuel. This is clearly the case for idle, climb and climb+ conditions, where CO emissions are higher across all fuel-air ratios. The approach condition shows a trend reversal where the ATJ-SKA fuel CO levels are the same or lower at the higher fuel-air ratios.

6.2.3.3 UHC Emissions

The flame tube exhaust gas was extracted via the gas sampling probe for four test conditions (Test Conditions 2 through 5 in Table 9) and processed via a UHC analyzer. Figure 26 shows the measured UHC EI for the four operating conditions over a range of fuel-air ratios.

Figure 26 shows the UHC EI are similar between the ATJ-SKA and Jet A for the higher power conditions (approach, climb and climb+). At idle condition, however, the ATJ-SKA fuel produces higher UHC levels.

6.2.3.4 Combustion Efficiency

Combustion efficiency is derived from the gaseous emission measurements. Figure 27 depicts combustion efficiency for the four operating conditions over a range of fuel-air ratios.

In general, combustion efficiency suffers with the ATJ-SKA synthetic fuel. Figure 27 shows the combustion efficiency is lower with ATJ-SKA fuel for idle, climb and climb+ operating conditions. For the approach condition, ATJ-SKA and Jet A fuels have similar combustion efficiency.

Because the UHC and CO are main contributors to combustion inefficiencies, the higher measured values of the two pollutants for the ATJ-SKA explain the lower combustion efficiency.

6.2.3.5 Smoke Emissions

The formation of soot in the primary zone of the combustor is largely dependent on fuel composition, together with combustor geometry and operating conditions. The aromatic content in a fuel is one of the leading fuel properties contributing to soot formation. In addition to the gaseous emissions (NOx, CO, UHC), particulate emissions were measured. Smoke as recorded using the ARP1179 protocols are shown in Figure 28 for three operating conditions over a range of fuel-air ratios.

In general, the smoke numbers between ATJ-SKA and Jet A fuels are similar at the different conditions. There is some scatter in the smoke readings; however, this is mostly the measurement resolution of the technique. The smoke emission test results for the ATJ-SKA fuel are considered acceptable, when considering experience with other fuels and the expected variation of the test precision.

6.2.4 Metal Wall Temp Testing

Metal wall temperature of the flame tube was assessed to determine if the ATJ-SKA had an effect on the heat load that differed from conventional Jet A. Lower combustor liner temperatures can result in enhanced durability of the combustor and hot section components. Excessive heat load to the liner through flame radiation and convection from hot flow within combustor can significantly reduce life of liner or even cause liner failure in extreme cases. The radiation component of the heat load is controlled by the flame luminosity, which in turn is a function of the soot concentrations in the combustion zone. Because the soot formation is dependent upon higher aromatic content, the fuel composition is considered one of the major factors impacting liner wall temperatures.

Thermocouples were placed along the flame tube to record metal temperatures on the “cold” side surface of the wall (reference Figure 29). The thermocouples were arranged so the dome section (forward panel of flame tube the fuel injector is mounted upon) and liner section (cylindrical tube containing the flame) temperatures are monitored. Two thermocouple stations are mounted on the dome panel and two axial rows with six thermocouple stations per row are

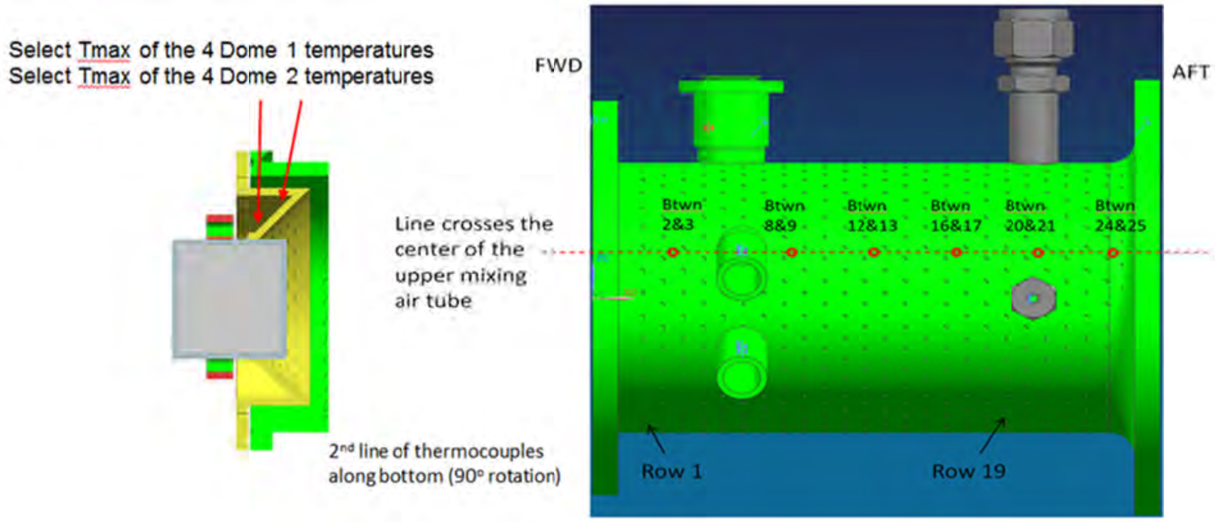


Figure 29. Thermocouple placement.

positioned along the liner section. The dome thermocouples are the first two axial stations shown on the plots. The remaining axial stations are the liner wall thermocouples. For these liner wall temperatures, the six solid symbols show temperatures along an axial line extending along the length of the liner wall at a specific azimuthal plane. Similarly, the open symbols show wall temperatures along an axial line that is rotated 180 degrees from the open symbol thermocouples.

Metal wall temperatures were recorded during the high pressure flame tube test. The thermocouple measurements are shown in Figure 30.

In general, the ATJ-SKA synthetic fuel does not significantly impact wall temperatures. Figure 30 shows wall temperatures for four conditions. Two f/a settings were selected at approach condition (top row of plots) to show the impact of f/a ratio on wall temperatures. Then, high f/a settings at climb and climb+ conditions are shown (bottom row of plots) to record the maximum wall temperatures. All plots show a circumferential wall temperature gradient as one side of the liner shows higher wall temperatures than the opposing side. The difference in temperatures from side to side is larger than the difference observed for the fuel type burned. The differences in wall temperatures due to fuel type are most pronounced at the forward section of the liner (stations at axial distance less than 3 inches).

6.2.5 Flame Tube Test Conclusions

The high pressure flame tube rig tests provided preliminary information on lean stability, combustion steady-state performance, and metal wall temperatures. Analyses of the flame tube test results reveal some performance similarities and differences between the ATJ-SKA fuel and the baseline Jet A fuel as follows:

- Lean stability deteriorated slightly with the ATJ-SKA with an average f/a ratio that is 7% higher

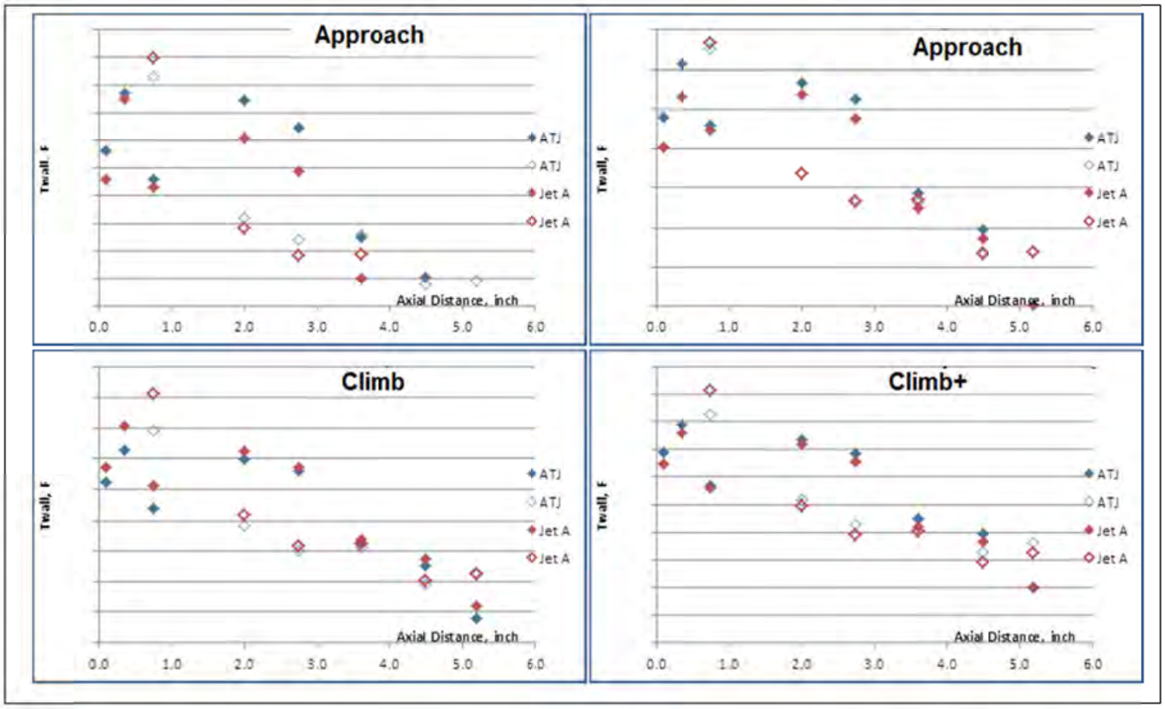


Figure 30. Thermocouple temperatures for selected operating points of interest.

- NOx emissions indices are similar for most test conditions and fuel-air ratios and insensitive to fuel type
- CO EI for the ATJ-SKA fuel are higher than Jet A.
- UHC EI is similar between the ATJ-SKA and Jet A for higher power conditions but elevated at low power conditions.
- The ATJ-SKA's higher CO and UHC emissions led to lower combustion efficiency.
- Smoke numbers between ATJ-SKA and Jet A fuels are similar at the different conditions.
- ATJ-SKA does not significantly impact wall temperatures with similar measurements.

In general, flame tube testing showed some deterioration in lean stability, with higher CO and UHC emissions that led to lower combustion efficiency. However similar results were found for NOx, CO, smoke number, and wall temperatures.

6.3 Elastocon Testing of Elastomer Seal Performance

Under the CLEEN II program Rolls-Royce assessed elastomeric seal material performance using the innovative Elastocon rig capability developed and demonstrated under CLEEN I. Building upon that success, we further developed the Elastocon rig capability by improving the test jigs and monitoring system to allow fuel switching by a fuel flow system, thus enhancing rig capability. We developed the ability to thermally age O-ring test specimens, so the condition of the elastomer material was more representative of in-service examples where physical and chemical properties are degraded and may be less able to withstand fuel aromatic shifts. Cyclic, fuel-switching testing between conventional and blends of ATJ-SKA fuels for a number of elastomer seal materials were tested allowing us to better understand the fuel's impact on seal performance. Results from this testing are discussed in the following subsections EDNS01000794774 [Ref. 17].

6.3.1 Background

The Rolls-Royce CLEEN I Program examined the effect of various fuels (including low aromatic fuel) on elastomer O-ring seals performance by characterizing compression stress relaxation. This work was previously reported in “Rolls-Royce Alternative Fuels Program – Rig Test of Candidate Fuels: Elastomer Testing” [Ref. 18]. That method used the proprietary Elastocon units, which were modified to provide an O-ring groove/plate representing a face seal arrangement. A representative selection of three engine O-ring material types (AS568-113 size) were installed into the Elastocon. The O-ring materials included: fluorocarbon, fluorosilicone, and nitrile rubber. These O-ring materials represent legacy and more recently developed elastomer materials used in the aerospace industry. The sealing force was monitored real time while seals were exposed to various fuels, at the same time temperature was cycled between +30 and -40°C.

The Elastocon test method used in CLEEN I compressed the elastomer seal under test either between flat plates (plattens) or in a groove/plate arrangement that was approximately representative of an engine face seal arrangement. Compression was achieved by manual movement of a lead screw, which pushed the Elastocon foot (or top plate) and compressed the seal under test. Force was continuously monitored with an inline load cell. Where the face seal arrangement was used, compression was such that there was no contact between the metallic parts that contacted the seal. The Elastocon unit is shown in Figure 31.

It is well known that nitrile rubber swells considerably in aromatic species found in jet fuel. This is taken into account in the various design standards that are used for commercial fuel system sealing. The results from CLEEN I showed a strong correlation between aromatic content and

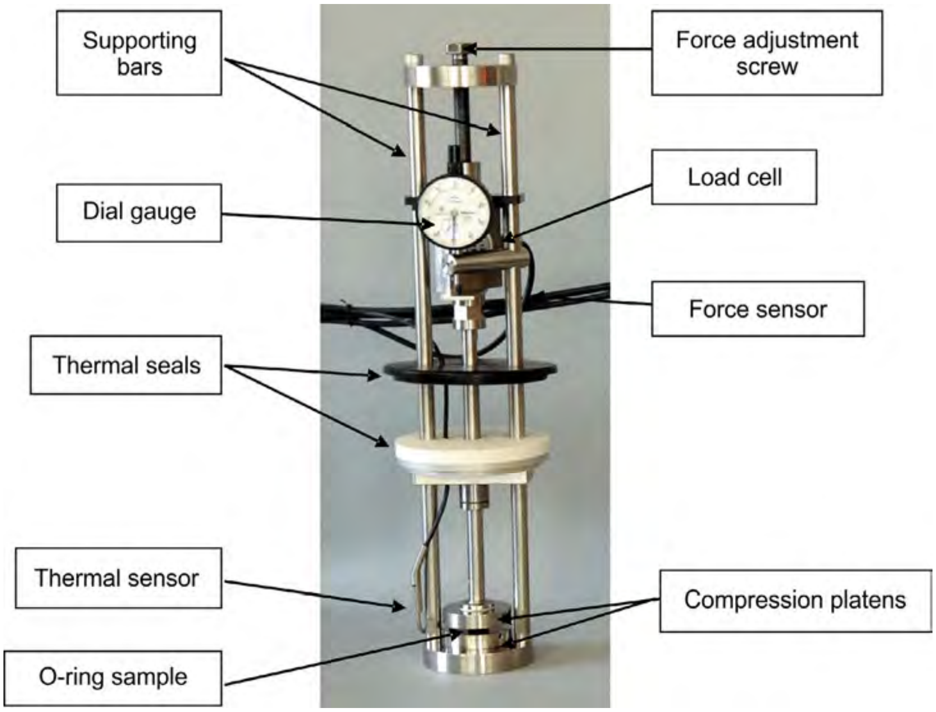


Figure 31. Elastocon test unit.

sealing force for nitrile rubber, where increased swell produced increased sealing force, which has also been found in previous studies. The relationship between aromatic content and swell, (therefore sealing force) is less for fluorosilicone than nitrile rubber, and lower still for fluorocarbon.

Similarly, CLEEN I demonstrated a strong correlation between test temperature and sealing force, with as expected, the lowest sealing force being measured at -40°C. This is because elastomeric materials have greater thermal expansion coefficients than the surrounding metallic parts, thus a very low temperature gives less interference, therefore less sealing force. Again, design standards take this into account.

Thus it can be appreciated that the worst case situation for jet fuel system sealing would be where nitrile rubber seals were in a zero aromatic fuel at low temperature.

Theoretically, the method developed under CLEEN I could be used to select a minimum level of aromatics in jet fuel to produce acceptable elastomer swell performance, with a minimum retained sealing force of 10% of the original sealing force. However, such a method has limitations and would make the assumption that no significant seal degradation takes place. Whereas in reality, seals suffer from compression set in service. This would manifest itself as a gradual decline in retained sealing force if the same effect were to be measured by compression stress relaxation. Thus, it can be appreciated that for an acceptable minimum level of aromatic content in fuel to be determined, a minimum level of sealing force should be retained for an elastomer seal in an end of life condition, while still at low temperature.

The above presents a practical challenge as compression stress relaxation cannot reliably be measured on used seals. Once compression is removed, compression set can be measured, but re compressing the seal such as would occur in compression stress relaxation will produce a very different physical response to a new seal being installed. To overcome this challenge, seals under test would need to be pre-aged in laboratory conditions such that compression was maintained over the period of aging and during compression stress relaxation measurements, with no or minimal removal of compression between. This could be done by using the Elastocon units over a long period of time and at elevated temperatures. However, a better method would be to age the seals in separate fixtures that could then be transferred to the Elastocon units for the sealing force measurements without removing the compression from the seals. The intent of the Elastocon work in CLEEN II was to pursue this representative ageing method, testing compression set after seals were aged in compression fixtures.

Rolls-Royce plc worked with Wallace Instruments some years ago to develop test jigs that retained elastomer O-ring seals in a face seal arrangement under approximately 20% compression. The actual level of compression was accurately controlled as described below. Over many years these jigs were loaded with O-rings and exposed to high temperatures and engine fluids so as to degrade the O-rings. After removal from the oven, the jigs would then be cooled to ambient temperature and the retained sealing force measured on a Shawbury-Wallace C11 Relaxometer. That provided single data points at ambient temperature only, but it enabled the stress relaxation process to be followed in a similar way to the real time measurement method the Elastocon system uses. It also had the significant advantage that seals could be aged at elevated temperatures without needing measurement systems that were capable under those conditions, and long duration aging without expensive long duration measurement. The health and safety problems associated with fuel at elevated temperature are also greatly reduced as only relatively small jigs have to be made safe rather than the much larger measurement equipment.

6.3.2 Elastocon Test Methodology

The CLEEN II Elastocon test effort was carried out by Sheffield University with considerable support from Rolls-Royce plc. Test fuels were supplied directly to Sheffield by Rolls-Royce Corporation. Within this section when Jet A1 is referred to it should be understood as being a single batch of Jet A1 fuel, sourced by Sheffield University. The No. 4 fuel is a 4% aromatic LanzaTech ATJ-SKA, and No. 13 fuel is the same 13% aromatic LanzaTech ATJ-SKA used throughout the entire CLEEN II program. These two aromatic levels give an indication on elastomeric response based on aromatic content.

6.3.2.1 Initial Setup

The newly developed method reported herein combines the real-time measurement under representative conditions of the Elastocon method with the ability to produce heavily degraded O-rings of the Rolls-Royce/Wallace method. The new method developed was as follows:

1. O-ring were loaded into the Rolls-Royce/Wallace C11 jigs, under approx. 20% compression.
2. The jigs were placed in the Elastocon units and a further 5% (i.e., 25% in total) compression was applied. At that point, the total force on the O-rings passed through the Elastocon units and compression stress relaxation data was able to be recorded (Figure 32).
3. The loaded C11 jigs were removed from the Elastocon units and subjected to elevated temperature aging in fuel.
4. At set intervals, the jigs were cooled to 30°C, then put back into the Elastocon units under the additional 5% compression as previously described. Of importance, the Elastocon unit foot is in exactly the same axial position as when the initial loading took place. The following detailed method explains how that is achieved. Conventional compression stress relaxation now takes place allowing temperatures, fuel cycling, and real-time data collection to occur.
5. Steps 3 and 4 can be repeated indefinitely to represent the number of cycles and time that is desired.
6. In addition, capability was gained to test seals at low temperatures down to -40°C.

The cross-sectional diameter (CSD) of O-rings were measured by a ±0.01 mm dial gauge before placing the seal in the test jig. All C11 test jig parts were measured using a micrometer ±0.01 mm and Vernier caliper (see Figure 32).

6.3.2.2 Compression Stress Relaxation Conditions

All the data reported has been collected at 30°C, cycling down to -40°C for the low temperature testing. Test durations and fuel immersion details are shown in Figure 33 and Figure 34. All the compression stress relaxation testing and high temperature aging was carried out with test seals fully immersed in fuel. In both cases care was taken that seals were not allowed to dry out.

6.3.2.3 High Temperature Seal Aging

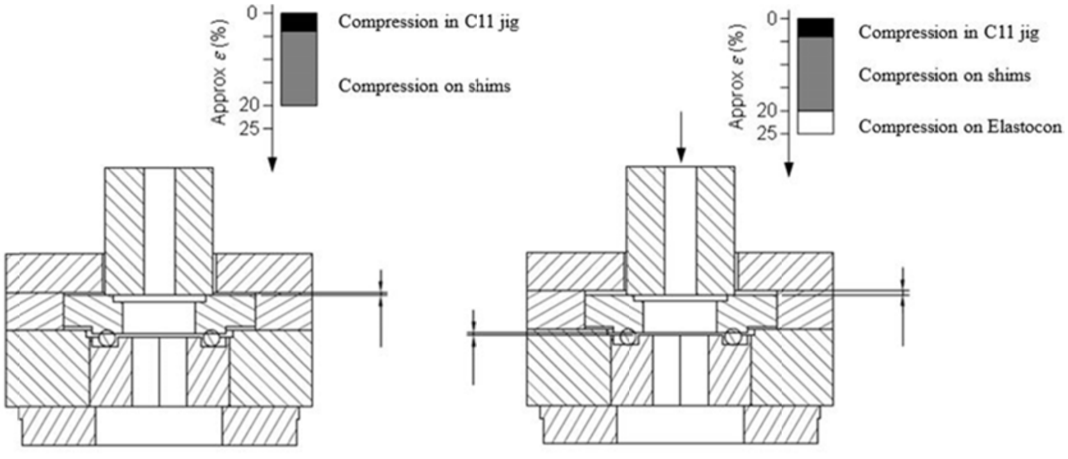
Seal aging was carried out while the seals were fully immersed with the Jet A1 reference fuel in sealed containers. Fluorocarbon and fluorosilicone seals were aged at 180°C, and nitrile seals were aged at 120°C. The aging times are indicated on the plots in the results section. No high temperature aging was carried out in the test fuels.

6.3.2.4 Low Temperature Testing

As a key part of this program, seals were also tested at -40°C as this was planned to be a direct follow-on from the main body of the testing (i.e., 30°C work) that is reported here. However, there was a considerable delay (approximately 2 months) between ending the main testing and starting the low temperature testing. The jigs/seals were kept under Jet A1 fuel during the waiting period and it was determined this waiting period did not significantly affect the test results. This is believed to be true as it is thought there was only minimal degradation in sealing force because the seals were at room temperature. This can be observed from the test result slopes towards the end of the testing periods in Figure 33 and Figure 34. Testing was carried out in the same manner as for the 30°C testing, except a purpose-built cooling unit was used to reduce the temperature around the test units.

6.3.2.5 Materials Selection

Three grades of fluorocarbon were used in the test: AMS7276 material, AMS7287 material, and a material supplied by Sheffield University that was described as ‘Fluorocarbon 60C7’. The first



Approx 20% compression on shims Approx 25% compression in Elastocon

Figure 32. Rolls-Royce / Wallace C11 jig and the foot of the Elastocon unit showing the application of 5% extra compression

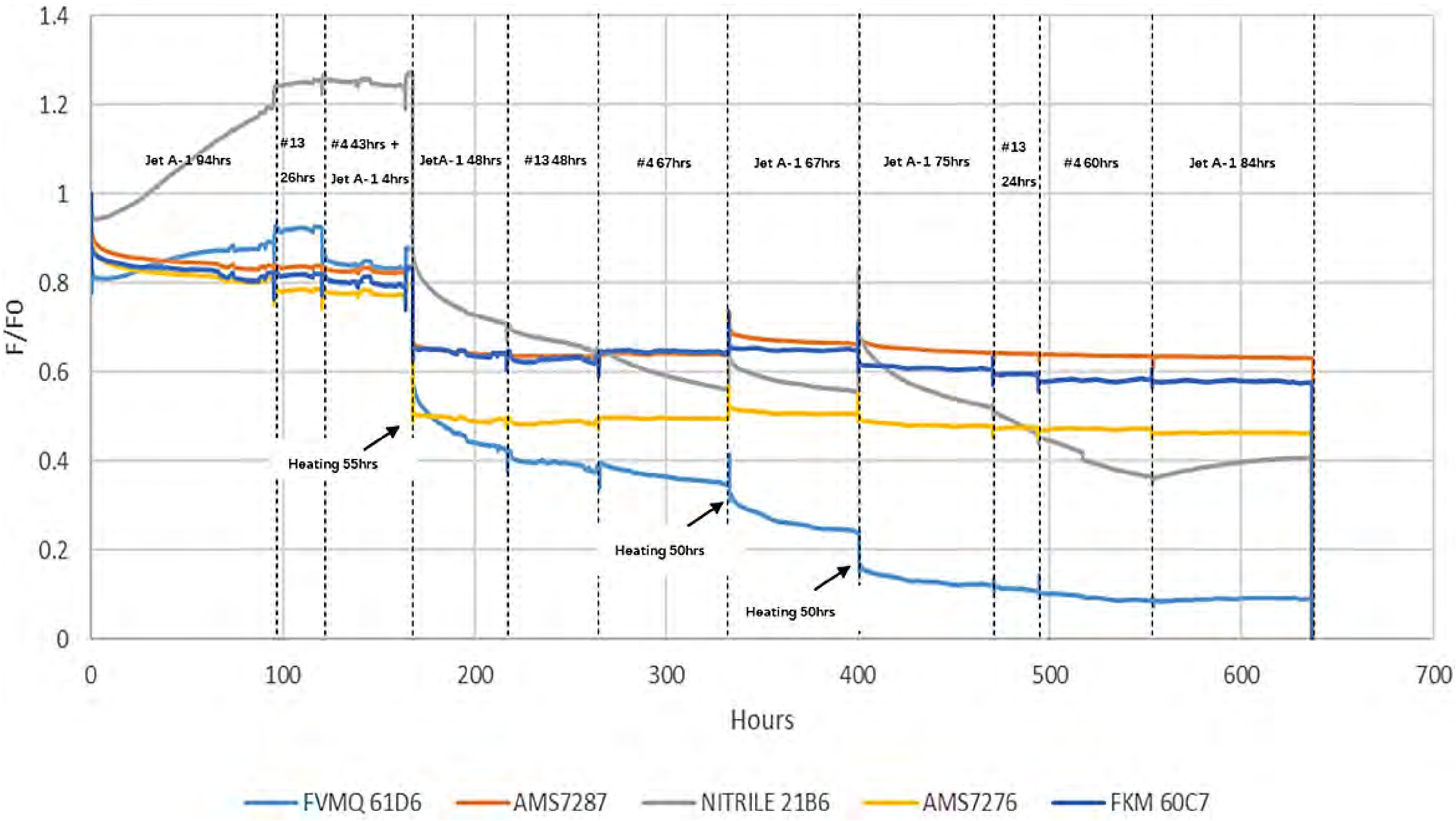


Figure 33. Compression stress relation data plot for Set 6.

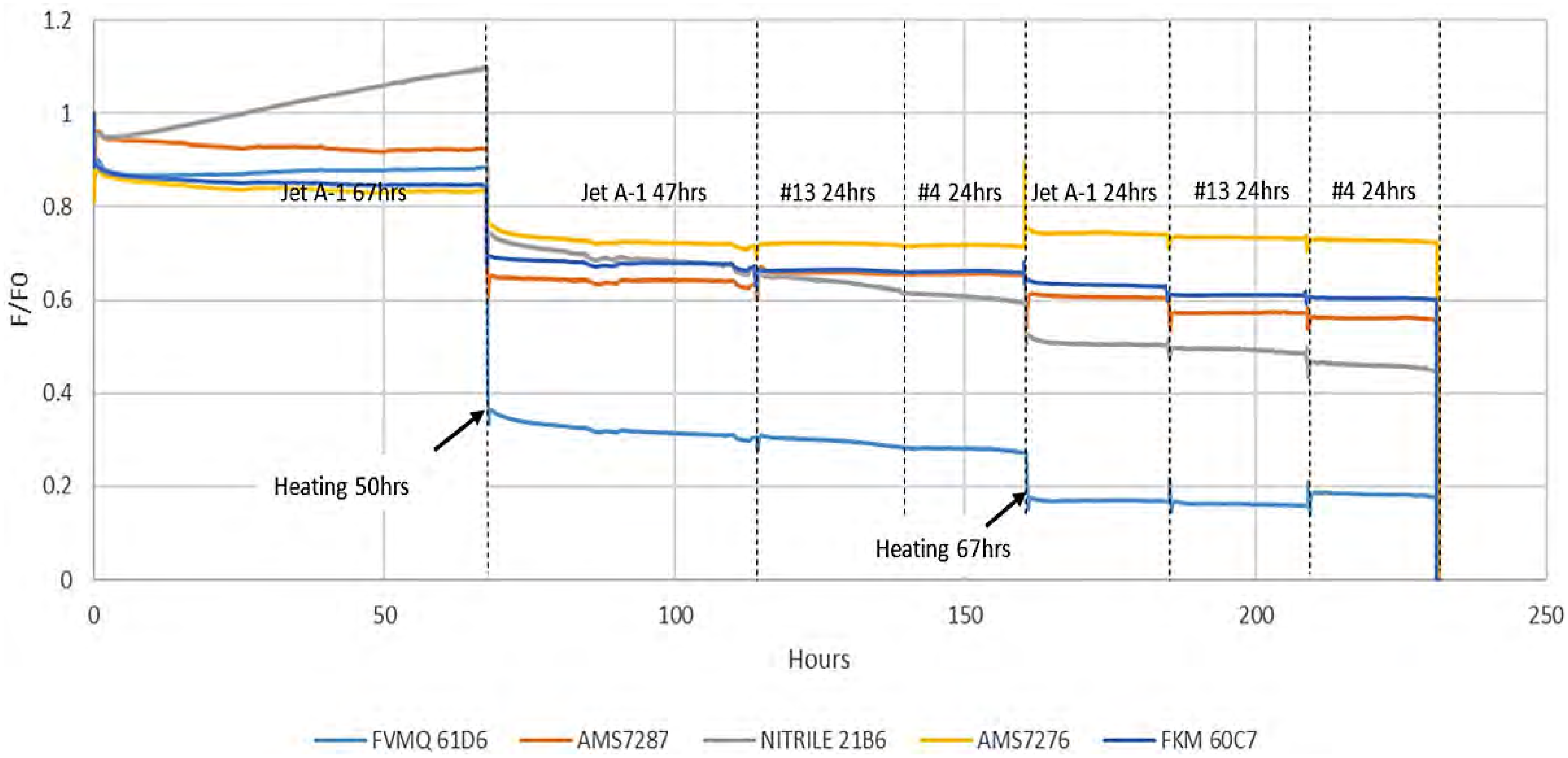


Figure 34. Compression stress relaxation data plots for Set 7.

two materials are representative of current Rolls-Royce engine design. Single nitrile and fluorosilicone elastomer material types were supplied by Sheffield University. They were described as ‘21B6’ and ‘61D6’, respectively. All the materials supplied by Sheffield University were chosen by them and are believed to be representative of current aerospace usage.

6.3.2.6 Examination of Seals Post Test

The seal test specimens were examined post-test and subjected to hardness testing by Rolls-Royce Materials Engineering staff.

6.3.3 Elastocon Rig Test Results

The elastomer O-rings were tested at both 30°C and 40°C in the Elastocon rig. Results from the testing will be discussed in the following subsections.

6.3.3.1 30°C Testing

Results from the 30°C testing regime are presented (Figure 33 and Figure 34) as normalized sealing force (Fo/F) versus time, while stress relaxation data are being generated. The annotated heating times in hours represent the time the O-rings were high temperature aged in Jet A1 fuel, where no stress relaxation data are being generated. The immersion fuels used and the associated times during data generation are also shown on both plots. Set 6 and Set 7 consisted of identical materials, although test conditions varied slightly as shown in the figures.

6.3.3.2 General Considerations

As can be seen in Figure 33 through Figure 37, the test results for Set 6 and Set 7 are not exact duplicates as test conditions had to be varied somewhat for practical reasons. It should be appreciated that the precision and accuracy of this method is yet to be determined, therefore the test results should be treated with caution.

The C11 test jigs used in this work have been used many times previously, although only for single measurement type work. In the past, testing was always done in triplicate, three separate jigs with three identical O-rings. Measurements were always taken in triplicate as well, with results being averaged for each jig, then the median result being reported between jigs. Over time it was found that there could be a considerable scatter on the data between jigs, less so in the measurements on the same jig. This should be kept in mind when interpreting the results presented herein, as current testing is in duplicate, not triplicate, and the data exhibits some scatter.

There is a level of general variation associated with some of the test results. At the end of a heat aging period when the jig/seal is put back into the Elastocon unit, a downward step change in sealing force is to be expected. Typically the greater the expected seal degradation, the greater the downward step change. However there are times where the data show a small upward step change. This trend should be discounted. An example of this erroneous trend can be found in the 160 hours in Set 7 for AMS7276. Similarly there are occasional small step changes either upwards or downwards when fuel is changed without any alternation in compression. The reason for this trend is not known. Actual changes in sealing force due to fuel type would occur slowly as the O-ring swell process takes time. An example of this behavior can be seen at 550 hours for nitrile in Set 6, where the higher swell caused by Jet A1 reference fuel as compared to Fuel No. 4 can be seen in the form of a gradual force increase.

A discussion of the individual elastomer seal types test results will be discussed below. Refer to Figure 33 through Figure 37 for data and trends.

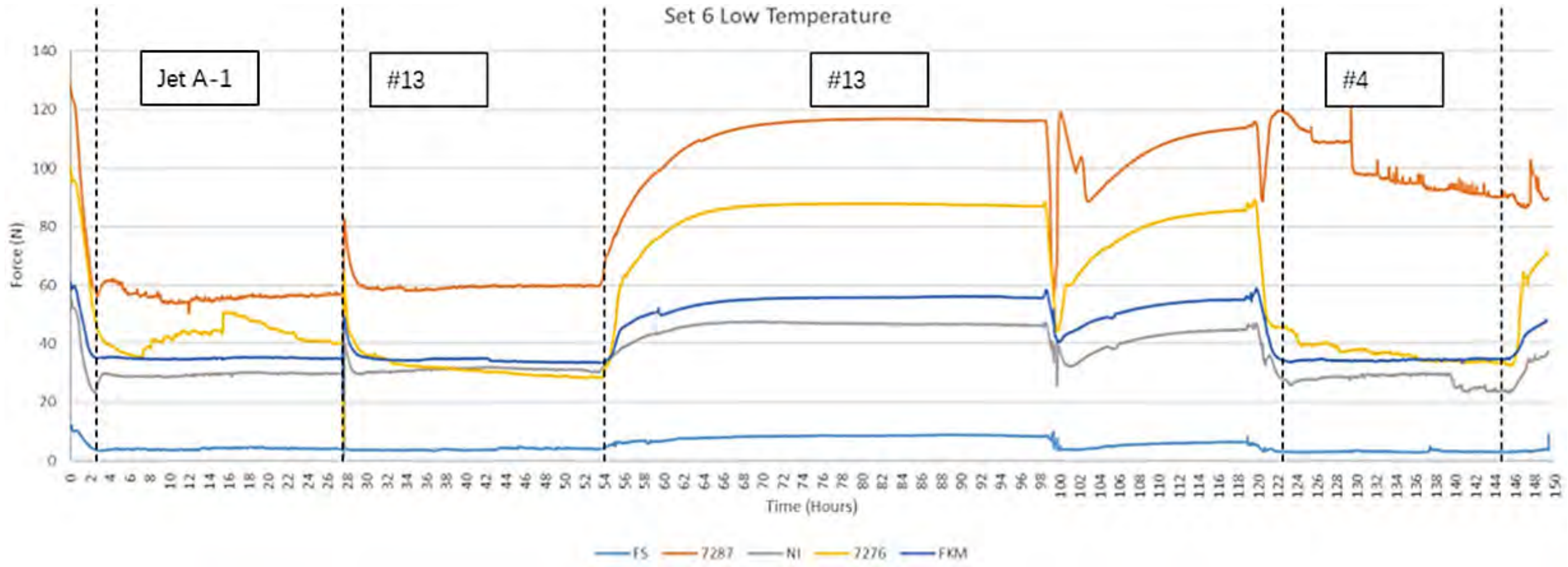


Figure 35. Set 6 Compression stress relaxation data plots at low temperature (absolute sealing force in Newton's).

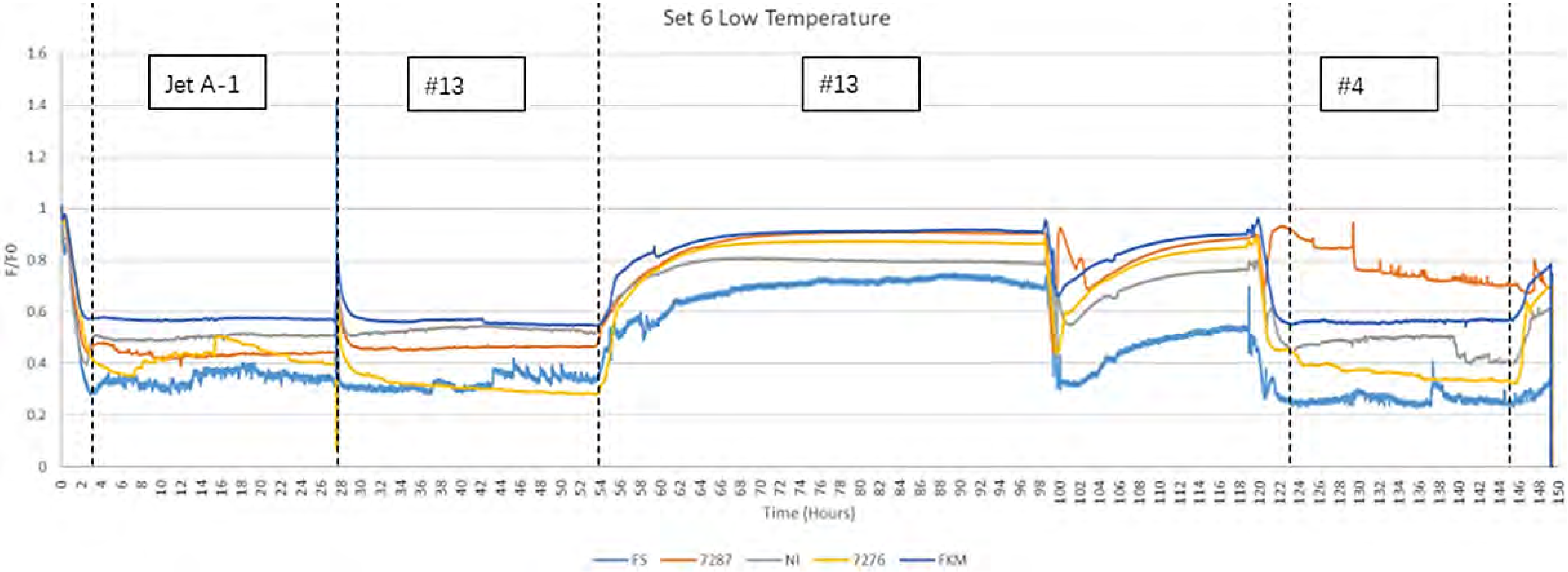


Figure 36. Set 6 Compression stress relaxation data plots at low temperature (normalized sealing force has been set to zero at start of test).

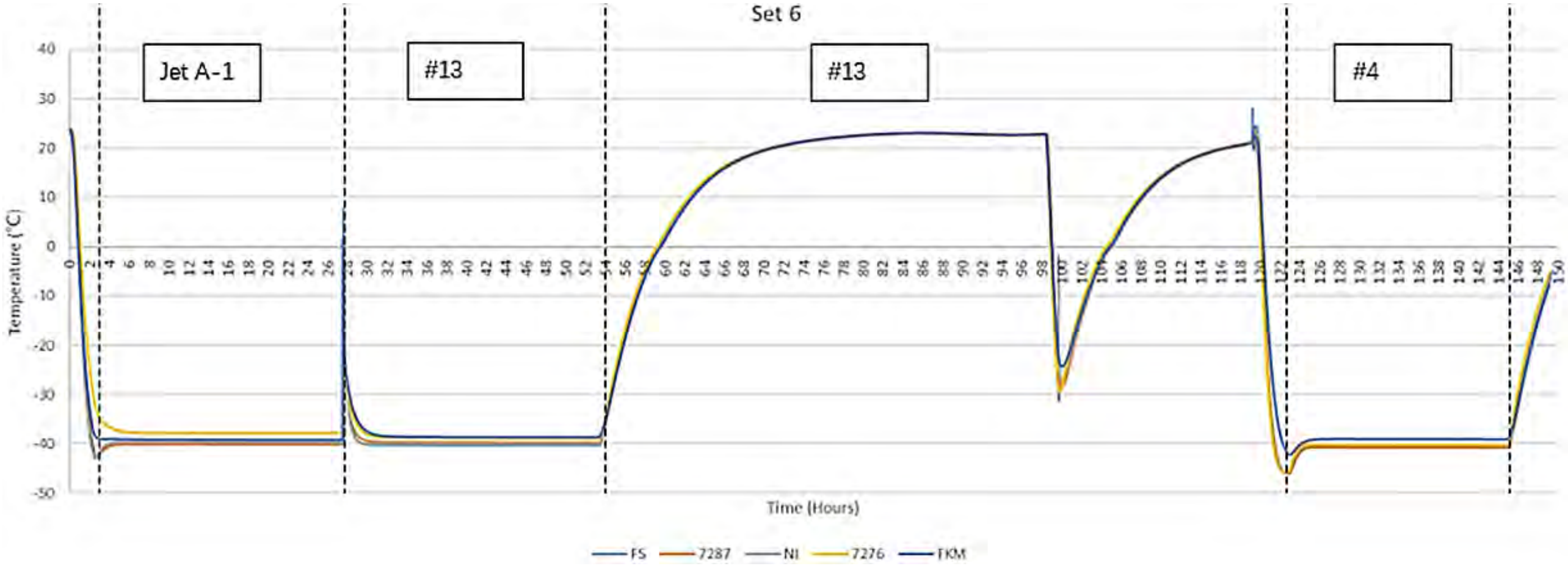


Figure 37. Set 6 low temperature cycling.

6.3.3.3 Nitrile Rubber

The results indicate the nitrile rubber shows an initial loss of sealing force after initial compression (as was expected) but then the sealing force rises, in marked contrast to the other seals. This rise is due to the nitrile elastomer seal swelling in response to the aromatic content of the fuel. This effect was not seen on CLEEN I as nitrile seals were pre-aged in fuels to allow for such swell to be initially present.

Degradation (sealing force loss) of the nitrile was more rapid than for the fluorocarbon seals. This is considered to be consistent with the aging temperature and duration of the test. Set 6 specimens at 155 hours and elevated temperature (and approximately 620 hours at 30°C) led to approximately 35% retained sealing force in Fuel No. 4. While Set 7 at 117 hours (and approximately 230 hours at 30°C) led to around 45% retained sealing force in the same fuel. For these specimens it is believed the majority of the degradation took place during the high temperature exposure, which manifests itself as sealing force loss during measurement.

Post-test it was observed that the nitrile seals showed considerable compression set. This was noted to be similar to ex-service high life (but still functioning correctly) seals that have previously been seen in the field. Figure 38 shows the condition of the nitrile seal from Set 6. The high level of compression set can clearly be seen in the cross section where the shape is oval instead of round.

The nitrile seal hardness was measured to be 77 IRHD for Set 6 and 76 IRHD for Set 7. The initial hardness was not determined, making it impossible to assess the level of degradation that had taken place during testing. Although the final recorded hardness was considered acceptable for a correctly functioning nitrile seal.

6.3.3.4 Fluorosilicone Rubber

On initial compression the fluorosilicone specimens showed an expected fall in sealing force, followed by a rise in sealing force due to the effect of seal swell. This effect was less when compared to nitrile rubber, which reflects the lower level of expected swell in fuel.

The fluorosilicone seals were subject to aggressive aging at a temperature of 180°C, thus considerable degradation was expected. The first high temperature exposure performed as expected, causing a substantial sealing force degradation. Set 6 showed approximately a 30% reduction in sealing force after 55 hours of heat aging, while Set 7 showed a 45% reduction after 50 hours of aging. The reason for this difference in reduction in sealing force between the sets is not known but shows the level of difference that may be present between sets. It is

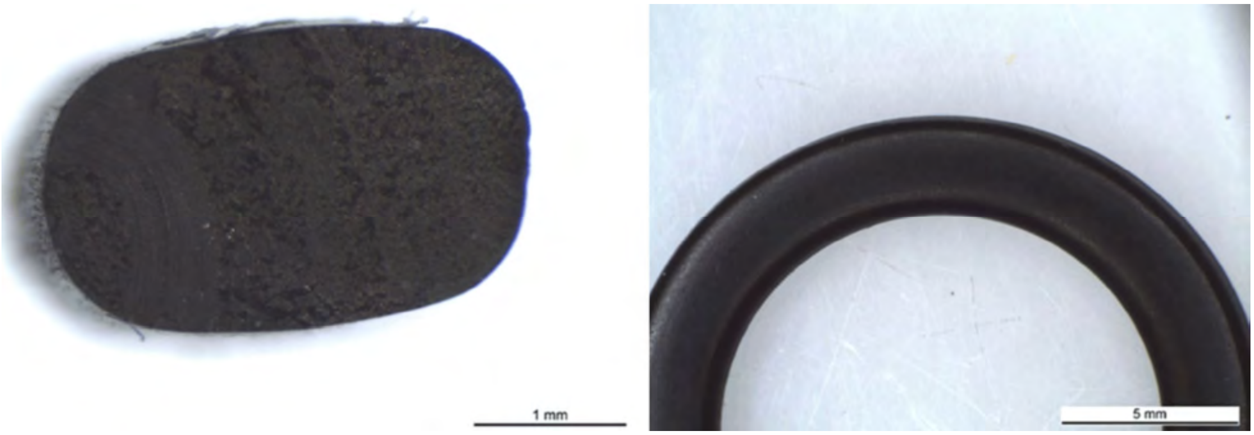


Figure 38. Nitrile rubber O-ring from Set 6 posttest.

expected that periods of heat aging will lead to sealing force reduction. The nitrile rubber shows there is a basic consistency within the results that longer heat aging (and longer 30°C exposure) total times caused greater sealing force reduction. For Set 6 fluorosilicone there was <10% retained sealing force remaining at the end of the test (155 hours heating), compared to <20% for Set 7 (117 hours heating). This amount of retained sealing force is likely sufficient for adequate sealing, but the measurements were obtained at an elevated temperature of 30°C. In contrast, at -40°C the seals showed even lower retained sealing force, possibly to the level of being ineffective.

The post-test seals were examined and found to be in very poor condition. The degradation is significantly worse than would be expected to be seen in service. These results are expected given the high temperature exposure these seals have been subjected to as fluorosilicone O-rings do not maintain performance as well as fluorocarbon materials at high temperatures. They showed a moderate level of compression set and had softened considerably. In addition there was extruded material (see Figure 39) visible, which is indicative of excessive seal swell and degradation.

The measured hardness was found to be 34 IRHD for Set 6 and >30 IRHD (i.e., off the bottom of the scale) for Set 7. The initial hardness was not known, but it is believed to be approximately 75 IRHD. Such softening is indicative of substantial degradation, making the seal nonfunctioning in service.

6.3.3.5 Fluorocarbon Rubber

The fluorocarbon seals were heat aged at 180°C. Given the relatively short duration of aging as compared to fluorocarbon capability in service, minimal thermal degradation was expected. But sealing force reduction due to physical relaxation was expected.

Upon initial compression the expected reduction in sealing force occurred. Unlike nitrile and fluorosilicone where there was little or no subsequent increase due to seal swell, this reaction is as expected because fluorocarbon materials are known to exhibit little swell in jet fuel.

Generally, all three fluorocarbon materials showed much less initial thermal degradation than fluorosilicone or nitrile seals. Over the course of testing between 55 and 75% sealing force was retained. Data show the AMS7287 and AMS7276 fluorocarbon traces swap positions between Set 6 and Set 7. The reason for this behavior is unknown.

The overall fluorocarbon results are broadly consistent as these materials have good resistance to elevated temperatures and performed well compared to fluorosilicone seals as expected. Fluorocarbon seals in these test conditions would be expected to function correctly in an engine.

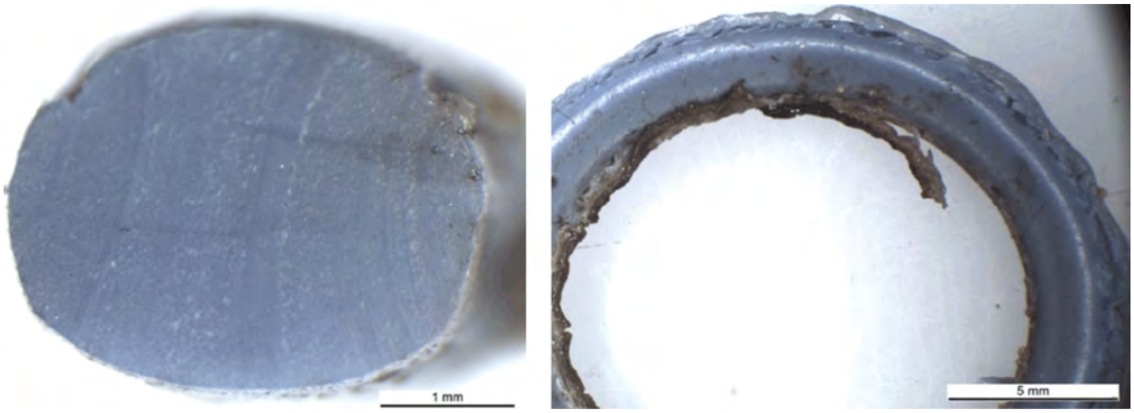


Figure 39. Post-test fluorosilicone O-ring from Set 6.

Upon post-test examination, all fluorocarbon seals were found to be in good condition, showing some level of compression set and softening, but consistent with correctly functioning seals not nearing end of life condition. The images in Figure 40 demonstrate the seal condition showing very little compression set and no adverse physical characteristics.

The hardness values of the fluorocarbon seals are shown in Table 10. Untested hardness values were approximately 75 Shore A nominal, so it can be seen that only a little softening has occurred due to minimal decrease in hardness, which is consistent with the general good seal condition.

Table 10. Post-test hardness for fluorocarbon materials (Shore A).

Material	Set 6	Set 7
‘FKM’	68	68
FKM 7276	64	65
FKM7287	67	68

6.3.3.6 Comparing Fuels

There were three fuels tested in this evaluation. A baseline reference Jet A1 fuel was compared to two fully-synthetic ATJ-SKA’s. The No. 4 fuel was a 4% aromatic LanzaTech ATJ-SKA and No. 13 fuel is the same 13% aromatic LanzaTech ATJ-SKA used throughout the entire CLEEN II program. Understanding if there are any fuel related effects to the performance of the elastomer seals was a key focus in this test.

Results indicate there are relatively few places where clear differences exist regarding the retained sealing force due to fuel exposure. This is partially due to there being no significant differences between the seal swell caused by the two ATJ-SKA test fuels and the reference fuel. Another contributing factor is the effect of heat aging did not appear to impact differences significantly. This heat aging added an additional influence on performance that has not been seen on previous test programs that utilized the Elastocon units and further. But there were a few small differences noted.

Figure 34 shows that at 550 hours the traces for nitrile and fluorosilicone show clear gradual sealing force increase following the change from Fuel No. 4 to Jet A1. This is considered to be due to expected increased seal swell caused by the higher aromatic content of Jet A1 (approximately 17%) compared to Fuel No. 4 (4%). This effect is clear for nitrile but barely

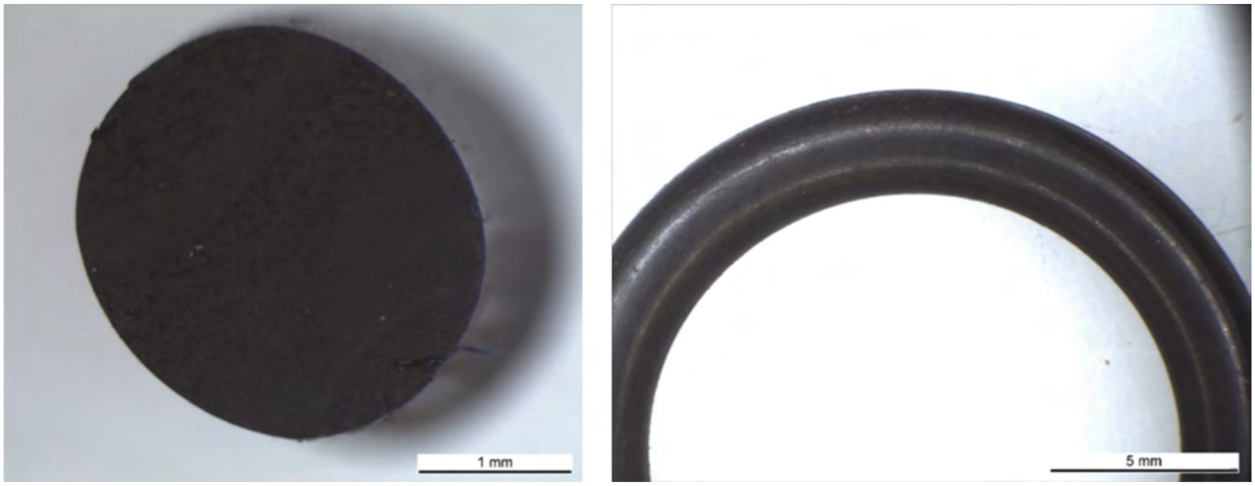


Figure 40. Post-test fluorocarbon O-ring from Set 6.

discernible for fluorosilicone, which is as expected given the known swell behavior of the two materials.

The nitrile seal traces are the best place to observe seal swell differences between fuels. Such differences are suggested by the data. The data do marginally support the theory that the seal swell effect of the fuels under test was ranked Jet A1 > Fuel No. 13 > Fuel No. 4, which given the decreasing percent of aromatic content would be expected. The swell effect of the mesitylene aromatic molecule compared to conventional aromatic content of jet fuels is not known, although the data here suggest there may be little difference. Further testing with different aromatic molecules could be investigated in future work.

6.3.3.7 Low Temperature Testing

Data presented for low temperature testing herein are for Set 6 only. Data were collected for Set 7 but the results were of poor quality and difficult to interpret, despite being collected in exactly the same way as was for Set 6. The low temperature testing was conducted on the seal sets after high temperature testing, so the elastomer materials had already experienced a significant level of testing and degradation by that point but may better simulate long-term use in the field. It was determined that Set 6 was more representative and will be reported upon.

It can be seen from Figure 37 that the test temperature was cycled from 30 to -40°C, while the Set 6 seals were in both test fuels and in the Jet A 1 reference fuel. Compression stress relaxation data were collect during the testing period and will be presented in two ways.

Firstly, the normalized sealing force is shown plotted against time (Figure 36). This is the same data handling method was used in Figure 33 and Figure 34. The data were normalized from the start of the low temperature testing, rather than as a continuation of the 30°C testing shown in Figure 33. The effect of that technique is the observed low sealing force at the start of the low temperature testing as it is rezeroed and thus not apparent in the data. To allow for this effect, actual sealing force against time is shown in Figure 35. Here it can be seen that the seals that completed the first phase of testing (Figure 33) with low sealing force started the second phase of testing with similarly low sealing force.

The data show there is a general relationship between a reduction in test temperature demonstrating a reduction in sealing force. This is as expected and is a result of greater thermal expansion coefficients of elastomers compared to the surrounding metal work.

It is notable that throughout the phase of low temperature testing the sealing force is primarily temperature dependent, with no discernible dependency on either time or fuel type.

For Set 6 the data are generally consistent, as discussed above. However, the FKM 7287 data start to look unusual from around 100 hours and after the final temperature change at 119 hours, where the sealing force appears to be anomalously high. The reasons for this are not clear, but it is obvious the sealing force is reading far too high.

6.3.4 Elastocon Test Conclusions

The testing yielded the following results:

- A new method (known as the Rolls-Royce/Elastocon method) has been developed to evaluate compression stress relaxation behavior in representative seals. This new method allows for a previously unobtainable level of O-ring degradation to be included in test, thereby allowing seals to be tested in an approximately end-of-life condition.

- Results suggest Fuel No. 4 and Fuel No. 13 produce less seal swell in the three elastomer materials tested as compared to reference Jet A1. Results also suggest Fuel No. 4 produces slightly lower swell than Fuel No. 13.
- The post-test seal condition is consistent with the stress relaxation data for all seals (i.e., low retained sealing force was associated with high levels of compression set).
- The seals tested had a minimum retained sealing force of approximately 10% at 30°C, which is considered marginally acceptable. This low sealing force is considered the worst case where a seal is capable of functioning.
- Temperature cycling to -40°C reduced the retained sealing force for all seals. The retained sealing force did not reach zero even for the worst condition seals. The performance of such degraded seals at this temperature is considered likely to be poor.
- It is notable that throughout the phase of low temperature testing the sealing force is primarily temperature dependent, with no discernible dependency on either time or fuel type.

7. Conclusions

The Rolls-Royce CLEEN II Sustainable Aviation Fuel program has succeeded in promoting the introduction of a viable 100% sustainable aviation fuel as a possible future candidate fuel, thus contributing to the achievement of FAA's NextGen Air Transportation System goals. This program was designed to push past the current 50% blend wall by determining the feasibility of using fully-synthetic sustainable aviation fuels in aircraft systems. The LanzaTech ATJ-SKA fuel was characterized under engine representative conditions and found to have the potential to be included in national and international aviation fuel specifications. This program advanced the scientific understanding of these fuels; therefore supporting the longer-term aim to increase the use of sustainable fuel within the aviation transport sector and thus improving the overall environmental performance relative to current operations. The results and information from this program will contribute to existing industry work streams aimed at enabling increased use of sustainable fuels for aviation. In addition, the outcomes of this program complement current work under the auspices of several organizations, including the Commercial Aviation Alternative Fuels Initiative (CAAFI), ASTM International, and European Union (EU) and the U.S. Government.

Overall each element of the test program concluded the following:

- Fuel selection:
    - An 87% by volume blend of LanzaTech ATJ-SKA with 13% Swift aromatic was the final fuel chosen for the CLEEN II program.
    - This test fuel meets program goals of promoting higher synthetic blend percentages, along with offering the potential to reduce carbon footprint of aviation.
    - The fuel has commercial viability, is readily available, and demonstrates suitability in aviation.
- Laboratory evaluation:
    - Composition – As compared to conventional Jet A, similar hydrocarbons, different distribution, predominantly iso-paraffinic.
    - Acceptable volatility and fluidity characteristics.
    - Fluidity – Similar viscosity profile and good low temperature performance.
    - Good thermally stability, thus anticipated low risk to fuel system deposits.
    - Acceptable energy content with minimal impact anticipated to aircraft range due to fuel's slightly lower energy content on a volume basis.
    - Combustion and thermal stability-suitable and within experience, indicating minimal impact to aircraft range and good deposit resistance.
- Fuel spray characterization:
    - In general, spray performance of the ATJ-SKA fuel was similar to the Jet A fuel, with only minor differences noted.
    - The visual spray recordings show similar sprays for all test fluids whether illuminated by natural light or by flash laser illumination. No divergence in visual spray behavior was noted for atmospheric test conditions evaluated.
    - The spray's density, uniformity, and liquid radial distribution as characterized through the optical patternation measurement showed only minor differences between Jet A and ATJ-SKA fuels.
    - For ambient temperature conditions, droplet sizes were quite similar between the Jet A and ATJ-SKA fuels as the line ensemble droplet size measured with the Malvern showed drop sizes within 1 μm with effective atomization independent of fuel type.

  - The pointwise PDI measurements confirmed the droplet sizes were similar, with differences in droplet size occurring at the periphery of the spray where larger droplets were recorded for the ATJ-SKA fuel. Axial droplet velocity falls off a bit faster with the ATJ-SKA fuel at the outer portions of the spray cone. For the ATJ-SKA fuel, the accompanying radial and swirl velocities are slightly higher toward central part of the spray as compared to the Jet A fuel spray.
- High pressure flame tube:
  - Lean stability deteriorated slightly with the ATJ-SKA with an average f/a ratio that is 7% higher.
  - NOx emissions indices are similar for most test conditions and fuel-air ratios, and insensitive to fuel type.
  - CO EI for the ATJ-SKA fuel are higher than Jet A.
  - UHC EI are similar between the ATJ-SKA and Jet A for higher power conditions, but elevated at low power conditions.
  - The ATJ-SKA's higher CO and UHC emissions led to lower combustion efficiency.
  - Smoke numbers between ATJ-SKA and Jet A fuels are similar at the different conditions.
  - ATJ-SKA does not significantly impact wall temperatures with similar measurements.
  - In general, flame tube testing showed some deterioration in lean stability, with higher CO and UHC emissions that led to lower combustion efficiency. But similar results were found for NOx, CO, smoke number, and wall temperatures.
- Elastocon testing:
  - A new method (known as the Rolls-Royce/Elastocon method) has been developed to evaluate compression stress relaxation behavior in representative seals. This new method allows for a previously unobtainable level of O-ring degradation to be included in test, allowing seals to be tested in an approximately end-of-life condition.
  - Results suggest Fuel No. 4 and Fuel No. 13 produce less seal swell in the three elastomer materials tested as compared to reference Jet A1. Results also suggest Fuel No. 4 produces slightly lower swell than Fuel No. 13.
  - The post-test seal condition is consistent with the stress relaxation data for all seals (i.e., low retained sealing force was associated with high levels of compression set).
  - The seals tested had a minimum retained sealing force of approximately 10% at 30°C, which is considered marginally acceptable. This low sealing force is considered the worst case where a seal is capable of functioning.
  - Temperature cycling to -40°C reduced the retained sealing force for all seals. The retained sealing force did not reach zero even for the worst condition seals. The performance of such degraded seals at this temperature is considered likely to be poor.
  - It is notable that throughout the phase of low temperature testing the sealing force is primarily temperature dependent, with no discernible dependency on either time or fuel type.

8. References

[1] ASTM D4054-20b *"Standard Practice for Evaluation of New Aviation Turbine Fuels and Fuel Additives"*, ASTM International, West Conshohocken, PA September 1, 2020.

[2] ASTM D7566-20b *"Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons"*, ASTM International, West Conshohocken, PA September 1, 2020.

[3] ASTM D1655-20c *"Standard Specification for Aviation Turbine Fuels"*, ASTM International, West Conshohocken, PA September 1, 2020.

[4] ASTM Research Report, *"Evaluation of LanzaTech-PNNL Ethanol Based Alcohol-to-Jet (LT-PNNL ATJ) Synthetic Paraffinic Kerosenes (ATJ-SPKs)"*, version 1.02, LanzaTech Inc., September 2017.

[5] ASTM D7171-20 *"Standard Test Method for Hydrogen Content of Middle Distillate Petroleum Products by Low-Resolution Pulsed Nuclear Magnetic Resonance Spectroscopy"*, ASTM International, West Conshohocken, PA May 1, 2020.

[6] ASTM D5291-16 *"Standard Test Method for Instrumental Determination of Carbon, Hydrogen, and Nitrogen in Petroleum Products and Lubricants"*, ASTM International, West Conshohocken, PA September 1, 2016.

[7] ASTM D86-20 *"Standard Test Method for Distillation of Petroleum Products and Liquid Fuels at Atmospheric Pressure"*, ASTM International, West Conshohocken, PA September 1, 2020.

[8] ASTM D56-16a *"Standard Test Method for Flash Point by Tag Closed Cup Tester"*, ASTM International, West Conshohocken, PA September 1, 2016.

[9] ASTM D4052-18a *"Standard Test Method for Density, Relative Density, and API Gravity of Liquids by Digital Density Meter"*, ASTM International, West Conshohocken, PA December 15, 2018.

[10] ASTM D5972-16 *"Standard Test Method for Freezing Point of Aviation Fuels"*, ASTM International, West Conshohocken, PA June 1, 2016.

[11] ASTM D445-19a *"Standard Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (and Calculation of Dynamic Viscosity)"*, ASTM International, West Conshohocken, PA December 1, 2019.

[12] ASTM D4809-18 *"Standard Test Method for Heat of Combustion of Liquid Hydrocarbon Fuels by Bomb Calorimeter (Precision Method)"*, ASTM International, West Conshohocken, PA August 1, 2018.

[13] ASTM D3241-20 *"Standard Test Method for Thermal Oxidation Stability of Aviation Turbine Fuels"*, ASTM International, West Conshohocken, PA September 1, 2020.

[14] ASTM D5001-19 *"Standard Test Method for Measurement of Lubricity of Aviation Turbine Fuels by the Ball-on-Cylinder Lubricity Evaluator (BOCLE)"*, ASTM International, West Conshohocken, PA December 1, 2019.

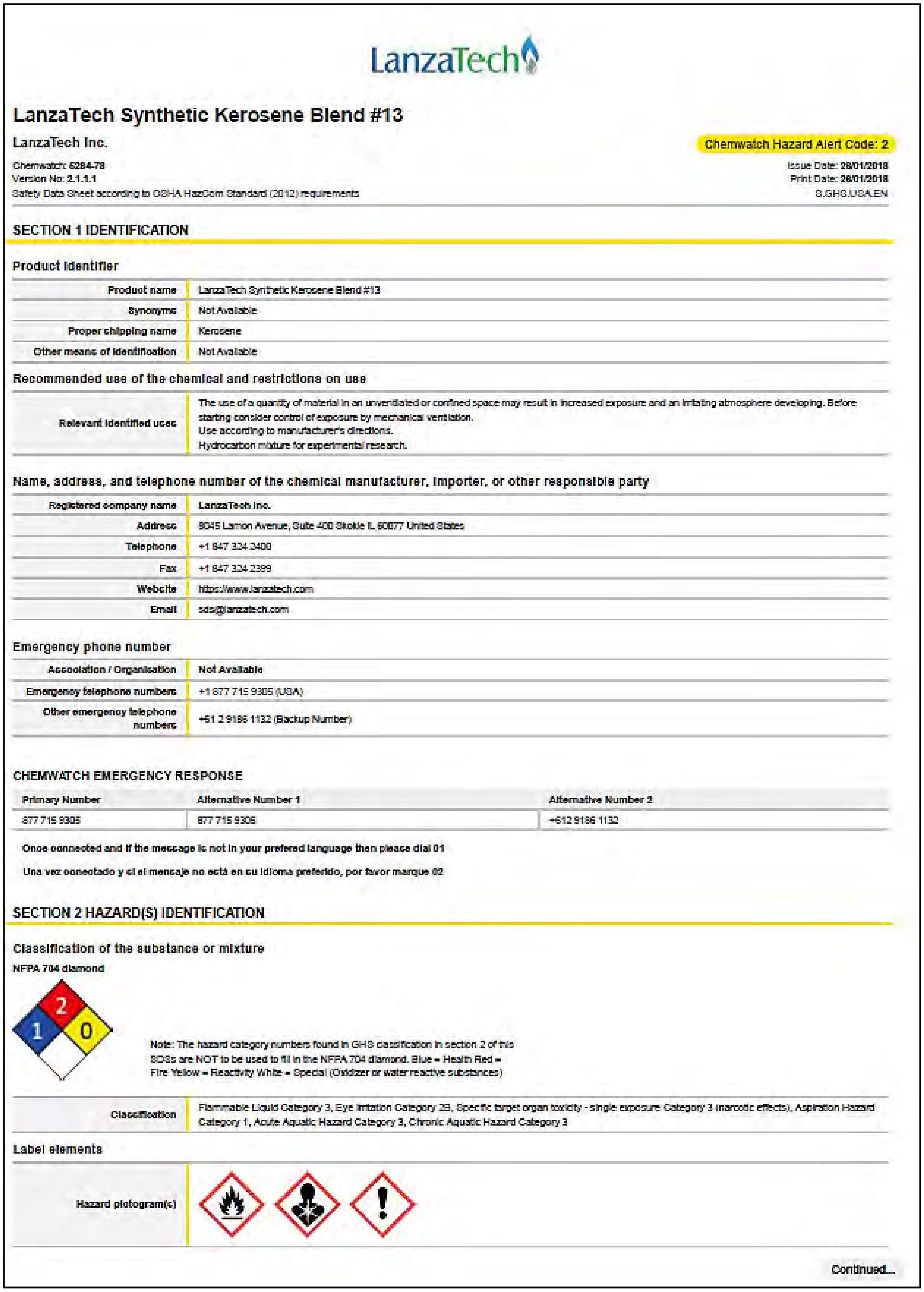
[15] D. Smith, September 19, 2018, *"Fuel Spray Evaluation of Jet A, ATJ synthetic fuel and test fluid MIL-PRF-7024"*, Rolls-Royce Technical Report.

[16] D. Smith, June 19, 2018, *"High Pressure Flame Tube Rig Test Results"*, Rolls-Royce Technical Report.

[17] B. Shaw, December 20, 2019 *"CLEEN II Elastomer Testing Final Report"*, Rolls-Royce Technical report: EDNS01000794774.

[18] C. Lewis, May 2015, *"Rolls-Royce Alternative Fuels Program-Rig Testing of Candidate Fuels: Elastomer Testing"*, Rolls-Royce Technical report: DOT/FAA/AEE/2015-07.

Appendix A. LanzaTech ATJ-SKA Safety Data Sheet



LanzaTech Synthetic Kerosene Blend #13

LanzaTech Inc.

Chemwatch Hazard Alert Code: 2

Chemwatch: 5284-78
Version No: 2.1.1.1
Safety Data Sheet according to OSHA HazCom Standard (2012) requirements

Issue Date: 28/01/2018
Print Date: 28/01/2018
S.GHS.USA.EN

SECTION 1 IDENTIFICATION

Product identifier

Product name	LanzaTech Synthetic Kerosene Blend #13
Synonyms	Not Available
Proper shipping name	Kerosene
Other means of identification	Not Available

Recommended use of the chemical and restrictions on use

Relevant identified uses	The use of a quantity of material in an unventilated or confined space may result in increased exposure and an irritating atmosphere developing. Before starting consider control of exposure by mechanical ventilation. Use according to manufacturer's directions. Hydrocarbon mixture for experimental research.

Name, address, and telephone number of the chemical manufacturer, importer, or other responsible party

Registered company name	LanzaTech Inc.
Address	8045 Lamon Avenue, Suite 400 Skokie IL 60077 United States
Telephone	+1 847 324 2400
Fax	+1 847 324 2399
Website	https://www.lanzatech.com
Email	sds@lanzatech.com

Emergency phone number

Association / Organisation	Not Available
Emergency telephone numbers	+1 877 715 9305 (USA)
Other emergency telephone numbers	+61 2 9186 1132 (Backup Number)

CHEMWATCH EMERGENCY RESPONSE

Primary Number	Alternative Number 1	Alternative Number 2
877 715 9305	877 715 9305	+612 9186 1132

Once connected and if the message is not in your prefered language then please dial 01

Una vez conectado y si el mensaje no está en su idioma preferido, por favor marque 02

SECTION 2 HAZARD(S) IDENTIFICATION

Classification of the substance or mixture

NFPA 704 diamond

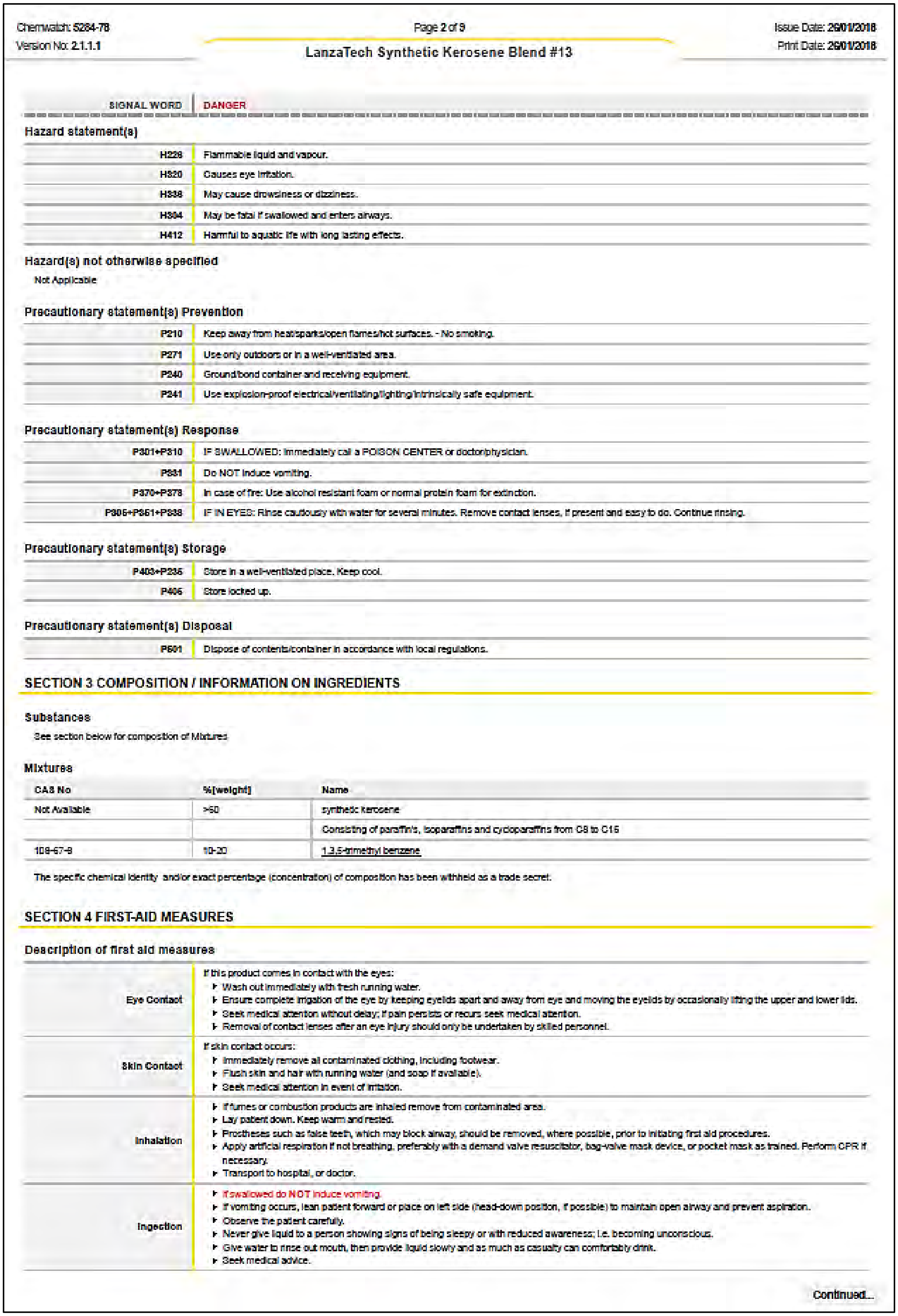
Note: The hazard category numbers found in GHS classification in section 2 of this SDSs are NOT to be used to fill in the NFPA 704 diamond. Blue = Health Red = Fire Yellow = Reactivity White = Special (Oxidizer or water reactive substances)

Classification	Flammable Liquid Category 3, Eye Irritation Category 2B, Specific target organ toxicity - single exposure Category 3 (narcotic effects), Aspiration Hazard Category 1, Acute Aquatic Hazard Category 3, Chronic Aquatic Hazard Category 3

Label elements

Hazard pictogram(s)	

Continued...



Chemwatch: 5264-78
Version No: 2.1.1.1

Page 2 of 9

LanzaTech Synthetic Kerosene Blend #13

Issue Date: 26/01/2018
Print Date: 26/01/2018

SIGNAL WORD	DANGER

Hazard statement(s)

H226	Flammable liquid and vapour.
H320	Causes eye irritation.
H336	May cause drowsiness or dizziness.
H304	May be fatal if swallowed and enters airways.
H412	Harmful to aquatic life with long lasting effects.

Hazard(s) not otherwise specified

Not Applicable

Precautionary statement(s) Prevention

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P271	Use only outdoors or in a well-ventilated area.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting/intrinsically safe equipment.

Precautionary statement(s) Response

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P331	Do NOT induce vomiting.
P370+P378	In case of fire: Use alcohol resistant foam or normal protein foam for extinction.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Precautionary statement(s) Storage

P403+P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.

Precautionary statement(s) Disposal

P501	Dispose of contents/container in accordance with local regulations.

SECTION 3 COMPOSITION / INFORMATION ON INGREDIENTS

Substances

See section below for composition of Mixtures

Mixtures

CAS No	%[weight]	Name
Not Available	>60	synthetic kerosene
		Consisting of paraffin's, isoparaffins and cycloparaffins from C8 to C16
108-67-8	10-20	1,3,5-trimethyl benzene

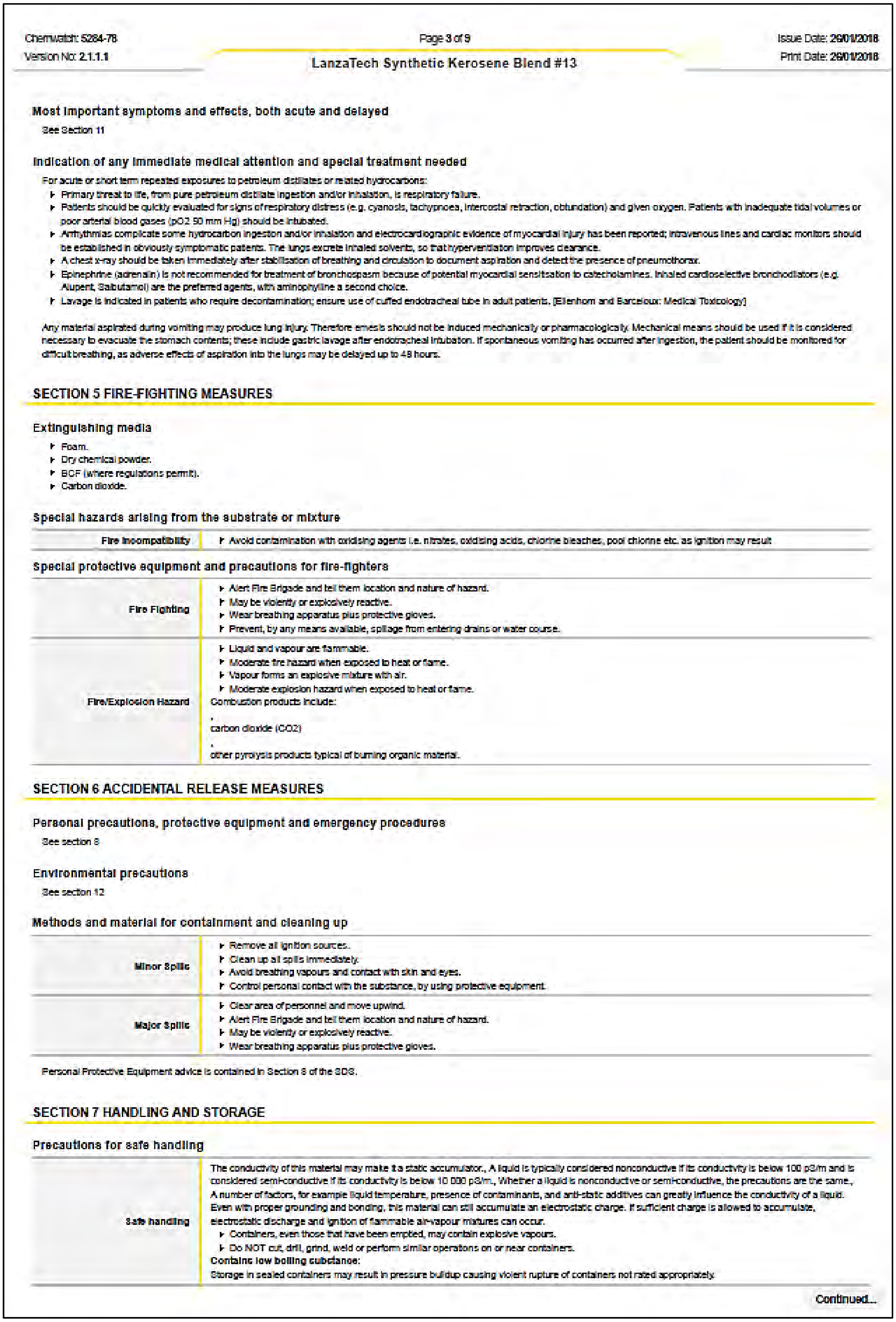
The specific chemical identity and/or exact percentage (concentration) of composition has been withheld as a trade secret.

SECTION 4 FIRST-AID MEASURES

Description of first aid measures

Eye Contact	If this product comes in contact with the eyes: ▸ Wash out immediately with fresh running water. ▸ Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids. ▸ Seek medical attention without delay; if pain persists or recurs seek medical attention. ▸ Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.
Skin Contact	If skin contact occurs: ▸ Immediately remove all contaminated clothing, including footwear. ▸ Flush skin and hair with running water (and soap if available). ▸ Seek medical attention in event of irritation.
Inhalation	▸ If fumes or combustion products are inhaled remove from contaminated area. ▸ Lay patient down. Keep warm and rested. ▸ Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures. ▸ Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary. ▸ Transport to hospital, or doctor.
Ingestion	▸ If swallowed do **NOT** induce vomiting. ▸ If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration. ▸ Observe the patient carefully. ▸ Never give liquid to a person showing signs of being sleepy or with reduced awareness; i.e. becoming unconscious. ▸ Give water to rinse out mouth, then provide liquid slowly and as much as casualty can comfortably drink. ▸ Seek medical advice.

Continued...



Chemwatch: 5284-78
Version No: 2.1.1.1

Page 3 of 9

LanzaTech Synthetic Kerosene Blend #13

Issue Date: 29/01/2018
Print Date: 29/01/2018

Most important symptoms and effects, both acute and delayed

See Section 11

Indication of any immediate medical attention and special treatment needed

For acute or short term repeated exposures to petroleum distillates or related hydrocarbons:

- Primary threat to life, from pure petroleum distillate ingestion and/or inhalation, is respiratory failure.
- Patients should be quickly evaluated for signs of respiratory distress (e.g. cyanosis, tachypnoea, intercostal retraction, obtundation) and given oxygen. Patients with inadequate tidal volumes or poor arterial blood gases (pO2 50 mm Hg) should be intubated.
- Arrhythmias complicate some hydrocarbon ingestion and/or inhalation and electrocardiographic evidence of myocardial injury has been reported; intravenous lines and cardiac monitors should be established in obviously symptomatic patients. The lungs excrete inhaled solvents, so that hyperventilation improves clearance.
- A chest x-ray should be taken immediately after stabilisation of breathing and circulation to document aspiration and detect the presence of pneumothorax.
- Epinephrine (adrenalin) is not recommended for treatment of bronchospasm because of potential myocardial sensitisation to catecholamines. Inhaled cardioselective bronchodilators (e.g. Alupent, Salbutamol) are the preferred agents, with aminophylline a second choice.
- Lavage is indicated in patients who require decontamination; ensure use of cuffed endotracheal tube in adult patients. [Ellenhorn and Barceloux: Medical Toxicology]

Any material aspirated during vomiting may produce lung injury. Therefore emesis should not be induced mechanically or pharmacologically. Mechanical means should be used if it is considered necessary to evacuate the stomach contents; these include gastric lavage after endotracheal intubation. If spontaneous vomiting has occurred after ingestion, the patient should be monitored for difficult breathing, as adverse effects of aspiration into the lungs may be delayed up to 48 hours.

SECTION 5 FIRE-FIGHTING MEASURES

Extinguishing media

- Foam.
- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.

Special hazards arising from the substrate or mixture

Fire Incompatibility	Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition may result

Special protective equipment and precautions for fire-fighters

Fire Fighting	Alert Fire Brigade and tell them location and nature of hazard. May be violently or explosively reactive. Wear breathing apparatus plus protective gloves. Prevent, by any means available, spillage from entering drains or water course.
Fire/Explosion Hazard	Liquid and vapour are flammable. Moderate fire hazard when exposed to heat or flame. Vapour forms an explosive mixture with air. Moderate explosion hazard when exposed to heat or flame. Combustion products include: , carbon dioxide (CO2) , other pyrolysis products typical of burning organic material.

SECTION 6 ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures

See section 8

Environmental precautions

See section 12

Methods and material for containment and cleaning up

Minor Spills	Remove all ignition sources. Clean up all spills immediately. Avoid breathing vapours and contact with skin and eyes. Control personal contact with the substance, by using protective equipment.
Major Spills	Clear area of personnel and move upwind. Alert Fire Brigade and tell them location and nature of hazard. May be violently or explosively reactive. Wear breathing apparatus plus protective gloves.

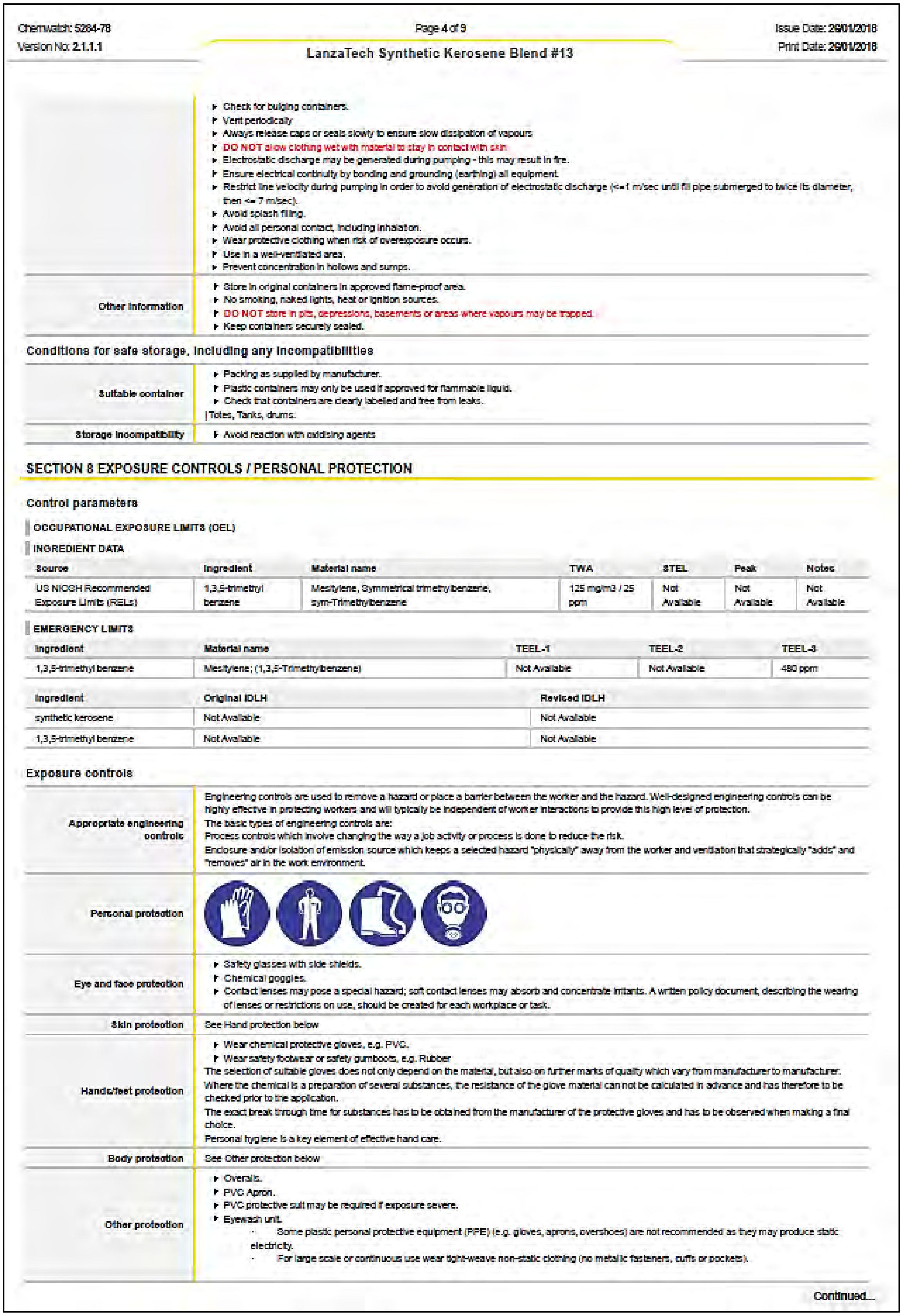
Personal Protective Equipment advice is contained in Section 8 of the SDS.

SECTION 7 HANDLING AND STORAGE

Precautions for safe handling

Safe handling	The conductivity of this material may make it a static accumulator., A liquid is typically considered nonconductive if its conductivity is below 100 pS/m and is considered semi-conductive if its conductivity is below 10 000 pS/m., Whether a liquid is nonconductive or semi-conductive, the precautions are the same., A number of factors, for example liquid temperature, presence of contaminants, and anti-static additives can greatly influence the conductivity of a liquid. Even with proper grounding and bonding, this material can still accumulate an electrostatic charge. If sufficient charge is allowed to accumulate, electrostatic discharge and ignition of flammable air-vapour mixtures can occur. Containers, even those that have been emptied, may contain explosive vapours. Do NOT cut, drill, grind, weld or perform similar operations on or near containers. **Contains low boiling substance:** Storage in sealed containers may result in pressure buildup causing violent rupture of containers not rated appropriately.

Continued...



Chemwatch: 5264-78
Version No: 2.1.1.1

Page 4 of 9

LanzaTech Synthetic Kerosene Blend #13

Issue Date: 29/01/2018
Print Date: 29/01/2018

	▸ Check for bulging containers. ▸ Vent periodically ▸ Always release caps or seals slowly to ensure slow dissipation of vapours ▸ DO NOT allow clothing wet with material to stay in contact with skin ▸ Electrostatic discharge may be generated during pumping - this may result in fire. ▸ Ensure electrical continuity by bonding and grounding (earthing) all equipment. ▸ Restrict line velocity during pumping in order to avoid generation of electrostatic discharge (<=1 m/sec until fill pipe submerged to twice its diameter, then <= 7 m/sec). ▸ Avoid splash filling. ▸ Avoid all personal contact, including inhalation. ▸ Wear protective clothing when risk of overexposure occurs. ▸ Use in a well-ventilated area. ▸ Prevent concentration in hollows and sumps.
Other information	▸ Store in original containers in approved flame-proof area. ▸ No smoking, naked lights, heat or ignition sources. ▸ DO NOT store in pits, depressions, basements or areas where vapours may be trapped. ▸ Keep containers securely sealed.

Conditions for safe storage, including any incompatibilities

Suitable container	▸ Packing as supplied by manufacturer. ▸ Plastic containers may only be used if approved for flammable liquid. ▸ Check that containers are clearly labelled and free from leaks. |Totes, Tanks, drums.
Storage incompatibility	▸ Avoid reaction with oxidising agents

SECTION 8 EXPOSURE CONTROLS / PERSONAL PROTECTION

Control parameters

OCCUPATIONAL EXPOSURE LIMITS (OEL)

INGREDIENT DATA

Source	Ingredient	Material name	TWA	STEL	Peak	Notes
US NIOSH Recommended Exposure Limits (RELs)	1,3,5-trimethyl benzene	Mesitylene, Symmetrical trimethylbenzene, sym-Trimethylbenzene	125 mg/m3 / 25 ppm	Not Available	Not Available	Not Available

EMERGENCY LIMITS

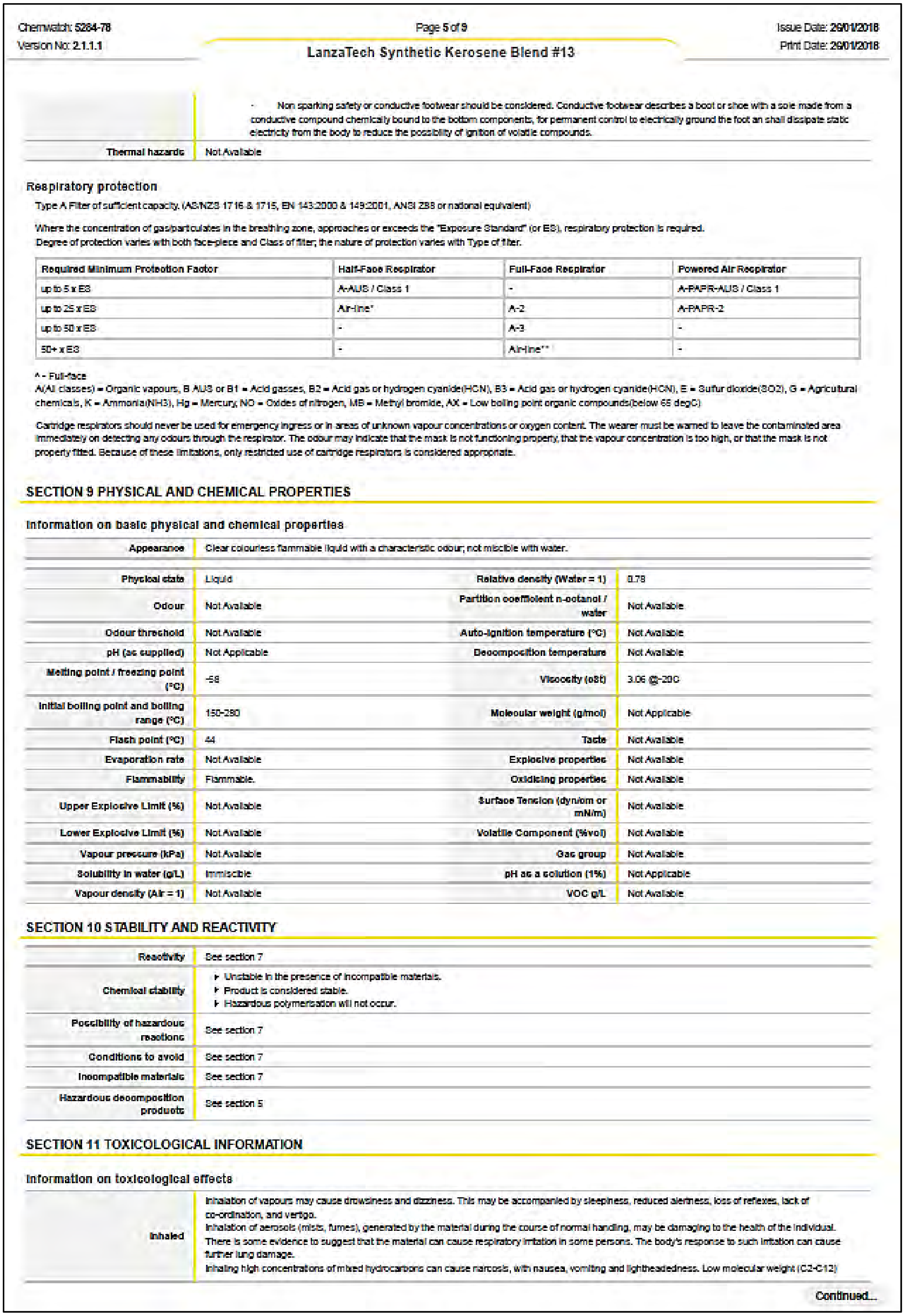
Ingredient	Material name	TEEL-1	TEEL-2	TEEL-3
1,3,5-trimethyl benzene	Mesitylene; (1,3,5-Trimethylbenzene)	Not Available	Not Available	480 ppm

Ingredient	Original IDLH	Revised IDLH
synthetic kerosene	Not Available	Not Available
1,3,5-trimethyl benzene	Not Available	Not Available

Exposure controls

Appropriate engineering controls	Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection. The basic types of engineering controls are: Process controls which involve changing the way a job activity or process is done to reduce the risk. Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.
Personal protection	
Eye and face protection	▸ Safety glasses with side shields. ▸ Chemical goggles. ▸ Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lenses or restrictions on use, should be created for each workplace or task.
Skin protection	See Hand protection below
Hands/feet protection	▸ Wear chemical protective gloves, e.g. PVC. ▸ Wear safety footwear or safety gumboots, e.g. Rubber The selection of suitable gloves does not only depend on the material, but also on further marks of quality which vary from manufacturer to manufacturer. Where the chemical is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application. The exact break through time for substances has to be obtained from the manufacturer of the protective gloves and has to be observed when making a final choice. Personal hygiene is a key element of effective hand care.
Body protection	See Other protection below
Other protection	▸ Overalls. ▸ PVC Apron. ▸ PVC protective suit may be required if exposure severe. ▸ Eyewash unit. · Some plastic personal protective equipment (PPE) (e.g. gloves, aprons, overshoes) are not recommended as they may produce static electricity. · For large scale or continuous use wear tight-weave non-static clothing (no metallic fasteners, cuffs or pockets).

Continued...



	· Non sparking safety or conductive footwear should be considered. Conductive footwear describes a boot or shoe with a sole made from a conductive compound chemically bound to the bottom components, for permanent control to electrically ground the foot an shall dissipate static electricity from the body to reduce the possibility of ignition of volatile compounds.
Thermal hazards	Not Available

Respiratory protection

Type A Filter of sufficient capacity. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

Where the concentration of gas/particulates in the breathing zone, approaches or exceeds the "Exposure Standard" (or ES), respiratory protection is required.
Degree of protection varies with both face-piece and Class of filter; the nature of protection varies with Type of filter.

Required Minimum Protection Factor	Half-Face Respirator	Full-Face Respirator	Powered Air Respirator
up to 5 x ES	A-AUS / Class 1	-	A-PAPR-AUS / Class 1
up to 25 x ES	Air-line*	A-2	A-PAPR-2
up to 50 x ES	-	A-3	-
50+ x ES	-	Air-line**	-

^ - Full-face
A(All classes) = Organic vapours, B AUS or B1 = Acid gasses, B2 = Acid gas or hydrogen cyanide(HCN), B3 = Acid gas or hydrogen cyanide(HCN), E = Sulfur dioxide(SO2), G = Agricultural chemicals, K = Ammonia(NH3), Hg = Mercury, NO = Oxides of nitrogen, MB = Methyl bromide, AX = Low boiling point organic compounds(below 65 degC)

Cartridge respirators should never be used for emergency ingress or in areas of unknown vapour concentrations or oxygen content. The wearer must be warned to leave the contaminated area immediately on detecting any odours through the respirator. The odour may indicate that the mask is not functioning properly, that the vapour concentration is too high, or that the mask is not properly fitted. Because of these limitations, only restricted use of cartridge respirators is considered appropriate.

SECTION 9 PHYSICAL AND CHEMICAL PROPERTIES

Information on basic physical and chemical properties

Appearance	Clear colourless flammable liquid with a characteristic odour; not miscible with water.

Physical state	Liquid	**Relative density (Water = 1)**	0.78
Odour	Not Available	**Partition coefficient n-octanol / water**	Not Available
Odour threshold	Not Available	**Auto-ignition temperature (°C)**	Not Available
pH (as supplied)	Not Applicable	**Decomposition temperature**	Not Available
Melting point / freezing point (°C)	-58	**Viscosity (cSt)**	3.06 @-20C
Initial boiling point and boiling range (°C)	150-280	**Molecular weight (g/mol)**	Not Applicable
Flash point (°C)	44	**Taste**	Not Available
Evaporation rate	Not Available	**Explosive properties**	Not Available
Flammability	Flammable.	**Oxidising properties**	Not Available
Upper Explosive Limit (%)	Not Available	**Surface Tension (dyn/cm or mN/m)**	Not Available
Lower Explosive Limit (%)	Not Available	**Volatile Component (%vol)**	Not Available
Vapour pressure (kPa)	Not Available	**Gas group**	Not Available
Solubility in water (g/L)	Immiscible	**pH as a solution (1%)**	Not Applicable
Vapour density (Air = 1)	Not Available	**VOC g/L**	Not Available

SECTION 10 STABILITY AND REACTIVITY

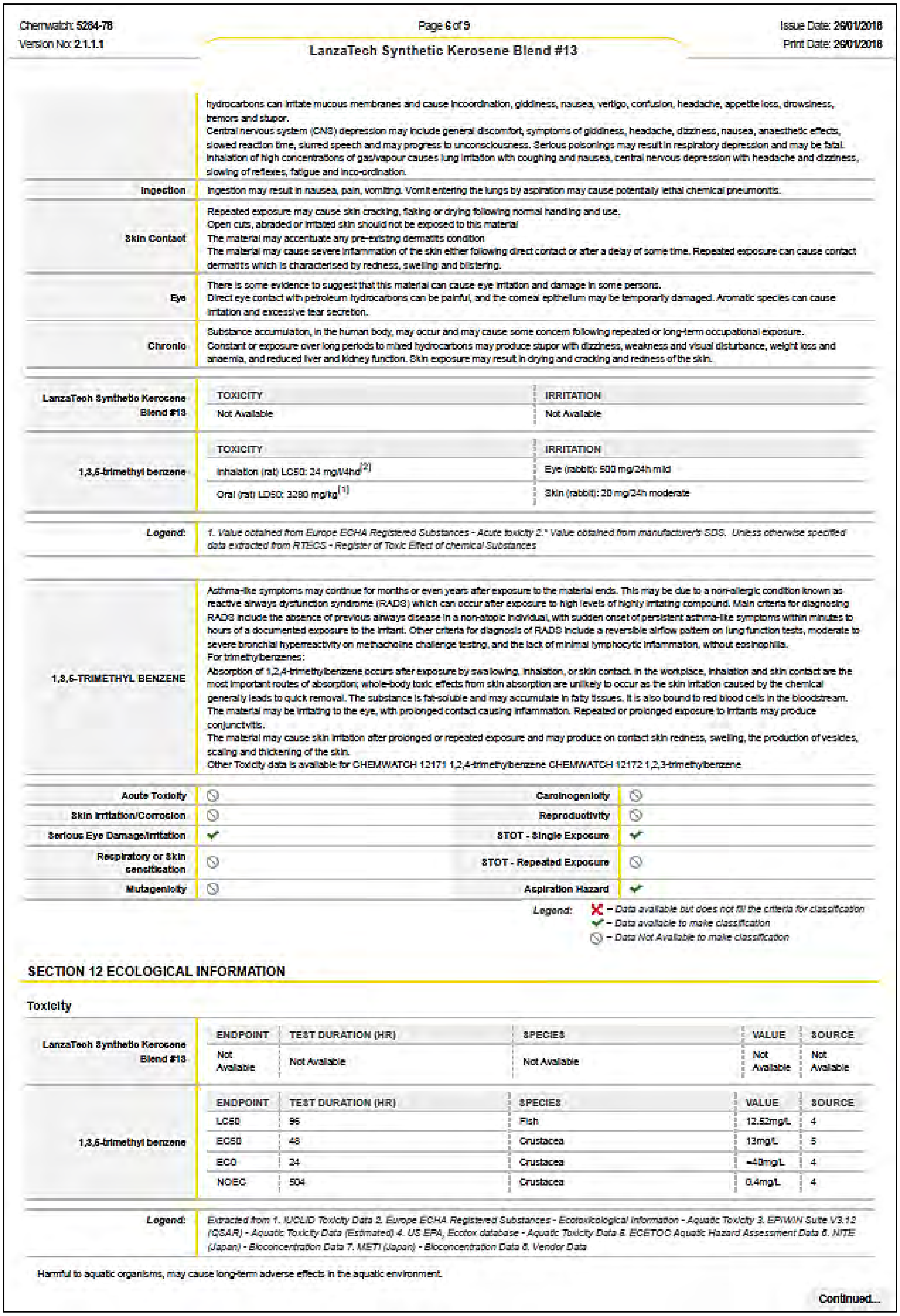
Reactivity	See section 7
Chemical stability	▸ Unstable in the presence of incompatible materials. ▸ Product is considered stable. ▸ Hazardous polymerisation will not occur.
Possibility of hazardous reactions	See section 7
Conditions to avoid	See section 7
Incompatible materials	See section 7
Hazardous decomposition products	See section 5

SECTION 11 TOXICOLOGICAL INFORMATION

Information on toxicological effects

Inhaled	Inhalation of vapours may cause drowsiness and dizziness. This may be accompanied by sleepiness, reduced alertness, loss of reflexes, lack of co-ordination, and vertigo. Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may be damaging to the health of the individual. There is some evidence to suggest that the material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage. Inhaling high concentrations of mixed hydrocarbons can cause narcosis, with nausea, vomiting and lightheadedness. Low molecular weight (C2-C12)

Continued...



Chemwatch: 5284-78
Version No: 2.1.1.1

Page 6 of 9

LanzaTech Synthetic Kerosene Blend #13

Issue Date: 29/01/2018
Print Date: 29/01/2018

	hydrocarbons can irritate mucous membranes and cause incoordination, giddiness, nausea, vertigo, confusion, headache, appetite loss, drowsiness, tremors and stupor. Central nervous system (CNS) depression may include general discomfort, symptoms of giddiness, headache, dizziness, nausea, anaesthetic effects, slowed reaction time, slurred speech and may progress to unconsciousness. Serious poisonings may result in respiratory depression and may be fatal. Inhalation of high concentrations of gas/vapour causes lung irritation with coughing and nausea, central nervous depression with headache and dizziness, slowing of reflexes, fatigue and inco-ordination.
Ingestion	Ingestion may result in nausea, pain, vomiting. Vomit entering the lungs by aspiration may cause potentially lethal chemical pneumonitis.
Skin Contact	Repeated exposure may cause skin cracking, flaking or drying following normal handling and use. Open cuts, abraded or irritated skin should not be exposed to this material The material may accentuate any pre-existing dermatitis condition The material may cause severe inflammation of the skin either following direct contact or after a delay of some time. Repeated exposure can cause contact dermatitis which is characterised by redness, swelling and blistering.
Eye	There is some evidence to suggest that this material can cause eye irritation and damage in some persons. Direct eye contact with petroleum hydrocarbons can be painful, and the corneal epithelium may be temporarily damaged. Aromatic species can cause irritation and excessive tear secretion.
Chronic	Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure. Constant or exposure over long periods to mixed hydrocarbons may produce stupor with dizziness, weakness and visual disturbance, weight loss and anaemia, and reduced liver and kidney function. Skin exposure may result in drying and cracking and redness of the skin.

	TOXICITY	IRRITATION
LanzaTech Synthetic Kerosene Blend #13	Not Available	Not Available

	TOXICITY	IRRITATION
1,3,5-trimethyl benzene	Inhalation (rat) LC50: 24 mg/l/4hd[2]	Eye (rabbit): 500 mg/24h mild
	Oral (rat) LD50: 3280 mg/kg[1]	Skin (rabbit): 20 mg/24h moderate

Legend:	*1. Value obtained from Europe ECHA Registered Substances - Acute toxicity 2.* Value obtained from manufacturer's SDS. Unless otherwise specified data extracted from RTECS - Register of Toxic Effect of chemical Substances*

1,3,5-TRIMETHYL BENZENE	Asthma-like symptoms may continue for months or even years after exposure to the material ends. This may be due to a non-allergic condition known as reactive airways dysfunction syndrome (RADS) which can occur after exposure to high levels of highly irritating compound. Main criteria for diagnosing RADS include the absence of previous airways disease in a non-atopic individual, with sudden onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. Other criteria for diagnosis of RADS include a reversible airflow pattern on lung function tests, moderate to severe bronchial hyperreactivity on methacholine challenge testing, and the lack of minimal lymphocytic inflammation, without eosinophilia. For trimethylbenzenes: Absorption of 1,2,4-trimethylbenzene occurs after exposure by swallowing, inhalation, or skin contact. In the workplace, inhalation and skin contact are the most important routes of absorption; whole-body toxic effects from skin absorption are unlikely to occur as the skin irritation caused by the chemical generally leads to quick removal. The substance is fat-soluble and may accumulate in fatty tissues. It is also bound to red blood cells in the bloodstream. The material may be irritating to the eye, with prolonged contact causing inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis. The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin. Other Toxicity data is available for CHEMWATCH 12171 1,2,4-trimethylbenzene CHEMWATCH 12172 1,2,3-trimethylbenzene

Acute Toxicity	⃠	**Carcinogenicity**	⃠
Skin Irritation/Corrosion	⃠	**Reproductivity**	⃠
Serious Eye Damage/Irritation	✓	**STOT - Single Exposure**	✓
Respiratory or Skin sensitisation	⃠	**STOT - Repeated Exposure**	⃠
Mutagenicity	⃠	**Aspiration Hazard**	✓

Legend:
✗ *– Data available but does not fill the criteria for classification*
✓ *– Data available to make classification*
⃠ *– Data Not Available to make classification*

SECTION 12 ECOLOGICAL INFORMATION

Toxicity

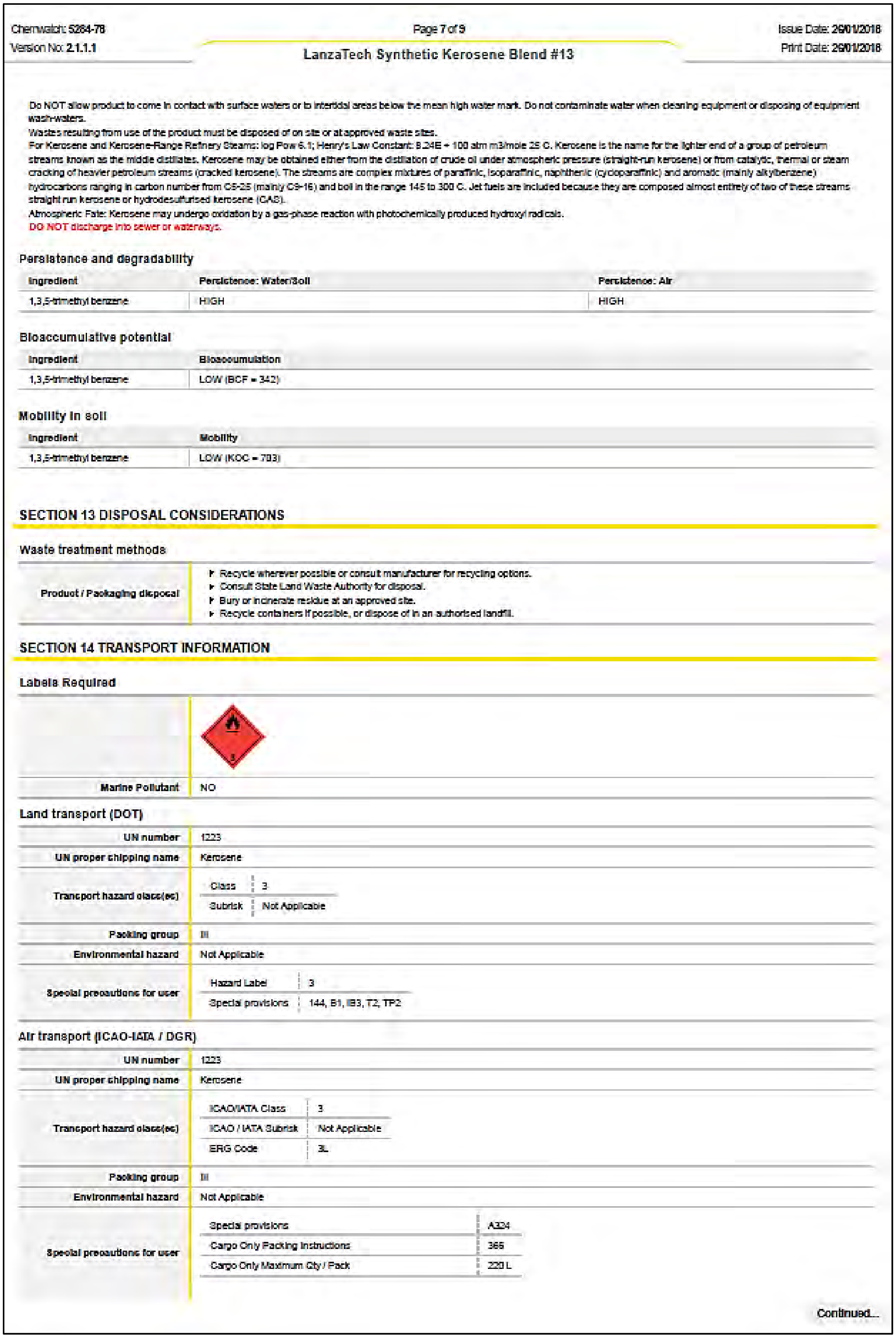
	ENDPOINT	TEST DURATION (HR)	SPECIES	VALUE	SOURCE
LanzaTech Synthetic Kerosene Blend #13	Not Available	Not Available	Not Available	Not Available	Not Available

	ENDPOINT	TEST DURATION (HR)	SPECIES	VALUE	SOURCE
1,3,5-trimethyl benzene	LC50	96	Fish	12.52mg/L	4
	EC50	48	Crustacea	13mg/L	5
	EC0	24	Crustacea	=40mg/L	4
	NOEC	504	Crustacea	0.4mg/L	4

Legend:	*Extracted from 1. IUCLID Toxicity Data 2. Europe ECHA Registered Substances - Ecotoxicological Information - Aquatic Toxicity 3. EPIWIN Suite V3.12 (QSAR) - Aquatic Toxicity Data (Estimated) 4. US EPA, Ecotox database - Aquatic Toxicity Data 5. ECETOC Aquatic Hazard Assessment Data 6. NITE (Japan) - Bioconcentration Data 7. METI (Japan) - Bioconcentration Data 8. Vendor Data*

Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Continued...



Chemwatch: 5284-78
Version No: 2.1.1.1

Page 7 of 9

LanzaTech Synthetic Kerosene Blend #13

Issue Date: 29/01/2018
Print Date: 29/01/2018

Do NOT allow product to come in contact with surface waters or to intertidal areas below the mean high water mark. Do not contaminate water when cleaning equipment or disposing of equipment wash-waters.
Wastes resulting from use of the product must be disposed of on site or at approved waste sites.
For Kerosene and Kerosene-Range Refinery Steams: log Pow 6.1; Henry's Law Constant: 8.24E + 100 atm m3/mole 25 C. Kerosene is the name for the lighter end of a group of petroleum streams known as the middle distillates. Kerosene may be obtained either from the distillation of crude oil under atmospheric pressure (straight-run kerosene) or from catalytic, thermal or steam cracking of heavier petroleum streams (cracked kerosene). The streams are complex mixtures of paraffinic, isoparaffinic, naphthenic (cycloparaffinic) and aromatic (mainly alkylbenzene) hydrocarbons ranging in carbon number from C5-25 (mainly C9-16) and boil in the range 145 to 300 C. Jet fuels are included because they are composed almost entirely of two of these streams straight run kerosene or hydrodesulfurised kerosene (CAS).
Atmospheric Fate: Kerosene may undergo oxidation by a gas-phase reaction with photochemically produced hydroxyl radicals.
DO NOT discharge into sewer or waterways.

Persistence and degradability

Ingredient	Persistence: Water/Soil	Persistence: Air
1,3,5-trimethyl benzene	HIGH	HIGH

Bioaccumulative potential

Ingredient	Bioaccumulation
1,3,5-trimethyl benzene	LOW (BCF = 342)

Mobility in soil

Ingredient	Mobility
1,3,5-trimethyl benzene	LOW (KOC = 703)

SECTION 13 DISPOSAL CONSIDERATIONS

Waste treatment methods

Product / Packaging disposal	▸ Recycle wherever possible or consult manufacturer for recycling options. ▸ Consult State Land Waste Authority for disposal. ▸ Bury or incinerate residue at an approved site. ▸ Recycle containers if possible, or dispose of in an authorised landfill.

SECTION 14 TRANSPORT INFORMATION

Labels Required

Marine Pollutant	NO

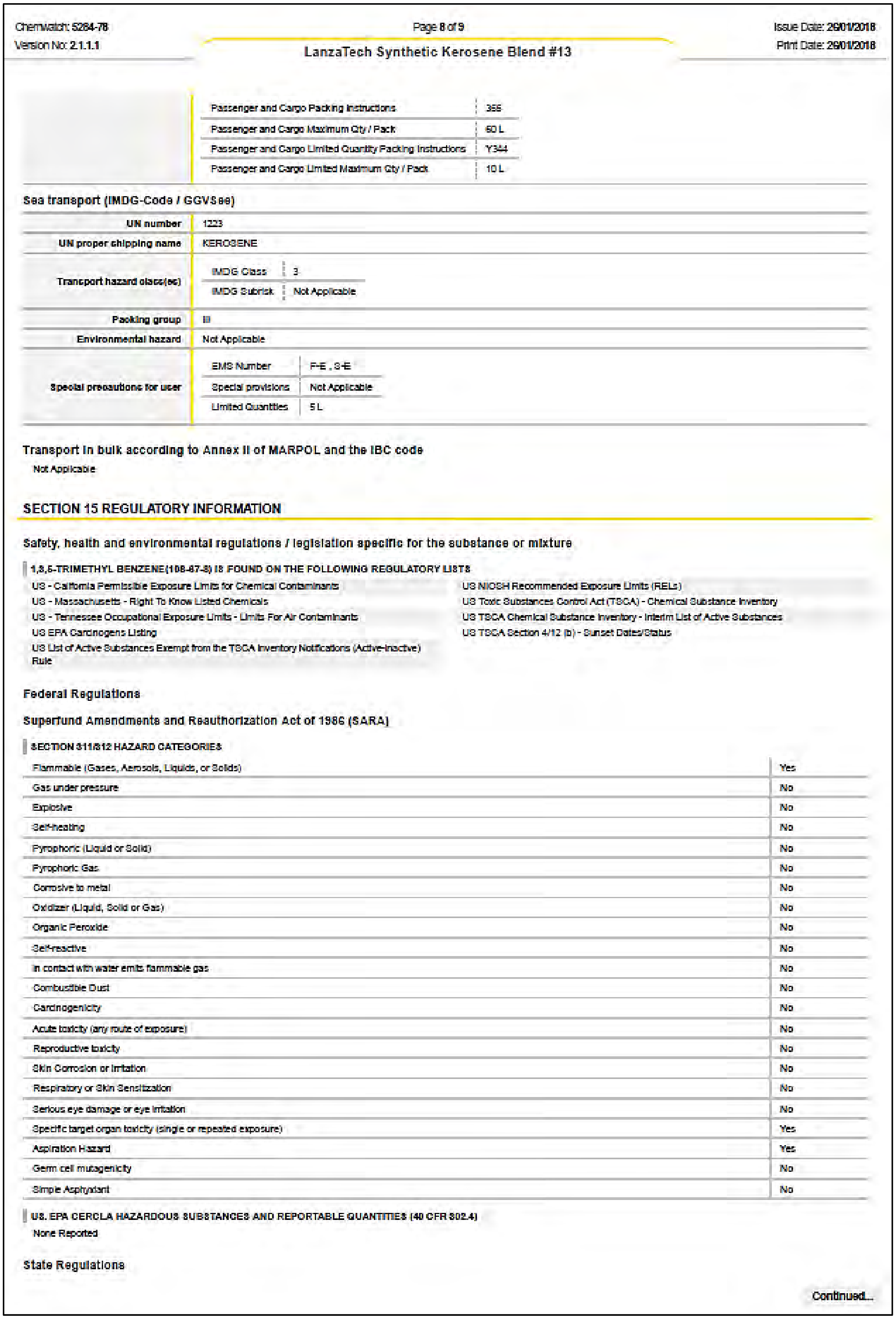
Land transport (DOT)

UN number	1223	
UN proper shipping name	Kerosene	
Transport hazard class(es)	Class	3
	Subrisk	Not Applicable
Packing group	III	
Environmental hazard	Not Applicable	
Special precautions for user	Hazard Label	3
	Special provisions	144, B1, IB3, T2, TP2

Air transport (ICAO-IATA / DGR)

UN number	1223	
UN proper shipping name	Kerosene	
Transport hazard class(es)	ICAO/IATA Class	3
	ICAO / IATA Subrisk	Not Applicable
	ERG Code	3L
Packing group	III	
Environmental hazard	Not Applicable	
Special precautions for user	Special provisions	A324
	Cargo Only Packing Instructions	366
	Cargo Only Maximum Qty / Pack	220 L

Continued...



	Passenger and Cargo Packing Instructions	355
	Passenger and Cargo Maximum Qty / Pack	60 L
	Passenger and Cargo Limited Quantity Packing Instructions	Y344
	Passenger and Cargo Limited Maximum Qty / Pack	10 L

Sea transport (IMDG-Code / GGVSee)

UN number	1223
UN proper shipping name	KEROSENE
Transport hazard class(es)	IMDG Class: 3 IMDG Subrisk: Not Applicable
Packing group	III
Environmental hazard	Not Applicable
Special precautions for user	EMS Number: F-E , S-E Special provisions: Not Applicable Limited Quantities: 5 L

Transport in bulk according to Annex II of MARPOL and the IBC code

Not Applicable

SECTION 15 REGULATORY INFORMATION

Safety, health and environmental regulations / legislation specific for the substance or mixture

1,3,5-TRIMETHYL BENZENE(108-67-8) IS FOUND ON THE FOLLOWING REGULATORY LISTS

US - California Permissible Exposure Limits for Chemical Contaminants
US - Massachusetts - Right To Know Listed Chemicals
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants
US EPA Carcinogens Listing
US List of Active Substances Exempt from the TSCA Inventory Notifications (Active-Inactive) Rule
US NIOSH Recommended Exposure Limits (RELs)
US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory
US TSCA Chemical Substance Inventory - Interim List of Active Substances
US TSCA Section 4/12 (b) - Sunset Dates/Status

Federal Regulations

Superfund Amendments and Reauthorization Act of 1986 (SARA)

SECTION 311/312 HAZARD CATEGORIES

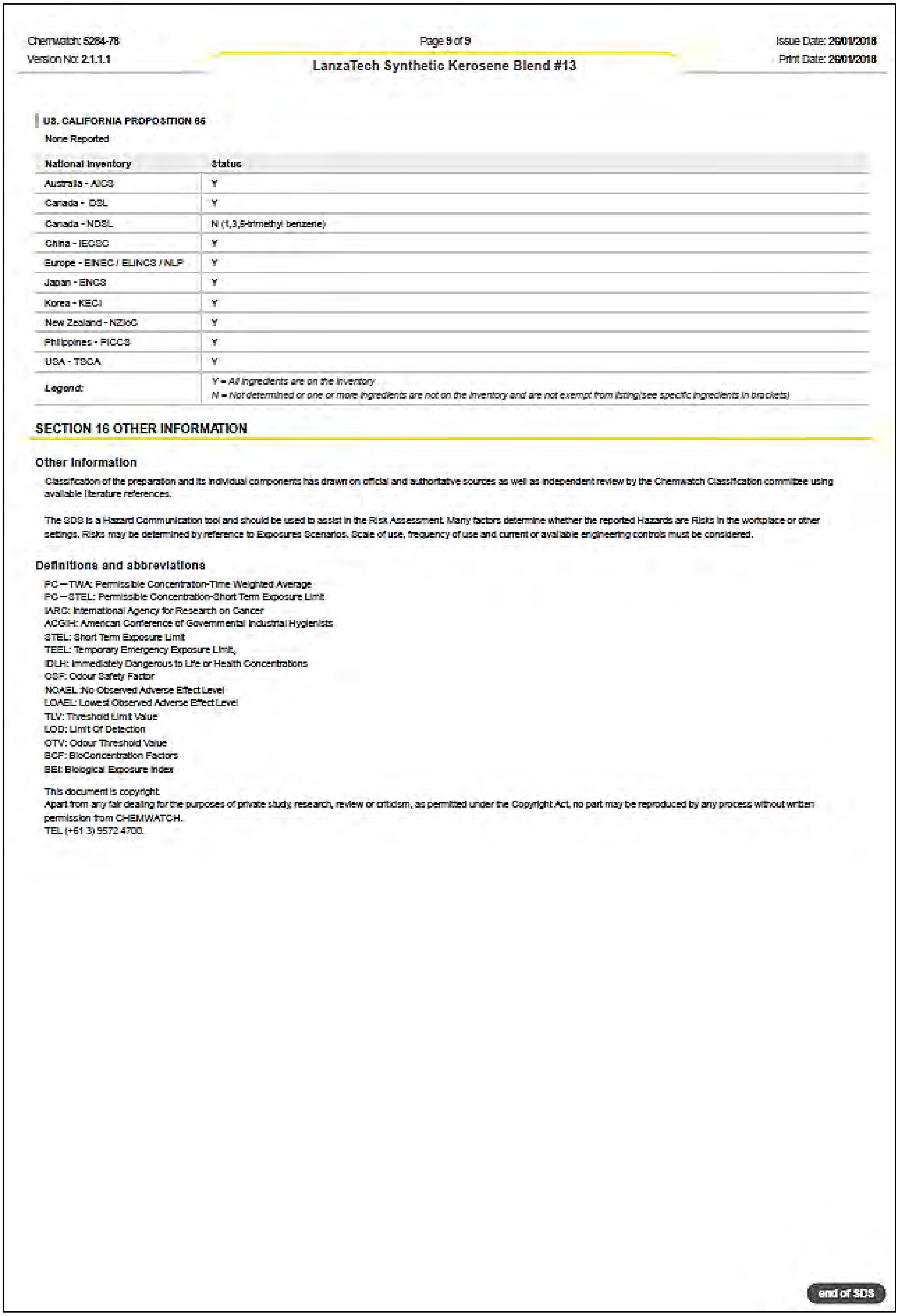
Flammable (Gases, Aerosols, Liquids, or Solids)	Yes
Gas under pressure	No
Explosive	No
Self-heating	No
Pyrophoric (Liquid or Solid)	No
Pyrophoric Gas	No
Corrosive to metal	No
Oxidizer (Liquid, Solid or Gas)	No
Organic Peroxide	No
Self-reactive	No
In contact with water emits flammable gas	No
Combustible Dust	No
Carcinogenicity	No
Acute toxicity (any route of exposure)	No
Reproductive toxicity	No
Skin Corrosion or Irritation	No
Respiratory or Skin Sensitization	No
Serious eye damage or eye irritation	No
Specific target organ toxicity (single or repeated exposure)	Yes
Aspiration Hazard	Yes
Germ cell mutagenicity	No
Simple Asphyxiant	No

US. EPA CERCLA HAZARDOUS SUBSTANCES AND REPORTABLE QUANTITIES (40 CFR 302.4)

None Reported

State Regulations

Continued...



Chemwatch: 5284-78
Version No: 2.1.1.1

Page 9 of 9

LanzaTech Synthetic Kerosene Blend #13

Issue Date: 29/01/2018
Print Date: 29/01/2018

US. CALIFORNIA PROPOSITION 65

None Reported

National Inventory	Status
Australia - AICS	Y
Canada - DSL	Y
Canada - NDSL	N (1,3,5-trimethyl benzene)
China - IECSC	Y
Europe - EINEC / ELINCS / NLP	Y
Japan - ENCS	Y
Korea - KECI	Y
New Zealand - NZIoC	Y
Philippines - PICCS	Y
USA - TSCA	Y
Legend:	*Y = All ingredients are on the inventory* *N = Not determined or one or more ingredients are not on the inventory and are not exempt from listing(see specific ingredients in brackets)*

SECTION 16 OTHER INFORMATION

Other Information

Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

Definitions and abbreviations

PC－TWA: Permissible Concentration-Time Weighted Average
PC－STEL: Permissible Concentration-Short Term Exposure Limit
IARC: International Agency for Research on Cancer
ACGIH: American Conference of Governmental Industrial Hygienists
STEL: Short Term Exposure Limit
TEEL: Temporary Emergency Exposure Limit。
IDLH: Immediately Dangerous to Life or Health Concentrations
OSF: Odour Safety Factor
NOAEL :No Observed Adverse Effect Level
LOAEL: Lowest Observed Adverse Effect Level
TLV: Threshold Limit Value
LOD: Limit Of Detection
OTV: Odour Threshold Value
BCF: BioConcentration Factors
BEI: Biological Exposure Index

end of SDS

Appendix B. Spray Visualization Images

B.1 Spray Imaging - Flash - dP/P=4%, F/A=0.030

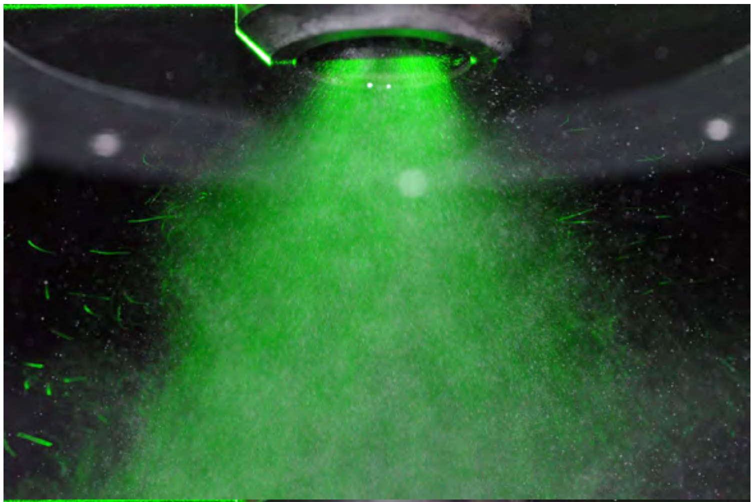
a) Jet A

b) Alt Fuel

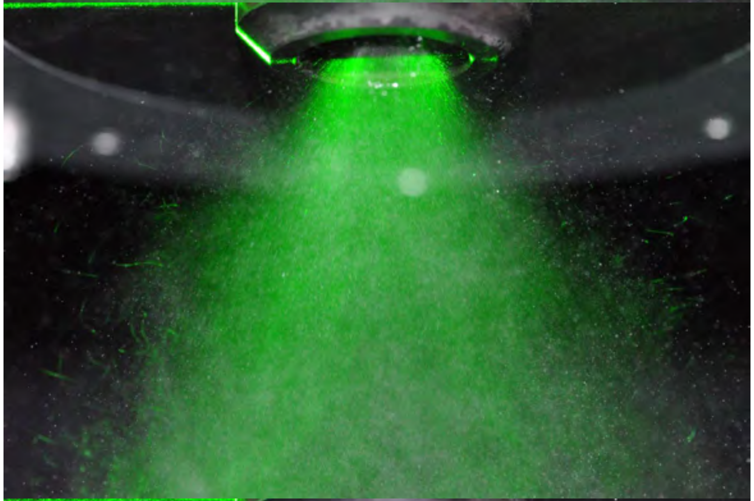
c) 7024 Fuel

B.2 Flash and Laser Sheet - dP/P=4%, F/A=0.030

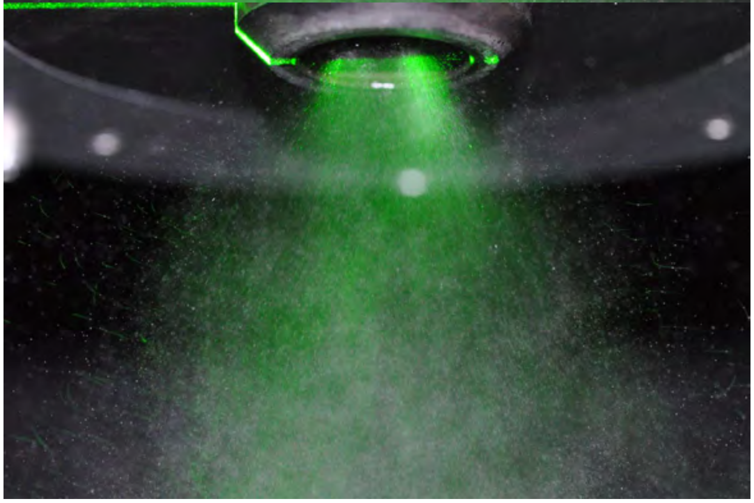
a) Jet A



b) Alt Fuel

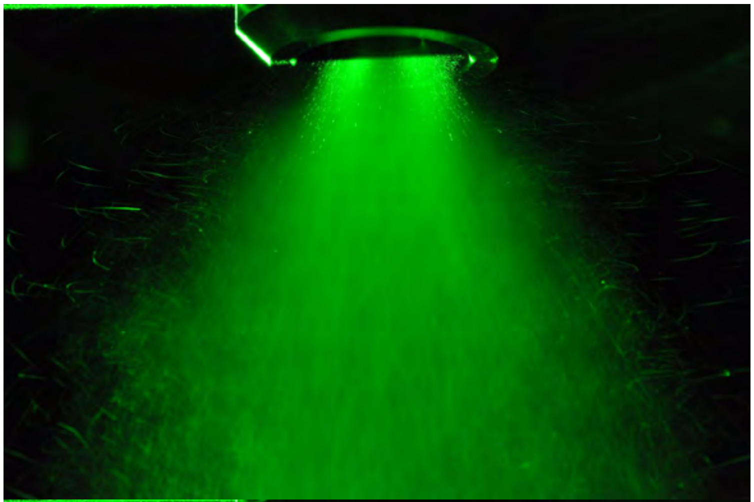


c) 7024 Fuel



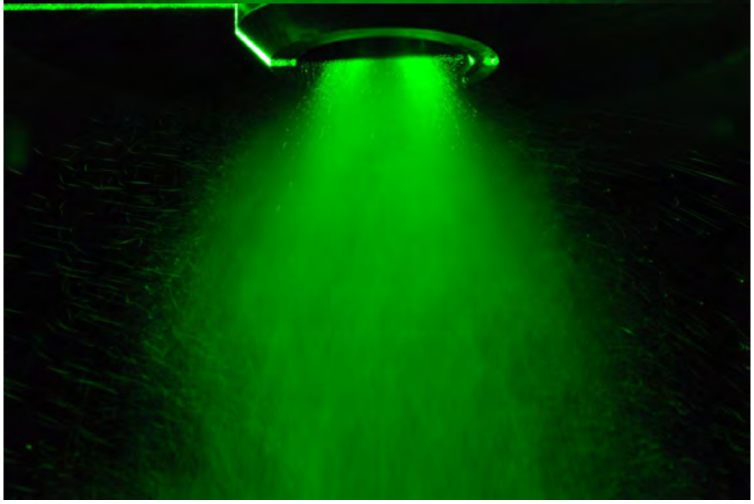
B.3 Laser Sheet (1/50 sec) - dP/P=4%, F/A=0.030

a) Jet A



b) Alt Fuel

c) 7024 Fuel



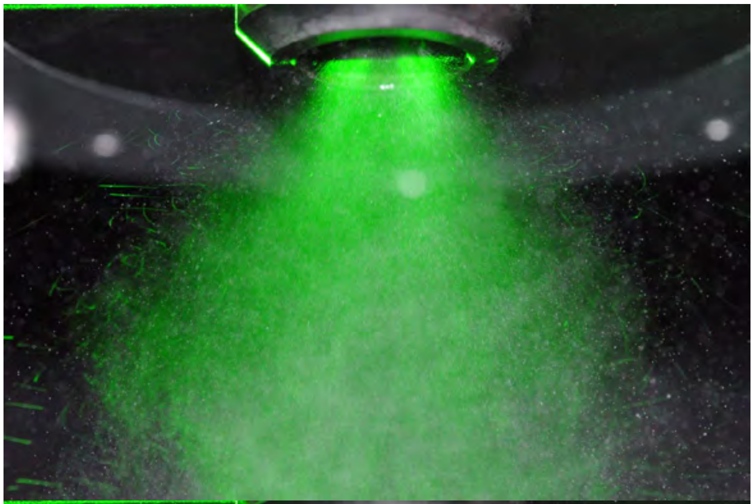
B.4 Flash - dP/P=4%, F/A=0.050

a) Jet A

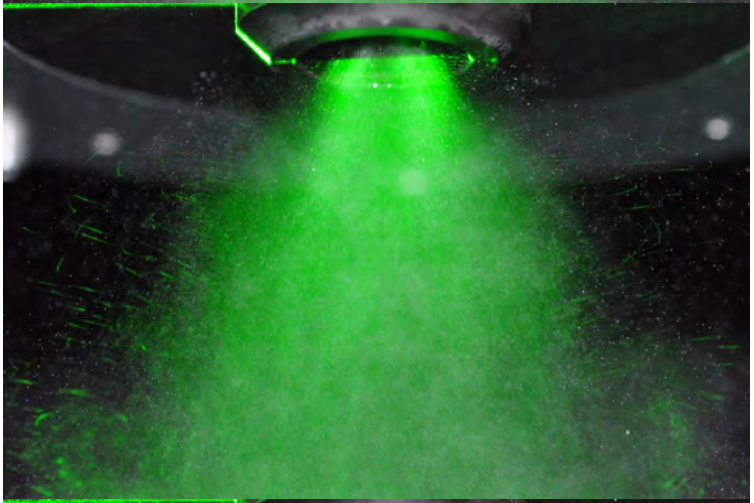
b) Alt Fuel

c) 7024 Fuel

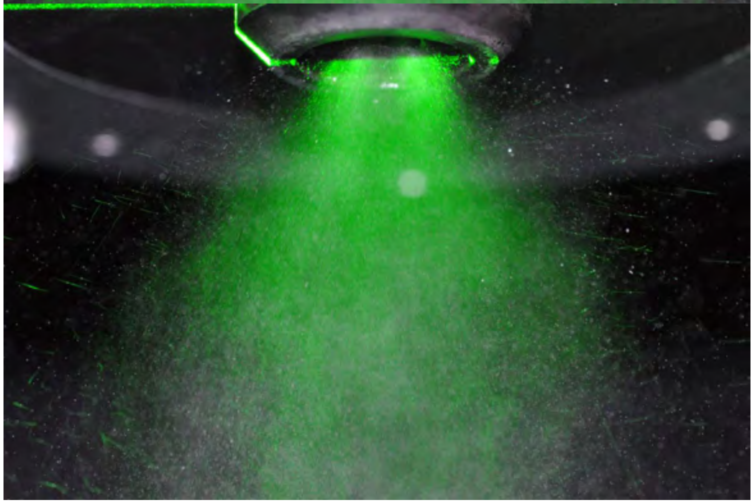
B.5 Flash and Laser Sheet - dP/P=4%, F/A=0.050



a) Jet A



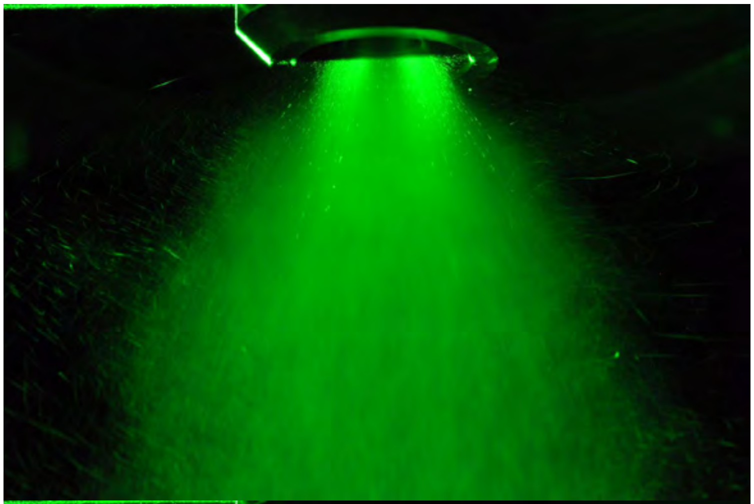
b) Alt Fuel



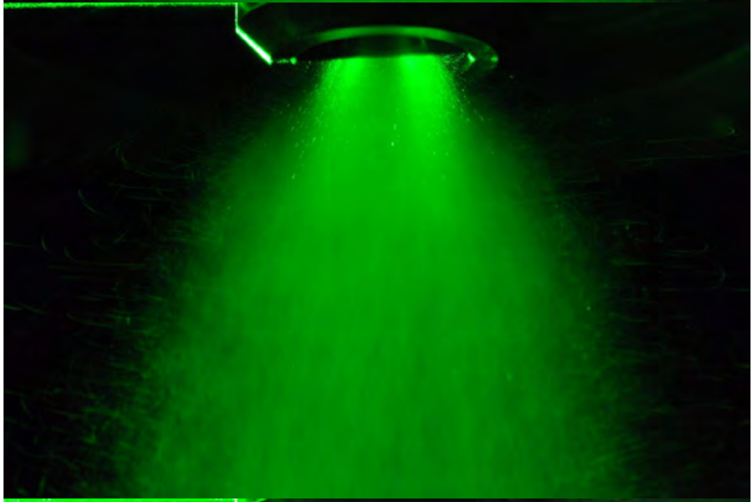
c) 7024 Fuel

B.6 Laser Sheet (1/50 sec) - dP/P=4%, F/A=0.050

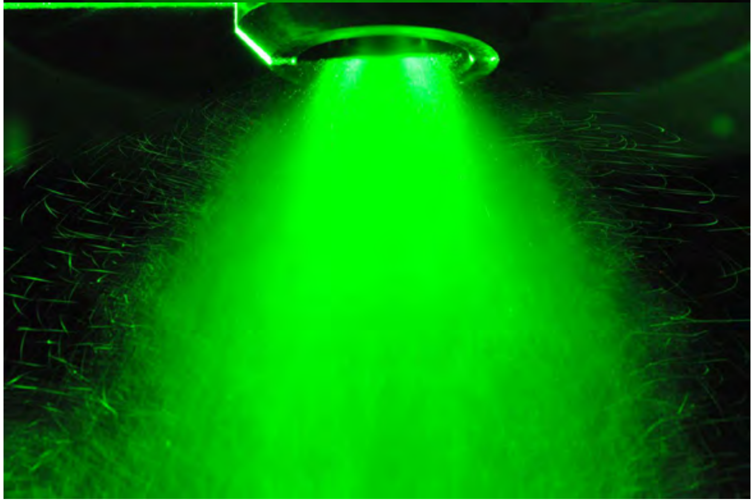
a) Jet A



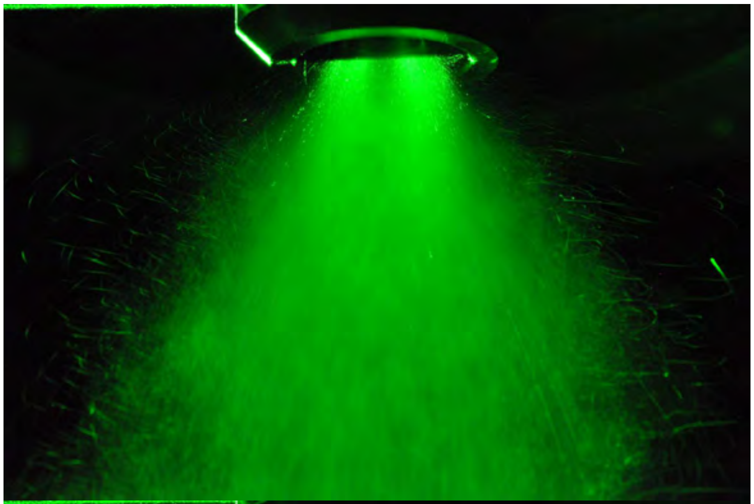
b) Alt Fuel



c) 7024 Fuel

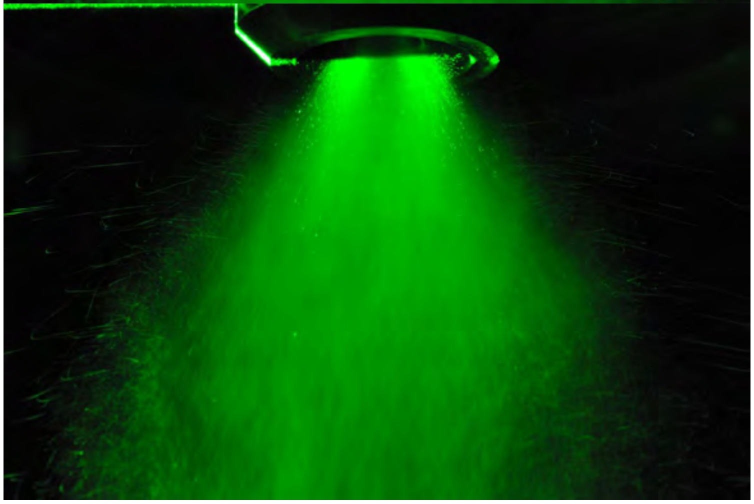


B.7 Laser Sheet (1/100 sec) - dP/P=4%, F/A=0.050



a) Jet A

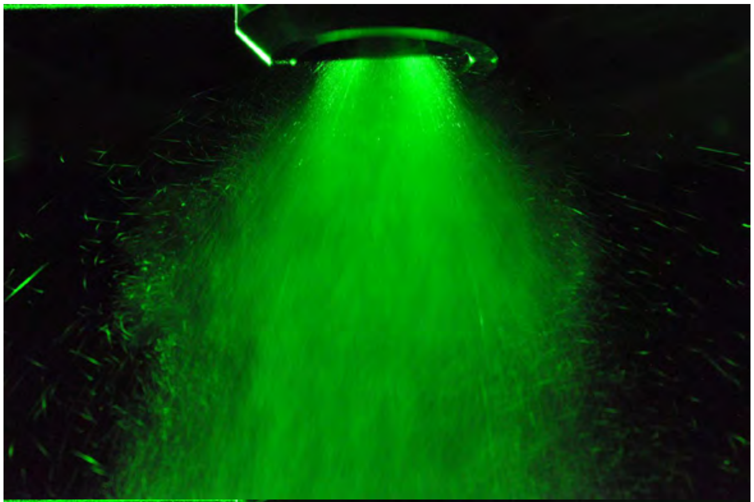
b) Alt Fuel



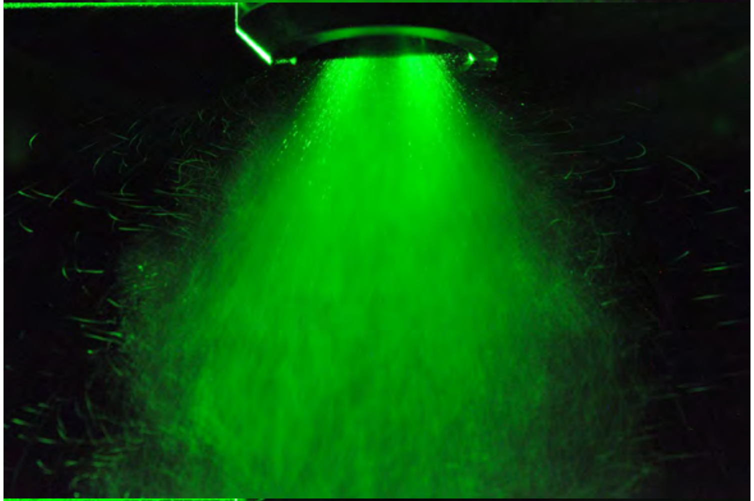
c) 7024 Fuel

B.8 Laser Sheet (1/200 sec) - dP/P=4%, F/A=0.050

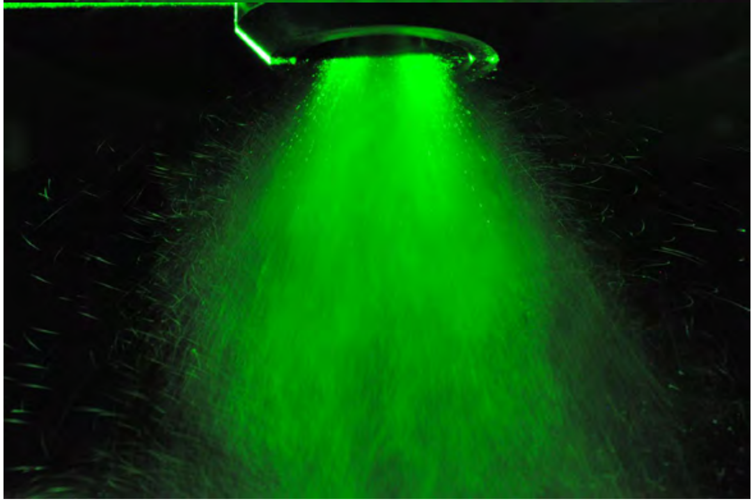
a) Jet A



b) Alt Fuel



c) 7024 Fuel

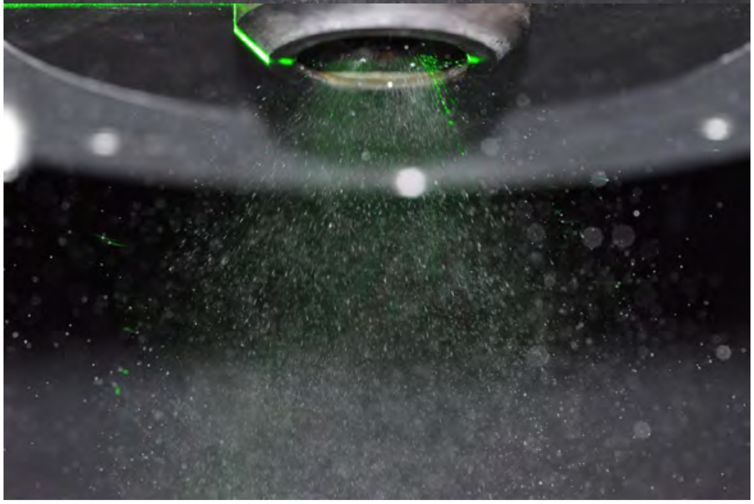


B.9 Flash - dP/P=2%, F/A=0.015

a) Jet A

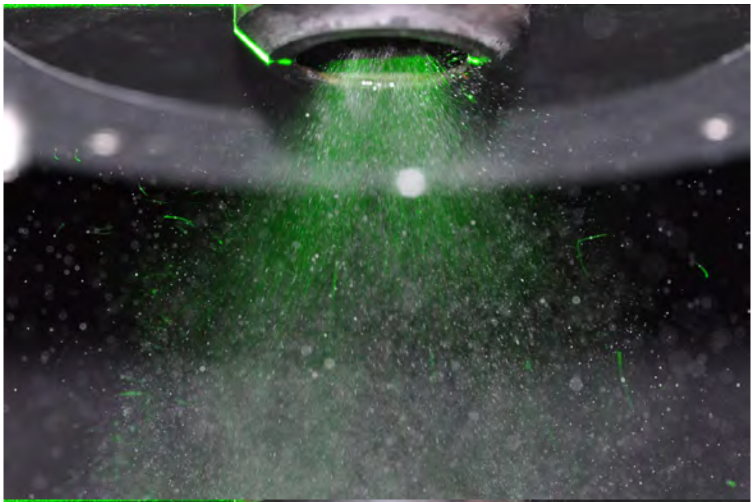
b) Alt Fuel

c) 7024 Fuel



B.10 Flash and Laser Sheet - dP/P=2%, F/A=0.015

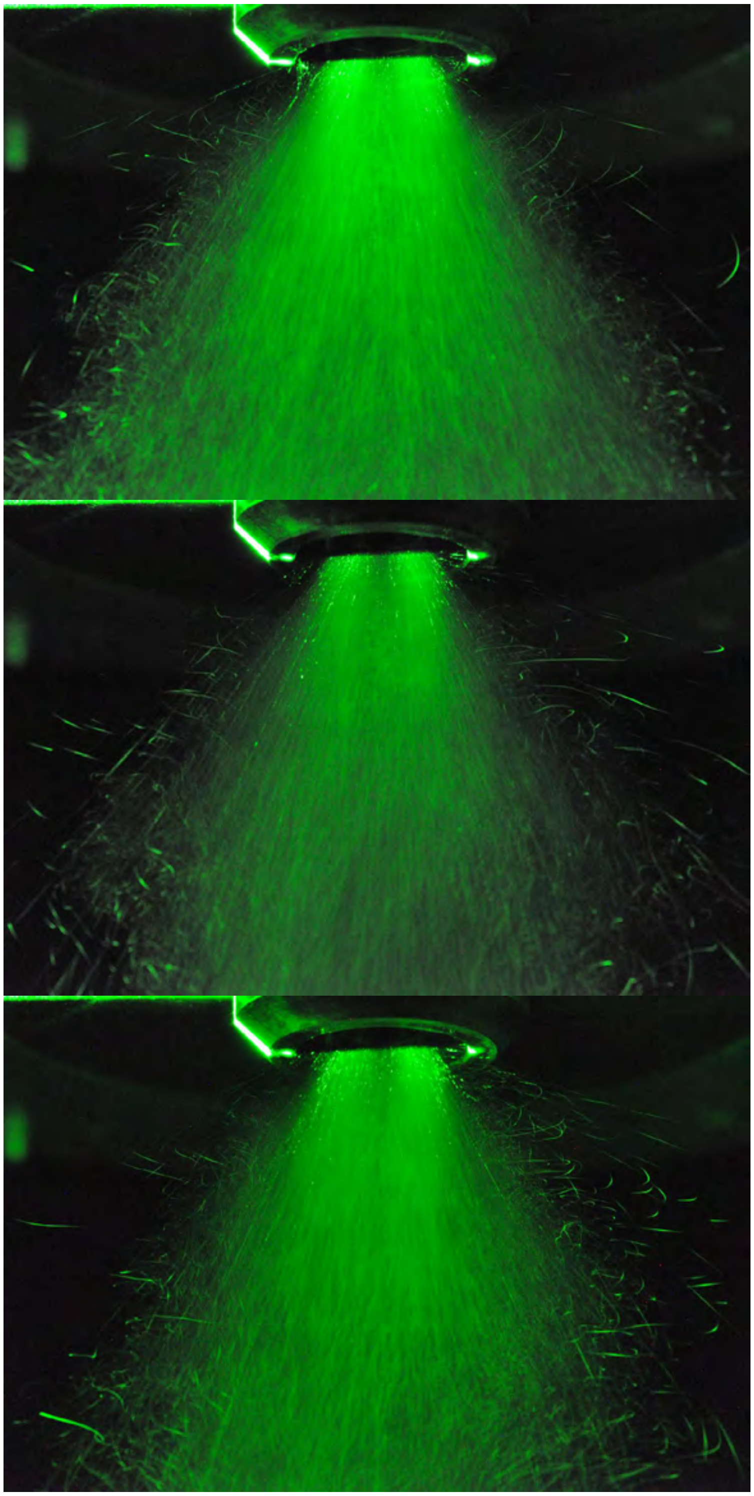
a) Jet A



b) Alt Fuel

c) 7024 Fuel

B.11 Laser Sheet (1/50 sec) - dP/P=2%, F/A=0.015



a) Jet A

b) Alt Fuel

c) 7024 Fuel

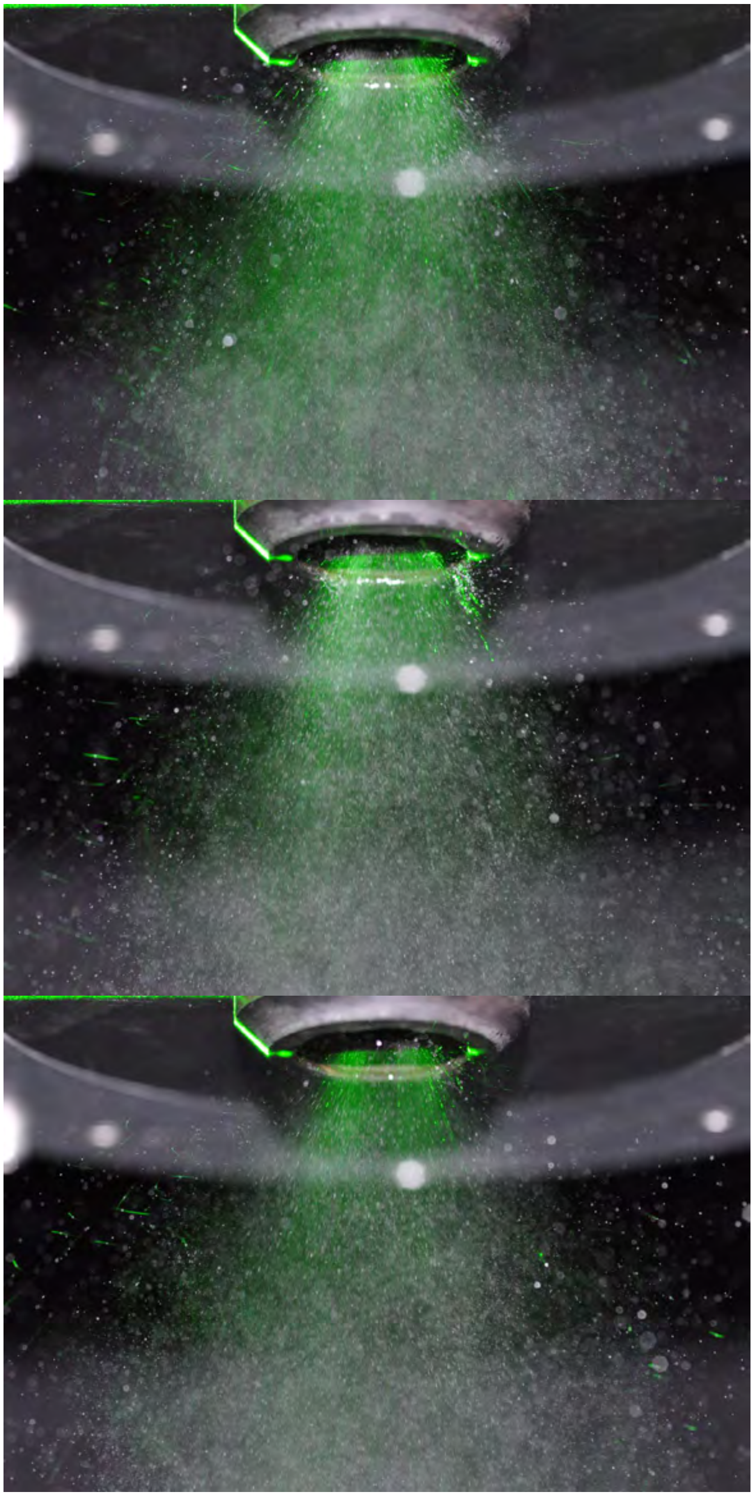
B.12 Flash - dP/P=2%, F/A=0.030

a) Jet A

b) Alt Fuel

c) 7024 Fuel

B.13 Flash and Laser Sheet - dP/P=2%, F/A=0.030



a) Jet A

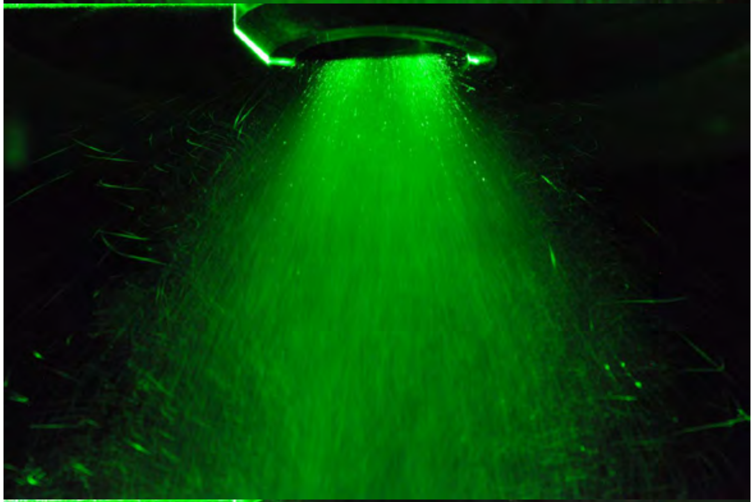
b) Alt Fuel

c) 7024 Fuel

B.14 Laser Sheet (1/50 sec) - dP/P=2%, F/A=0.030

a) Jet A

b) Alt Fuel



c) 7024 Fuel

Rolls-Royce Corporation
P.O. Box 420
Indianapolis, Indiana
46206-0420 USA

www.rolls-royce.com

APPROVED FOR PUBLIC RELEASE