COMPARATIVE EVALUATION OF SEMI-SYNTHETIC JET FUELS

FINAL REPORT

Prepared for

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EXECUTIVE SUMMARY

This report compares the properties and characteristics of five blends of individual synthetic paraffinic kerosenes with petroleum-based Jet A, Jet A-1 or JP-8 fuel to make semi-synthetic jet fuels (SSJF). The study was requested by the aviation fuel community to provide technical support for the acceptance of synthetic paraffinic kerosenes (SPK) derived from synthesis gas as blending streams up to 50%(v) in fuel specifications for aviation turbine fuel. The methodology for comparison was to be the properties and characteristics used in the original evaluation of the Sasol semi-synthetic jet fuel (SSJF) which has experienced 9 years of successful service since it was approved for use as commercial jet fuel by DEF STAN 91-91 in 1998.

The SPK used by Sasol in the original SSJF was produced by a Fischer-Tropsch (F-T) process using synthesis gas derived from coal. The synthesis gases for the four new candidates were produced from natural gas. The details of the F-T process conditions and the downstream processing differed among the five SPK fuels.

Although all five SPK fuels were comprised almost entirely of saturated hydrocarbons, i.e., normal, iso-, and cyclo-paraffins, there were distinct differences in the ratio of the three families and in the distribution of carbon numbers. Despite these differences, when blended at 50%(v) with conventional jet fuels, these five SPK fuels produced semi-synthetic jet fuels that were very similar to each other and had fit-for-purpose properties and characteristics that were very typical of conventional jet fuel. Moreover, all five SPKs met all of the requirements of Table 1 with the exception of density. It is important to realize there are no new chemical compositions involved in SSJF, just a change in the ratios of the aromatics to the saturates, i.e., the paraffin families.

It is believed that these five fuels covered a large range of SPK compositions likely to result from F-T catalysis of synthesis gas based on the ratios of the paraffin families and the variation in the range of carbon numbers.

It is concluded that semi-synthetic kerosenes produced by blending conventional jet fuels with up to 50%(v) SPK derived from synthesis gas by F-T catalysis and downstream processing and having compositions similar to that described in this report are fit-for-purpose as jet fuel. This conclusion has been validated by nine years of operation on one SSJF and in-depth flight-testing and test experience in ground support systems on another two of the five SSJFs evaluated here.

Based on the property data of the five SPKs evaluated, it was possible to develop a composition and performance based definition of SPK derived from synthesis gas through an F-T process that would assure that SSJF with up to 50%(v) such SPK would be fit-for-purpose as jet fuel and certifiable under major fuel specifications. This definition is based on meeting a modification of Table 1 requirements designed to assure that the producer has control over the processes for making SPK and to assure a minimum quality of product, both as an item of commerce and for making SSJF.

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Table of Contents

1. BACKGROUND	
2. OBJECTIVE	
3. APPROACH	
4. SPK FUELS OF CONSIDERATION	
5. COMPARISON OF SPKs	
5.1 Comparison of Synthetic Paraffinic Kerosenes	
5.2 Comparison of 50/50 Blends of SPK with Conventional Jet Fuel	9
5.2.1 Boiling Point Distribution	
5.2.2 Bulk Physical Properties	
5.2.3 Dielectric-Density Correlation	
5.2.4 Lubricity	
5.2.5 Electrical Conductivity	
5.2.6 Thermal Stability	
5.2.7 Storage Stability	
5.2.8 Alternate Test Methods	
5.2.9 Additive Compatibility	
5.2.10 Fuel Compatibility	
5.2.11 Water Solubility	
5.2.12 Elastomer Compatibility	
5.3 Summary of Comparison of Properties	
6. FLIGHT EXPERIENCE ON SSJF	
6.1 South African Airlines, Johannesburg, South Africa	
6.2 US Air Force	
6.3 Airbus	
7. DEFINITION OF SPK	
8. SUMMARY AND CONCLUSIONS	
9. RECOMMENDATIONS	
REFERENCES	
APPENDICES	

List of Figures

Figure 1. Hydrocarbon Composition of Five SPK Fuels Using GCxGC	5
Figure 2. Distribution of Hydrocarbons in Five SPK Fuels Using GCxGC	5
Figure 3. Boiling Point Distributions of SPK Fuels (D86)	6
Figure 4. Boiling Point Distributions of SSJF Blends	11
Figure 5. Kinematic Viscosity Characteristics of Five SSJF	12
Figure 6. Density Characteristics of Five SSJF	12
Figure 7. Specific Heat Characteristics of Five SSJF	13
Figure 8. Thermal Conductivity Characteristics of Five SSJF	13
Figure 9. Surface Tension Characteristics of Five SSJF	14
Figure 10. Bulk Modulus Characteristics of SSJF	14
Figure 11. Correlation of Density and Dielectric Constant for SSJF	15
Figure 12. Response of SSJF to Lubricity Improver Additive (DCI-4A)	16
Figure 13. Response of SSJF to Static Dissipator Additive	17
Figure 14. Effect of Blending on JFTOT Deposit Characteristics	
Figure 15. Peroxide Formation During Accelerated Storage (ASTM D3703)	19
Figure 16. Comparison of the Solubility of Water in Sasol SSJF	22
Figure 17. Effect of Sasol IPK on Properties of O-Ring Materials	25
Figure 18. Effect of S-8 on Properties of O-Ring Materials	
Figure 19. Effect of Sasol and Shell GTL Fuels on Properties of O-Ring Materials	27
Figure 20. Correlation of Boiling Range for SPKs	

List of Tables

Table 1.	Comparison of Resources and Process Used in Producing the Test SPKs	
Table 2.	Comparison of the Synthetic Paraffinic Kerosenes	
Table 3.	Slopes of the Boiling Point Curves for the SPK Fuels	6
Table 4.	Thermal Stability of SPKs	7
Table 5.	Analyses of Trace Organics and Sulfur in SPK Fuels	7
Table 6.	Analyses of Trace Metals in SPK Fuels	
Table 7.	Density and Freezing Points of SPK Fuels	
Table 8.	Properties and Characteristics of 50/50 Blends of the SPK and Jet Fuel	10
Table 9.	Slopes of the Boiling Point Curves for the SSJF Blends	11
Table 10	. JFTOT Breakpoint Temperatures of SPK Fuels	17
Table 11	. Gum Formation During Accelerated Storage at 100°C	19
Table 12	. Comparison of Alternate Test Methods for Determining Freezing Point	20
Table 13	Comparison of Alternate Test Methods for Determining Specific Energy	
Table 14	Aromatic Content of Fuels Used in Elastomer Compatibility Tests	22

1.0 BACKGROUND

Prior to the introduction of Sasol's semi-synthetic jet fuel (SSJF) at Johannesburg International Airport in July 1999, all commercial aviation fuel had been derived solely from conventional sources. The specifications controlling the quality of those fuels had evolved around the characteristics and properties of those fuels, assuming a relatively constant, or slowly evolving, range of crude resource and refining techniques. The Sasol request for the use of synthetic hydrocarbons derived from coal through their Fischer-Tropsch (F-T) processing was a significant departure from experience. Since many of the inherent properties of kerosenes that make them "fit-for-purpose" as jet fuels are not a part of the specification and quality control system and are rarely measured, the United Kingdom Aviation Fuels Committee (AFC), which guides the Defence Standard (DEF STAN) 91-91 [1] fuel specification for Jet A-1, developed a new set of guidelines for fuels containing synthetic products as blending stocks.

If accepted under DEF STAN 91-91, specific approved synthetic kerosenes can currently be used in concentrations up to 50%(v) providing there are at least 8%(v) aromatics in the final blend, all of which must come from the petroleum-derived blending streams.

Sasol iso-paraffinic kerosene (IPK) is the only synthetic kerosene that has been approved at the time of this writing. The blend with petroleum-derived jet fuel is termed semi-synthetic jet fuel (SSJF). The blend has been recognized by ASTM D1655 [2] as an acceptable fuel for commercial aviation to maintain compatibility with DEF STAN 91-91.

As currently written, any synthetic kerosene must be approved on an individual, site-specific basis. This puts the AFC, and other specification-writing bodies, in the position of having to approve every synthetic kerosene that is developed and offered for consideration – a time-consuming effort for all involved.

The Aviation Fuels Subcommittee of ASTM International is the cognizant body for the commercial jet fuel specification in the United States. The specification designating the jet fuel to be used in civil aviation is ASTM D1655, *Standard Specification for Aviation Turbine Fuels*. [2] However, ASTM has a policy that it does not approve products under its specifications. Instead, it provides the requirements that a fuel must meet to be certified for use.

Recognizing the growing interest in the United States and elsewhere in synthetic jet fuels from F-T processes, ASTM requested that the Aviation Committee of the Coordinating Research Council (CRC) develop a process to accept F-T kerosenes for use in jet fuel for civil aviation so that ASTM would not be in the position of having to approve individual candidate fuels. A Protocol for the Acceptance of Synthetic Fuels Under Commercial Specification was developed and is available on the CRC website. [3]

During the development of this acceptance protocol, it became apparent that the class of F-T kerosenes that contain no aromatic hydrocarbons may be sufficiently similar to the Sasol IPK that a general acceptance of these kerosenes as blending components might be considered. The aircraft-engine original equipment manufacturers (OEMs) requested a demonstration of the similarity of semi-synthetic fuels containing paraffinic F-T kerosenes. At that time, the synthetic

kerosene designated S-8 developed by Syntroleum for the US Air Force was the only other synthetic kerosene that had been analyzed and successfully flight-tested in a 50/50 blend. Properties and characteristics of a 50/50 blend of S-8 and JP-8 were compared and reported to be very similar in the CRC report on the approval protocol. [3]

Since the publication of that report, three other paraffinic fuels from F-T processes have been offered for evaluation to further solidify the belief that blends of these fuels are very similar to the original Sasol SSJF and form the foundation for the general acceptance in major jet-fuel specifications of synthetic paraffinic kerosenes from synthesis gas as blending stock up to 50% to make SSJF. Since the original Sasol IPK, these new synthetic kerosenes have been found to contain significant fractions of normal paraffins and a small fraction of cyclo-paraffins. Hence, the accepted terminology is now Synthetic Paraffinic Kerosene or SPK.

2. OBJECTIVE

The objective of this report is to compare the properties and characteristics of available synthetic paraffinic kerosenes (SPK) derived from synthesis gas and blends thereof with petroleum-based Jet A/A-1/JP-8 fuels. The purpose of the comparison is to define the acceptable range of compositions of SPK derived from synthesis gas that may be blended with conventional jet fuel to produce fit-for-purpose, semi-synthetic jet fuel

3. APPROACH

Four synthetic kerosenes representing different resources and processes are compared with the original Sasol IPK. The comparisons are made on the basis of the properties and characteristics used in the original approval process of the Sasol semi-synthetic jet fuel in accordance with the request of the engine OEMs.

Comparisons of the properties and characteristics of the 50/50 blends with petroleum-derived jet fuel are also made with conventional fuel using data from the CRC World Fuel Survey [4] where available and typical values from the CRC Handbook of Aviation Fuels [5].

Further information on flight experience is provided to support the general approval of SPK from synthesis gas for blending SSJF:

- Experience of South African Airlines using Sasol SSJF at OR Tambo International Airport, Johannesburg, South Africa
- US Air Force experience certifying the B52 aircraft on a 50/50 blend of S-8 with JP-8
- US Air Force experience with 50/50 blends of Shell GTL with JP-8 for engine tests and flight tests of C-17, B-1, F-15, and F-22 aircraft
- Experience of Airbus 380 flying on Blend of Shell GTL and Jet A-1

4. SPK FUELS OF CONSIDERATION

The five fuels compared in this study were all derived from synthesis gas using a Fischer-Tropsch process followed by downstream processing resulting in a kerosene fraction. However, the original resource for the synthesis gases differed, as did the F-T and downstream refining processes. The five SPK fuels are identified below; the first was derived from coal while the other four used natural gas as the source of the synthesis gas.

- 1. Sasol IPK: This coal-derived kerosene is used by Sasol to blend their semi-synthetic jet fuel. It was approved by DEF STAN 91-91 and has been supplied regularly at OR Tambo International Airport (formerly Johannesburg International Airport) since July 1999.
- 2. S-8: This fuel, derived from natural gas, was developed for the US Air Force by Syntroleum to demonstrate that a synthetic fuel could be made that met JP-8 specifications. Due to a concern over the need for aromatics and following the lead of the Sasol SSJF, it was used in 50/50 blends with JP-8 in the test flights of the B-52 leading ultimately to the certification of the B-52 on semi-synthetic jet fuel. A T-38 demonstration flight was planned for August 2008.
- 3. Shell GTL: This fuel was produced by Shell from natural gas at their gas-to-liquid (GTL) plant in Bintulu, Malaysia. It is currently being used by the US Air Force to certify more aircraft following the B-52 demonstration. 50/50 blends of the Shell GTL with JP-8 were used in a cross-country flight of a C-17, supersonic flights of both B-1 and F-15 aircraft, and an F-22 flight that included aerial refueling from a KC-135..
- 4. Sasol GTL-1: This fuel was a distillate cut from the GTL fuel currently produced by Sasol at the Oryx plant in Qatar. The plant is currently optimized for making diesel fuel, not jet fuel. As a result, the distillate cut was limited by the ability to make freeze point.
- 5. Sasol GTL-2: This fuel was made by isomerizing the Sasol GTL-1 to reduce the fraction of normal paraffins thus enabling a wider boiling range while still making freeze point.

A brief summary of the resources and processes used in producing these five SPK fuels is provided in Table 1. The down-stream processes following the F-T conversion process are considered typical of those found in conventional refineries.

SPK Fuel	Source Material	FT Process	FT Product	Refinery Processes to Make Kerosene
SASOL IPK	Coal	High temperature	C3 – C4 olefins	Oligamerization,
		Iron Catalyst	extracted from	hydrogenation, and
			C1 – C40 HC liquid	fractionation
Syntroleum S-8	Natural gas	Low temperature	C5 – C200+ paraffins	Hydrocracking
		Cobalt catalyst	and olefins	hydro-isomerization.
Shell GTL	Natural gas	Low temperature	Primarily C4 – C200 n-	Hydrocracking,
		Cobalt catalyst paraffins and olefinic isomer		isomerisation, and
			hydrocarbons	fractionation
Sasol GTL-1	Natural gas	Low temperature	Primarily C1 – C200 n-	Hydrocracking,
		Cobalt catalyst	paraffins and olefinic	hydrotreating, and
			hydrocarbons	fractionation
Sasol GTL-2	Natural gas	Low temperature	Primarily C1 – C200 n-	Hydrocracking,
		Cobalt catalyst	paraffins and olefinic	hydro-isomerization,
			hydrocarbons	and fractionation

Table 1. Comparison of Resources and Process Us	sed in Producing the Test SPKs
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Appendix A1 lists the jet-fuel specification properties for the five SPKs. These data demonstrate that the SPKs can be expected to meet all of the specification Table 1 requirements with the exception of density.

5. COMPARISON OF SPKs

The comparison of the properties and characteristics of the five SPK fuels is presented in two parts. The first compares pertinent properties of the SPKs themselves to identify important similarities and differences. The second comparison is of the 50/50 blends of each SPK with an appropriate petroleum-derived jet fuel, i.e., JP-8 for the S-8 and Shell GTL and Jet A/Jet A-1 for the commercial Sasol fuels.

5.1 COMPARISON OF SYNTHETIC PARAFFINIC KEROSENES

Table 2 provides a summary of the comparison tests that will be presented on the SPK fuels themselves as well as the figure or table associated with each comparison.

	Fuel Property or Characteristic	Location of Comparison
1	Hydrocarbon composition	Figure 1
2	Hydrocarbon distribution	Figure 2
3	Boiling point distribution (BPD)	Figure 3
4	Slope of BPD	Table 3
5	Thermal stability	Table 4
6	Trace organics and sulfur	Table 5
7	Trace metals	Table 6
8	Density and Freeze point	Table 7

 Table 2. Comparison of the Synthetic Paraffinic Kerosenes

The analyses of the five fuels were done at different times by different laboratories, using different methods. In each case, the methods were considered to be the best available at the time.

Figure 1 compares the hydrocarbon composition of the five fuels as determined by GCxGC analysis. Figure 2 shows how the hydrocarbon families are distributed by carbon number, also determined from GCxGC analysis. These fuels are primarily comprised of iso-paraffins and normal paraffins, with a very small fraction of cyclo-paraffins. Due to the processing differences, there are significant difference among the fuels in the spread of hydrocarbons as well as the ratio of normal to iso-paraffins and the presence of cyclo-paraffins. Sasol GTL-1 probably has the most normal paraffins that could be expected while still making freeze point requirements, while the Sasol IPK is at the other extreme with almost no normal paraffins. The Sasol GTL-2 range over 9-10 carbons numbers. Due to improved analytical techniques over the last ten years, the Sasol IPK has now been found to contain a significant fraction of cyclo-paraffins, typically in the range of 7 to 13%. The Shell GTL and the two Sasol GTLs typically have about 1% cyclo-paraffins.



Figure 1. Hydrocarbon Composition of Five SPK Fuels Using GCxGC



Figure 2. Distribution of Hydrocarbons in Five SPK Fuels Using GCxGC

Figure 3 compares the D86 boiling point distributions (BPD) of the 5 SPK fuels; the two fuels with the highest and lowest BPD from the CRC World Fuel Survey are provided for comparison. (Note: It is not expected that the SPKs would have BPD similar to full fuels since they are intended as blending streams; only the S-8 fuel was intentionally distilled to look like a conventional fuel.) As would be expected from the distributions of Figure 1, the Sasol IPK and Shell GTL fuels have relatively flat BPDs. Table 3 presents data comparing the slopes of the boiling point distributions with the highest and flattest slopes from the CRC World Fuel Survey. The S-8 and Sasol GTL-2 fuels have fairly typical slopes; the other three are relatively flat.



Figure 3. Boiling Point Distributions of SPK Fuels (D86)

SPK Fuel	$T_{50} - T_{10}$	T ₉₀ -T ₁₀
Sasol IPK	7 °C	29 °C
S-8	39 °C	89 °C
Shell GTL	7 °C	22 °C
Sasol GTL-1	17 °C	40 °C
Sasol GTL-2	30 °C	60 °C
CRC W Survey	14 to 42°C	55 to 85°C

Table 3. Slopes of the Boiling Point Curves for the SPK Fuels

One major characteristic of the SPKs is their very high thermal stability; all had JFTOT breakpoints over 340°C as shown in Table 4. This is due to the lack of reactive species, metals, and heteroatoms in the SPKs.

SPK Fuel	JFTOT Breakpoint, °C
Sasol IPK	>340
S-8	370
Shell GTL	370
Sasol GTL-1	>340
Sasol GTL-2	>340

Table 4. Thermal Stability of SPKs

The five SPKs were analyzed for trace organics and metals to evaluate the possibility of contaminants that could affect fuel quality. Table 5 presents a summary of the trace organics; all were essentially below the detection limit. Table 6 summarizes the metals analysis and compares the results with the few metals analyzed in the analysis of the CRC World Fuel Survey.

	Trace Material / Test Method					
SPK Fuel	Carbonyls as MEK, ppm	Alcohols as EtOH, ppm	Esters as KOH, ppm	Phenols, ppm	Acids, mg KOH/g	Sulfur ppm
Sasol IPK	<25	<100	<1	<1	0.001	<10
Sasoi IPK	E411	UOP 656	Sasol 2.72	Sasol H175	D3242	D2622
6.0	<20	<20	<20	<20	0.004	<100
S-8	HPLC	HPLC	HPLC	HPLC	D3242	D4294
Shell GTL	not	not	not	<50	0.001	<3
Shell GTL	detectable ^{1,2}	detectable ^{1,2}	detectable ^{1,2}	EPA 8270C	D3242	D2622
Sasol GTL-1	not	not	not	<50	0.021	<1
Sasol GIL-1	detectable ^{1,2}	detectable ^{1,2}	detectable ^{1,2}	EPA 8270C	D3242	D5453
Sasol GTL-2	not	not	not	<50	0.003	1.3
Sasor GTL-2	detectable ^{1,2}	detectable ^{1,2}	detectable ^{1,2}	EPA 8270C	D3242	D5453

 Table 5. Analyses of Trace Organics and Sulfur in SPK Fuels

Notes: 1. Volatile species – modified EPA 8015B; detection limit 5 ppm

2. Semi-volatile species – modified EPA 8260B; detection limit 50ppm

It can be seen that these five fuels are high-purity hydrocarbons; other organics and most metals were below the detection limit of the analysis. Metals and sulfur from the original resource, i.e., natural gas or coal, are separated out during the formation of the synthesis gas. Thus, the starting point of synthesis gas makes an excellent "fire wall" for any inorganic impurities. The various stages of hydrotreatment remove any oxygenates.

Issues that exist with the SPK are their low lubricity, low electrical conductivity, low density, and lack of aromatics. The first two are due to the absence of organics acids in the SPK fuels that are normally present in conventional fuel. Low density is due to the lack of aromatics and

cyclo-paraffins in SPK. Table 7 lists the densities of the SPK fuels showing that they are all below the minimum specification requirement of 775 kg/m³. It will be seen in Figure 6 that the low density of the SPKs can be a limiting factor in the blending ratio by causing the density of the blend to drop below the minimum density requirement for Jet A/Jet A-1/JP-8. This limiting blend ratio will depend upon the density of the petroleum fraction.

	Trace Metal Content, ppb					
Metal	Sasol IPK (ICP/MS)	S-8 (ASTM D7111)	Shell GTL (ASTM D5185)	Sasol GTL-1 (ASTM D7111)	Sasol GT	
Ag	na ¹	<100	<1000	<100	<100	na
Al	na	<100	<1000	<100	108	na
Ва	na	<100	<1000	<100	<100	na
Са	na	<100	<1000	<100	<100	0 - 42
Cr	na	<100	<1000	<100	<100	na
Cu	<10	14	<1000	<100	<100	0 - 195
Fe	10 - 50	<100	<1000	<100	<100	0 - 3
К	na	<500	<5000	<1000	<1000	na
Li	na	na	na	103	<100	na
Mg	na	<100	<1000	<100	<100	na
Mn	na	<100	<1000	<100	<100	0 - 103
Мо	na	<100	<1000	<100	<100	na
Na	na	<1000	<5000	<1000	<1000	na
Ni	na	<100	<1000	<100	<100	na
Pb	< 50	<100	<1000	<100	<100	na
Si	na	<100	<1000	3000	395	na
Ti	na	<100	<1000	<100	<100	na
V	na	<100	<1000	<100	<100	na
Zn	na	118 - 266	<1000	<100	<100	0 - 32

Table 6. Analyses of Trace Metals in SPK Fuels

1. na: fuel was not analyzed for this metal

Table 7. De	ensity and	Freezing	Points	of SPK Fuels
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SPK Fuel	Density@ 15°C, kg/m ³	Freezing Point, °C
Specification	775.0 (min.)	-40/-47/-47 ¹ (max)
Sasol IPK	768.8	<-65 (D2386)
S-8	755	-51 (D5972)
Shell GTL	736.1	-54 (D5972)
Sasol GTL-1	733.3	-49 (D2386)
Sasol GTL-2	761.6	-60 (D2386)

1. Jet A/Jet A-1/JP-8 limits, respectively

Also listed in Table 7 are the freezing points of the SPK fuels. All are lower than the specification limits. The freezing point is directly related to the fraction of normal paraffins in the SPK, but it also depends upon their carbon-number distribution (distillation end-point). The ratio of normal to iso-paraffins is a function of the hydro-isomerization process conditions for the SPK produced from F-T wax. The distillation end-point is controlled by the fractionation process.

In summary, the five fuels meet all the jet-fuel specification property requirements except for density. It is believed that this set of fuels represents a reasonable range of chemical composition and hydrocarbon distribution that would be expected of SPK kerosenes from synthesis gas and F-T processing. They are noted for their high thermal stability, lack of aromatics and sulfur, and their relatively low density. Those with low concentration of normal paraffins will have very low freezing points. Also, since SPKs have no natural anti-oxidants or electrical conductivity, appropriate additives should be considered for storage and handling.

It will be shown in the next section that the notable differences in paraffin ratios and carbon distribution have very little impact on the properties and characteristics of the 50/50 blends with the exception of density.

5.2 COMPARISON OF 50/50 BLENDS OF SPK WITH CONVENTIONAL JET FUEL

Each of the five SPK fuels was blended in a 50/50 ratio with a conventional fuel as follows:

- Sasol IPK/Jet A-1
- S-8/JP-8
- Shell GTL/JP-8
- Sasol GTL-1/Jet A
- Sasol GTL-2/Jet A

All of the 50/50 blends met all of the property requirements of the appropriate fuel specification with the exception of two blends that did not meet the minimum density requirements; this deficiency will be addressed later. Tables A2 to A5 in the Appendix compare the specification properties of each 50/50 blend with the relevant base fuel.

Table 8 provides a summary of the tests that were conducted on the 50/50 blends of each SPK with a conventional jet fuel. Following the convention used with the original Sasol blend, these fuels will now be termed semi-synthetic fuels (SSJF). In each case, the test method is provided along with the table or figure that shows the actual comparison for each property.

As previously noted, wherever possible, the properties of the five SSJF are compared to data from the CRC World Fuel Survey [4] and the CRC Handbook of Aviation Fuel Properties [5]. However, it must be recognized that the purpose of these data sources is to provide guidance on typical values and temperature functions. They do not define the limits of experience with petroleum fuels; other surveys, notable those by QinetiQ [6] and the Petroleum Quality Information System [7], provide evidence that many fuels lie outside the bounds of the CRC World Survey. It is not expected that all fuel properties will fall within the bounds of the World Survey or have exactly the same temperature sensitivity as the "max" and "min" examples. The data presented in the CRC Handbook are for a typical fuel; in many cases that may have been a

typical fuel of many years ago or may have been calculated values, not test data. It has been established that bulk physical properties of various jet fuels blend linearly.[8] Therefore, it is reasonable to expect that the SSJF blends will have properties and characteristics that are typical of conventional fuels as represented by these data sources.

Fuel Property or Characteristic		Test Method	Location of Comparison
1	Boiling point distribution	D86	Section 5.2.1; Figure 4
2	Slopes of boiling point distribution	D86	Section 5.2.1; Table 9
3	Viscosity vs temperature	D445	Section 5.2.2; Figure 5
4	Density vs temperature	D4052	Section 5.2.2; Figure 6
5	Specific heat vs temperature	E1269	Section 5.2.2; Figure 7
6	Thermal conductivity vs temperature	D2717	Section 5.2.2; Figure 8
7	Surface tension vs temperature	D1331	Section 5.2.2; Figure 9
8	Bulk modulus	D6793	Section 5.2.2; Figure 10
9	Density-dielectric constant	D924	Section 5.2.3; Figure 11
10	Lubricity	D5001	Section 5.2.4; Figure 12
11	Electrical conductivity	D2624	Section 5.2.5; Figure 13
12	Thermal stability Breakpoint	D3241	Section 5.2.6; Table 10
13	Deposit thickness	pending	Section 5.2.6; Figure 14
14	Storage stability Peroxides	D3703	Section 5.2.7; Figure 15
15	Gums	D5304	Section 5.2.7; Table 11
16	Alternate test methods Freezing	D2386	Section 5.2.8; Table 12
	point	D5972	
17	Alternate test methods Specific	D3338	Section 5.2.8; Table 13
	energy	D4529	
		D4809	
18	Additive compatibility	D4054/B	Section 5.2.9
19	Fuel compatibility	D4054/B	Section 5.2.10
20	Water solubility	D3241	Section 5.2.11; Figure 16
21	Materials compatibility Volume Swell	D471	Section 5.2.12; Figures 17 - 19
22	Hardness	D412	
23	Tensile strength	D2240	

Table 8. Properties and Characteristics of 50/50 Blends of the SPK and Jet Fuel

5.2.1 Boiling Point Distribution Figure 4 presents the boiling point distributions of the five SSJFs, and Table 9 presents the corresponding values for $[T_{50}-T_{10}]$ and $[T_{90}-T_{10}]$. The five fuels all have boiling point distributions that are quite normal when compared to the CRC World Fuel Survey and meet the specification limits, also provided on the graph. The values of $[T_{90}-T_{10}]$ for the blends made from Sasol IPK and from Shell GTL both lie outside the range of values from the CRC World Fuel Survey; however, both of these fuels have been flown with no apparent issues.



Figure 4. Boiling Point Distributions of SSJF Blends

Fuel	$T_{50} - T_{10}$	$T_{90} - T_{10}$
Sasol IPK/Jet A-1	14 °C	46 °C
S-8/JP-8	36 °C	83 °C
Shell GTL/JP-8	17 °C	35 °C
Sasol GTL-1/Jet A	22 °C	68 °C
Sasol GTL-2/Jet A	32 °C	70 °C
CRC World Survey	14 to 42°C	55 to 85°C

Table 9. Slopes of the Boiling Point Curves for the SSJF Blends

5.2.2 Bulk Physical Properties Figures 5 through 10 demonstrate that the bulk properties of all the SSJF have values and temperature functions that are very typical of conventional jet fuels. The one exception is in Figure 6 where the densities of the 50/50 blends made from Shell GTL and from Sasol GTL-1 are below the minimum specification requirement; these two SPKs have the lowest density as was shown in Table 7. Since density blends linearly, this demonstrates that, depending upon the density of the conventional fuel, it may not be possible to achieve a 50/50 blend with some SPK. Specification writing bodies may want to consider reducing the minimum density specification and/or placing a restriction on the minimum density of SPK.

In the original evaluation of the Sasol SSJF with IPK, the specific heat data was invalid; this was not discovered until after the test fuel was expended and the report had been written. Hence, no data is shown for that property of IPK/Jet A-1. During this investigation, it was not possible to obtain data on the thermal conductivity of the Shell and Sasol GTLs due to a malfunction in the test equipment at SwRI; an alternate test lab was located but did not respond in a timely manner. This report will be amended to include these data when they become available.



Figure 5. Kinematic Viscosity Characteristics of Five SSJF



Figure 6. Density Characteristics of Five SSJF



Figure 7. Specific Heat Characteristics of Five SSJF



Figure 8. Thermal Conductivity Characteristics of Five SSJF



Figure 9. Surface Tension Characteristics of Five SSJF



Figure 10. Bulk Modulus Characteristics of SSJF

In Figure 10, the data show that blending with SPK causes a slight reduction in the bulk modulus. This reduction is related to the lower aromatic content because they have a higher bulk modulus than paraffins. The reduction is less than the difference between the two base fuels and, therefore, should not be problematic. No data was available on the minimum requirement for bulk modulus. If such a limit can be identified, it should be compared with the bulk modulus of a zero-aromatic SPK to evaluate a possible lower limit on aromatic content.

All in all, the bulk physical properties of the SPK blends are very typical of conventional fuels.

5.2.3 Dielectric-Density Correlation The dielectric-density correlation is important because it is used in the tank gauging system to determine the density of the fuel. Thus, it is important that the correlation between density and dielectric constant be typical of conventional jet fuel. Figure 11 shows that the dielectric-density data for the five fuel blends blends are very typical of the correlation from the CRC World Fuel Survey. The multiple data points for the S-8, Shell GTL, and Sasol GTL blends were taken at different temperatures which changed the density; the data, therefore, show that the dielectric constant changed appropriately.



Figure 11. Correlation of Density and Dielectric Constant for SSJF

5.2.4 Lubricity There is a natural concern about the lubricity of synthetic jet fuels since, due to their purity, they do not contain the organic acids or other polar compounds that provide lubricity in conventional fuels. The lubricity of SSJF will be determined by the lubricity of the petroleum-derived component; however, since commercial jet fuel does not have a lubricity requirement, there is no guarantee that SSJF will have adequate lubricity without the use of a

lubricity-improver additive. For this reason, when the Sasol SSJF was approved by DEF STAN 91-91, a requirement was placed on the fuel for a maximum lubricity rating of 0.85 mm WSD (wear scar diameter). The JP-8 specification requires a maximum lubricity rating of 0.65mmWSD; a lubricity additive is required in JP-8 to ensure adequate lubricity for all military use. Thus, it is important to demonstrate that SSJF respond well to lubricity improvers in case the petroleum component does not have good lubricity. Figure 12 shows that all the SSJF respond well to DCI-4A, a common corrosion-inhibitor/lubricity-improver additive. Α concentration of only 5 mg/l is sufficient to reduce the BOCLE wear scar diameter by about 0.1 mm. Beyond 5 mg/l the response factor is less, but the lubricity is adequate by that point so it doesn't matter. This is much less than the maximum allowable concentration, so the response is considered to be very good. Only 1 point is shown for the S-8/JP-8 and Shell GTL/JP-8 blends because of the JP-8 requirement for a corrosion inhibitor/lubricity improver additive. Also shown in Figure 12 are data for the Sasol IPK and Shell GTL demonstrating that SPK themselves respond well to a lubricity improver additive.



Figure 12. Response of SSJF to Lubricity Improver Additive (DCI-4A)

5.2.5 Electrical Conductivity Figure 13 shows that the electrical conductivity of the SSJFs responds linearly to the static dissipator additive (SDA) Stadis 450. The effect of SDA concentration is not shown for the S-8/JP-8 and Shell GTL/JP-8 blends because JP-8 has a required concentration of 2 mg/L.



Figure 13. Response of SSJF to Static Dissipator Additive

5.2.6 Thermal Stability Thermal stability is not considered an issue with SPK fuels from synthesis gas due to the lack of impurities, i.e., hetero-atoms, sulfur compounds, etc. The breakpoint temperatures are generally not measurable as the temperature is beyond the useful temperature of the aluminum JFTOT tubes. Table 10 lists the JFTOT breakpoint temperatures of the SSJF being evaluated.

SPK Fuel	JFTOT Breakpoint Temperature, °C		
SPR Fuel	Neat SPK	50/50 Blend	
Sasol IPK	>340 ¹	>3001	
S-8	370	>325 ¹	
Shell GTL	370	290	
Sasol GTL-1	>340 ¹	285	
Sasol GTL-2	>340 ¹	295	

Table 10. JFTOT Breakpoint Temperatures of SPK Fuels

Note: 1. Testing stopped at indicated temperature

Figure 14 presents data showing the effect of blending SPK with conventional fuel on the JFTOT deposit thickness as measured with an ellipsometer. Each set of data gives the deposit depth at the associated temperature of the JFTOT tube. As the tube temperature increases, the deposit depth at the end of the test increases. The black line on the left is for the petroleum Jet A, while the two data sets down and to the right are for the two unblended SPKs from Sasol. The two

curves in the middle show the effect of blending on the deposit characteristics. These data suggest that SPK could be used to upgrade fuels that are marginal on thermal stability.



Figure 14. Effect of Blending on JFTOT Deposit Characteristics

5.2.7 Storage Stability During long-term storage, fuels are known to form peroxides and gums unless anti-oxidants are present. Petroleum-derived fuels generally contain natural anti-oxidants unless they are removed by hydrotreating. Because SPK fuels do not contain natural antioxidants, DEF STAN 91-91 requires that an anti-oxidant be added to fuels containing synthetic hydrocarbons. All military jet fuels containing blending stocks that have been hydrotreated are required to contain 17 to 24 mg/l of anti-oxidant. Sasol adds 20 mg/l of anti-oxidant to the IPK in their production SSJF; the same concentration was added to the Sasol GTL blends. Figure 15 presents the results of accelerated storage tests for peroxide formation; for this test, all fuels did contain an approved anti-oxidant. None of the fuels developed more than 5 ppm of peroxides during heated storage at 65°C. According to ASTM D4625, six weeks of storage at 64°C is equivalent to 96 weeks at an ambient temperature of 21°C, or almost 2 years. Currently, there are no peroxide requirements in any of the major jet-fuel specifications, but the US Navy's JP-5 specification used to have a limit of 8ppm. Using this as a guideline, none of the SSJF fuels would be expected to generate significant peroxides as long as an anti-oxidant is used. (Note that for maximum efficacy the antioxidant should be added as soon as possible when the SPK is made, e.g. to the run down line of the distillation tower).



Figure 15. Peroxide Formation During Accelerated Storage (ASTM D3703)

Similarly, the fuels were also evaluated for potential gum formation according to ASTM D873. The fuels, also containing the same levels of anti-oxidant, were stored at 100°C under 800kPa of oxygen for 16 hours, which is equivalent to 40 months at ambient conditions according to ASTM D5204, Appendix X1. The major fuel specifications for jet fuel limit existent gum to 7mg/100ml. The results presented in Table 11 show that none of the fuels would have reached a gum concentration of more than 2 mg/100ml in that time period; even after storage at 96 hours, the gum concentration was still under 7 mg/100ml for all the SSJF.

Table 11. Gum Formation During Accelerated Storage at 100°C

Fuel	Gum Concentration mg/100ml		
	16 Hours	96 Hours	
Sasol IPK/Jet A-1 ¹	1.9, 1.9	3.4, 4.5	
S-5/JP-5 ²	0.7 – 0.9		
Shell GTL	0.4		
Sasol GTL-1/Jet A	1.2	1.1	
Sasol GTL-2/Jet A	1.4	2.1	

Notes: 1. Two samples tested

2. No data for S-8; S-5 was made for the US Navy to simulate JP-5; it was similar to S-8 except for flash point

5.2.8 Alternate Test Methods There are two property areas where the demonstration that "technically equivalent" methods of property determination are an issue:

- methods of determining freezing point
- methods of determining specific energy

Two different methods are used to measure freezing point in the United States, ASTM D2386 (manual method) and ASTM D5972 (automatic method). A third method, ASTM D5901 (automated method) was discontinued in recent years; it has been modified and published as ASTM D 7154. The new method was not available for comparison of the Shell and Sasol GTL blends. Since these work on different principles, it is important that they provide similar results with the accuracy of the methods.

Table 12 compares the results of the two methods available. While the results do not agree exactly, they are within the repeatability and reproducibility factors of the methods.

	Freezing Point, °C			
Fuel	ASTM D2386 ASTM D5972		ASTM D5901	
	(Manua Method)	(Automatic Method)	(Automated Method)	
Sasol IPK/Jet A	-54.6	-55.3	-56.8	
S-8/JP-8	Not analyzed	-51.0	Not analyzed	
Shell GTL/JP-8	-58.0	-58.9	Not analyzed	
Sasol GTL-1/Jet A	-47.0	-48.5	Not analyzed	
Sasol GTL-2/Jet A	-50.0	-49.4	Not analyzed	

Table 12. Comparison of Alternate Test Methods for Determining Freezing Point

There are three acceptable methods for determining the specific energy of jet fuel in MJ/kg, or equivalent. The referee method for determining specific energy is the bomb calorimeter method of ASTM D4809. There are two methods for calculating specific energy: ASTM D3338 calculates specific energy from a correlation with density, aromatic content, and boiling point distribution with a correction for sulfur content; ASTM D4529 calculates specific energy on a sulfur free basis from a correlation with density and aniline point. Table 13 compares the results of the three methods for the five SSJF. Although the "technically equivalent" methods were developed around traditional fuels, they appear to be valid for the SSJF blends which in general will have lower aromatics, lower density, and essentially zero sulfur.

Test	Specific Energy, MJ/kg				
Test Method	Sasol IPK/Jet A-1	S-8/JP-8	Shell GTL/JP-8	Sasol GTL-1/Jet A	Sasol GTL-2/Jet A
D3338	43.28	43.52	43.7	43.5	43.6
D4809	43.20	43.32	43.5	43.6	43.7
D4529	43.35	NA	43.7	43.7	43.7

 Table 13. Comparison of Alternate Test Methods for Determining Specific Energy

5.2.9 Additive Compatibility Five standard additives used in military and commercial jet fuel were evaluated for solubility and compatibility issues:

- Anti-oxidant
- Lubricity improver
- Static dissipator additive
- Metal deactivator additive
- Fuel system icing inhibitor

The effectiveness of lubricity improver, static dissipator additive, and anti-oxidant has already been demonstrated. (See Figures 12, 13, & 15 and Table 8.) All additives were found to be soluble at twice the normal treat rate. There was no visible cloudiness or discoloration after 24 hours at both -17.8°C and 38°C. It was concluded that there are no compatibility issues with any of the common additives.

5.2.10 Fuel Compatibility Fuel compatibility was evaluated in a manner similar to the hot and cold storage evaluation of the additives. All five of the SPKs were blended 50/50 with both a Merox jet fuel and a hycdrotreated jet fuel. All ten blends were stored for 24 hours at both - 17.8°C and 38°C. In all cases at both conditions, there was no visible cloudiness, separation, discoloration, or particulate formation. It was concluded that the SPKs could be blended with any jet fuel and there would be no compatibility issues.

5.2.11 Water Solubility Figure 16 illustrates the effect of blending SPK into a jet fuel on the solubility of water; data was not available for the SSJF based on S-8 and on Shell GTL. In the three cases shown, the solubility of water is reduced by the addition of the SPK. This is reasonable since it is detergents, heteroatoms, and polar compounds that increase water solubility. Since the SPKs contain none of these, their natural concentration in the conventional jet fuel would be reduced. Therefore, it is concluded that the addition of SPK to any fuel will not cause problems with coalescers or monitors.



Figure 16. Comparison of the Solubility of Water in Sasol SSJF

5.2.12 Elastomer Compatibility Elastomer compatibility was based on property tests on Orings made of the three most common elastomer materials: nitrile (Buna-N), fluorosilicone, and fluorocarbon (Viton). The comparison of elastomer compatibility for the five fuels is the most subjective of the comparisons due to variations in testing procedures, possible differences in the actual compounds used within basic families of elastomers, and the apparent lack of definitive pass/fail criteria. As a reference, the aromatic contents of the fuels used in the elastomer testing is summarized in Table 14.

Test Fuel	Aromatic Content, %(v)
All SPKs	0.0
25/75 IPK/Jet A-1	15.0
50/50 IPK/Jet A-1	11.0
Jet A-1	18.7
50/50 S-8/JP-8	9.8
JP-8	18.8
50/50 Shell GTL/Jet A	8.1
Jet A	15.9
50/50 Sasol GTL-1/Jet A	7.3
50/50 Sasol GTL-2/Jet A	8.3
Jet A	17.7

 Table 14. Aromatic Content of Fuels Used in Elastomer Compatibility Tests

The elastomer testing for SSJF made from S-8 was part of a very extensive matrix of materials testing conducted by the US Air Force.[8] This testing involved essentially all metallic, elastomeric, and other non-metallic materials found on aircraft. Temperatures and soak times were chosen as considered appropriate for military aircraft, specifically the B-52 in preparation for flight tests. The tests on the original Sasol SSJF blended from IPK were conducted under conditions considered more normal for commercial aircraft using soak times of 14 days at 75°F. The S-8 blend tests were for 28 days at 165°F for nitrile, 225°F for fluorosilicone, and 325°F for fluorocarbon. The Air Force chose not to conduct compatibility tests on the more recent Shell GTL/JP-8 blend, having concluded the chemical differences between S-8 and Shell GTL were not significant.

Tensile strength was the only test property common to both the Sasol IPK and S-8 fuel blend evaluations. For the Sasol IPK, change in mass and thickness, and modulus of elasticity were evaluated. These can be related to change in volume, which was included in the Air Force tests with the S-8 fuel in addition to compression set and shore hardness.

Elastomer tests were then conducted on the Shell GTL and the two Sasol GTLs at SwRI using the same conditions that were used during the original Sasol IPK evaluation. A possible detriment was that no record was made during the IPK tests of the specific compounds used for each of the three elastomer families. It is possible the more recent tests on the Shell and Sasol GTLs used somewhat different compounds within each of the three elastomer families.

Selection of appropriate pass/fail criteria also presented a challenge. It was concluded that the most relevant data would be provided from a comparison of the SSJFs with conventional jet fuel relative to the effect on elastomer properties.

The results shown in Figure 17 from the original IPK evaluation show very little difference as increasing amounts of IPK are added to the base Jet A-1. The results of the evaluation of S-8 presented in Figure 18 show a larger fuel effect than the IPK tests, but this is may be due to the more extreme temperature conditions used. The most significant effect was on volume swell in the nitrile o-rings; the swell decreased as the aromatic content was reduced, as expected. The results of the more recent tests at SwRI on the Shell and Sasol GTLs are presented in Figure 19. The variation in tensile strength is similar to the S-8 results, about $\pm 10\%$ with no real fuel trend. There was essentially no effect on the hardness of any of the materials. Volume swell with the Sasol and Shell SSJF blends of about 5% are very comparable to that of the S-8 blend. Likewise, the swell with the 100% GTLs was always less than the SSJF blends in line with the reduced aromatic content.

Despite the variations in test conditions and properties, the data on elastomer compatibility show that volume swell is the only property affected by the SPK and their blends. As expected, volume swell is basically related to the aromatic content. Since the primary concern is lack of swell, these data show that there should be little concern with any SSJF that has an aromatic content of at least 8%. This is supported by 9 years of flight experience as well as the more limited flight experience of the US Air Force. Research is still needed to determine the actual lower allowable limit for aromatic content.

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Figure 17. Effect of Sasol IPK on Properties of O-Ring Materials



Figure 18. Effect of S-8 on Properties of O-Ring Materials



Figure 19. Effect of Sasol and Shell GTL Fuels on Properties of O-Ring Materials

100

90

-No fuel soak



■ No Fuel soak

Shell GTL/JP-8

Sasol GTL-1/Jet A

Jet A

Sasol GTL-2/Jet A

Sasol GTL-1

Shell GTL

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5.3 SUMMARY OF COMPARISON OF PROPERTIES

The data presented above demonstrate that when the four new SPK fuels are blended at a 50/50 ratio with a conventional jet fuel, each of the resultant fuels has properties and characteristics that are very similar to the Sasol semi-synthetic fuel and moreover, very typical of conventional jet fuels when compared to the data from the CRC World Fuel Survey. It is safe to conclude that SSJF with less than 50% SPK will also have typical properties and characteristics.

Variations in the bulk physical properties are due primarily to changes in the ratios of the paraffin types (isomers). It is important to keep in mind that there are no new chemical compositions involved in SSJF – only a change in the proportions of the major hydrocarbon families and a reduction in trace materials such as sulfur, metals, and organics. It must be recognized that there are wide variations in the proportions of hydrocarbon families among conventional fuels due to crude sources and refining processes. These variations naturally lead to variations in fuel properties; for example:

- Reducing aromatics increases specific heat but reduces thermal conductivity, bulk modulus, viscosity, and density.
- Increasing the fraction of iso-paraffins lowers the viscosity and freezing point.

With the exception of viscosity, the bulk physical properties are linear with temperature and blend linearly. Viscosity is a complex log-log function with temperature; that functionality appears to blend linearly away from the freezing point. The reason is that all hydrocarbons, at least in the distillate range, have essentially the same temperature sensitivities for any given bulk property. The final value of a bulk property for any fuel is simply due to the blending ratios of the individual hydrocarbons.

Thus, since the SPKs are high-purity hydrocarbons in the kerosene boiling range, it is safe to conclude that they will have the bulk physical properties with the same values and temperature sensitivities as conventional, petroleum-derived fuels of the similar hydrocarbon composition.

Most of the other fit-for-purpose characteristics are related, either positively or negatively, to the presence of trace organics, metals, and/or hetero-atoms, materials which are reduced as SPK is added.

- The dielectric constant of the SSJFs was shown to have the same correlation with density as conventional fuels.
- The thermal stability is improved with the addition of the SPK.
- Water is somewhat less soluble after blending with SPK.
- Lubricity and electrical conductivity are reduced by the addition of SPK and will be controlled by the base fuel; both respond well to additives if necessary.
- Storage stability was not an issue, but all of the SSJF contained anti-oxidant (AO); AO was shown to be necessary in the original IPK study and should be continued with SSJF.
- There are no compatibility issues with either additives or other fuels. All conventional additives are soluble and effective in SSJF as with conventional fuel.
- The alternate test methods for freezing point and specific energy are valid for the SSJFs.

The only remaining issue is the question of elastomer compatibility. It was shown that blending SPK into conventional jet fuel had little or no significant effect on hardness, tensile strength, and elasticity – all properties that are considered to be measures of fluid compatibility by seal companies.[10] The major concern of the industry is that of volume swell, which is known to be affected by the presence of aromatics in the fuel, especially for nitrile elastomers. Generally, the SSJFs produced less swell than the base fuels and more swell than the SPKs alone. The concern is what might happen if fuels with very low aromatic content, i.e., approaching zero, are introduced into old aircraft with aged seals – will they shrink and start to leak? At present there are no data to answer this question. To alleviate any concerns, a minimum of 8%(v) was imposed on the aromatic content of the Sasol SSJF when approved by DEF STAN 91-91. Until further data is provided to answer this question, a minimum of 8%(v) aromatics should be required for SSJF.

6. FLIGHT EXPERIENCE ON SSJF

This section presents a summary of the flight and testing experience on three of the five fuels evaluated thus validating the results of the fit-for-purpose tests presented above.

6.1 SOUTH AFRICAN AIRLINES, JOHANNESBURG, SOUTH AFRICA

Over the last nine years there has been a considerable amount of flying on semi-synthetic jet fuel. By far the most of this has been on international and domestic flights out of Johannesburg, South Africa where the Sasol SSJF has been continuously supplied since July 1999. Sasol uses their IPK to augment the jet-fuel production from their local petroleum refinery. The blend ratio has varied over the years depending on the availability of the petroleum-derived fuel. The average has been around 20%, but has been in the 45 to 50% range for extended periods of time during refinery shutdowns. The IPK and Jet A-1 being used in these blends are the same as were used in the approval evaluation and, hence, the data presented here. The Operations Manager of South African Airlines has stated that the use of the Sasol SSJF has been totally transparent and that there have been no issues with air worthiness, safety, maintenance, or storage and handling when mixed with jet fuel from other sources in bulk storage tanks.

6.2 US AIR FORCE

During the Summer and Fall of 2006, the US Air Force successfully conducted a 50-hour engine test on a TF33 engine leading to flight tests and cold weather tests on B52 aircraft using the 50/50 blend of S-8 and JP-8. Based on the results of the tests with S-8 blends, the Air Force has certified the B-52 for flight on SSJF. The data presented here for S-8 and S-8/JP-8 were developed on the same fuels that were used for the engine tests and flight demonstrations of the B-52.

In December the US Air Force conducted a transcontinental flight with a C-17 Globemaster III using a 50/50 blend of the Shell GTL with JP-8. The C-17 has now also been certified to fly on SSJF. In March 2008, the US Air Force conducted the first supersonic flight SSJF with a B-1 Lancer using the same Shell GTL to blend the fuel. In August 2008, the US Air Force began flight tests of the F-15 and F-22 fighters using 50/50 blends of the Shell GTL with JP-8. The F-15 was flown at speeds greater than Mach 2 on the blend, while the F-22 tests included aerial
refueling from a KC-135 Stratotanker. The US Air Force did not conduct as much testing on the Shell GTL blends as they did with the S-8 because they considered the Shell GTL to be very similar to the S-8 that was tested so extensively.

Thus far, the Air Force certification process has detected no significant differences in performance, flight safety, durability, ground handling or storage between either the S-8/JP-8 or Shell GTL/JP-8 blends and conventional JP-8. Further testing is planned with the goal of certifying every engine and aircraft in the Air Force inventory by 2011 on semi-synthetic jet fuel.

6.3 AIRBUS

In February 2008, an Airbus 380 powered by Roll-Royce Trent 900 engines made a three-hour flight from Filton, UK to Toulouse, France on a SSJF blended with a Shell GTL that was very similar to the fuels tested by the US Air Force.[11] The fraction of GTL was limited to 37.4%, however, in order to meet the minimum density requirement. The demonstration flight included accels and decels as well as two altitude windmill airstarts.

Analysis of the data recorded while the aircraft was fuelled and during the flight, and from materials testing, showed that the use of the GTL blend had no adverse effect on the engine, aircraft systems or materials. Airbus concluded that the fuel behaved like a conventional Jet A-1 kerosene. Airbus supports the incorporation of SPK into the commercial fuel specifications for 50/50 blends.

All three organizations that have flight and engine test experience have reported no adverse affects on engine and aircraft systems or on storage and handling with ground systems. They have all concluded that SSJF should be included in the major fuel specifications, both commercial and military.[10]

7. DEFINITION OF SPK

The above results demonstrate and validate that a jet fuel containing up to 50% SPK produced from synthesis gas will have chemical and physical properties and characteristics that are typical of jet fuels on the world market and therefore, fit-for-purpose as jet fuel. It now becomes important to develop a working definition of such SPK fuels that can allow them to be incorporated into a fuel specification and available as an item of commerce. Such a definition should provide satisfactory limits on properties and ensure a quality so as to be able to guarantee that blends up to 50% will be not only certifiable but fit-for-purpose.

It is assumed here that the SPK is derived from synthesis gas through an F-T process followed by conventional downstream processing to produce a distillate in the kerosene boiling range. The resource used to produce the synthesis gas is immaterial; it may be bio-mass, coal, or natural gas. If processed correctly, the SPK should have the following characteristics:

- Comprised of saturated hydrocarbons, i.e., normal, iso-, and up to 15%(v) cyclo-paraffins
- Near-zero sulfur, organics, and metals
- Very high thermal stability
- Acceptable bulk physical properties, with the exception of density.

The following potential characteristics could create issues or problems if they are not controlled:

- Peroxide formation in storage
 - Control with an anti-oxidant in the SPK
- High freezing point depending on the concentration of normal paraffins
 - $\circ\;$ Should be limited to the same as the fuel specification.
- Potential presence of trace reactive organics, metals, and olefins
 A thermal stability limit will control these
- Potential presence of non-saturated hydrocarbons, i.e., aromatics and olefins
 - Aromatics should be controlled by analysis, e.g., ASTM D2425
 - Olefins will be controlled by thermal stability as above
- Low lubricity
 - o Control with an additive in the SPK if necessary

It is believed that controlling these items will be sufficient to control the quality of SPK produced from synthesis gas for the objective of making an SSJF that is fit-for-purpose providing the SPK has a significant boiling-point distribution. A very narrow-cut such as a pure solvent is not desirable since a high concentration could result in characteristics that are not typical of conventional fuels, e.g., a discontinuous boiling-point distribution.

A limit on the minimum value for $[T_{90}-T_{10}]$ can be use to ensure an adequate boiling-point distribution. The Sasol IPK and the Shell GTL have the two narrowest boiling ranges as shown in Figure 2 and Table 3. Since there has been significant flight and test experience with these two SPKs as 50/50 blends, using their boiling range as a minimum acceptable limit will cause no issues with regards to flight worthiness.

Figure 20 demonstrates the significance of using $[T_{90}-T_{10}]$ as a control for boiling range. The inset is a composite of the carbon number distribution for the five SPKs from Figure 2, i.e., all the families of a given carbon number are summed into a single value. The major graph then presents a correlation of $[T_{90}-T_{10}]$ with the number of "significant carbon numbers" in the distribution, where a "significant carbon number" is defined as having at least 10% of the fuel mass. A least-Squares fit to these data has an r²=0.90, so it is significant. It appears from this correlation that a minimum value of $[T_{90}-T_{10}]$ of 22°C will provide a distribution that has a width of at least four significant carbon numbers.



Figure 20. Correlation of Boiling Range for SPKs

Based on these arguments, the following is thought to be an adequate definition of SPK derived from synthesis gas using an F-T process and downstream processing, regardless of the original resource for the synthesis gas, i.e., bio-mass, coal, or natural gas:

- 1. SPK should meet relevant fuel-specification property requirements, i.e., Table 1, with a few modifications as noted in the following. This will provide assurance that the SPK product is essentially a jet fuel. It might be possible to eliminate some of the elements of Table 1.
- 2. The density of the SPK should be in the range of 730 to 770 kg/m³, also to ensure the SPK composition is similar to those evaluated and approved.
- 3. The cyclo-paraffins in the SPK should be limited to 15% to ensure the composition is similar to that which has been evaluated and approved.
- 4. No detectable aromatics by ASTM 5186 (<0.1%) or possibly D2425 (<0.5%). This will help ensure the refiner has control over the F-T and downstream processes to make SPK.
- 5. Require passing a JFTOT test conducted at 335°C. This will help ensure there has been a sufficient amount of hydrotreating so as to preclude the presence of organics, unsaturated compounds, catalytic metals, and other reactive species that could affect stability.
- 6. Sulfur should be less than 10 ppm. Again, this acts as a guarantee against contaminants.

- 7. An anti-oxidant should be required for the SPK to prevent peroxide formation in storage. This will preclude a new requirement for an anti-oxidant in the major fuel specification.
- 8. Finally, in addition to meeting the common requirements for boiling-point distribution of Table 1, a limit on $[T_{90}-T_{10}] \ge 22^{\circ}C$ will provide assurance that the SPK is not just a single compound but spread over at least 3 significant carbon numbers.

A few supplemental comments on SPK:

- 9. It may not be necessary to provide an upper limit to flash point. If the flash point is higher than that of the certified base fuel into which the SPK is blended, the flash point of the base fuel will control that of the blend. If the flash point of the SPK is lower, but still above 38°C, there is no issue.
- 10. A lubricity control may not be needed. The lubricity of the final blend will be controlled by the certified base fuel into which the SPK will be blended. If it is a military fuel, a lubricity additive will be present. Commercial fuels do not currently have a lubricity requirement.
- 11. The mutual densities of the SPK and the base fuel will determine the maximum amount of SPK that can be used without exceeding the minimum density of the final blend. It should not be necessary to control the density of the SPK unless it is desirable to always be able to go to a 50% blend.

It is believed that any SPK produced from synthesis gas, regardless of the initial resource, i.e., bio-mass, natural gas, or coal, through an F-T catalysis and downstream processing and meeting the definition described herein can be blended up to 50%(v) with petroleum-derived kerosene to produce a semi-synthetic jet fuel that is fit-for-purpose and can be certified as jet fuel under any of the major fuel specifications. The only limitation might be that meeting minimum density requirement will limit the amount of SPK that can be used. Note that this limitation has the benefit of rendering unlikely the possibility that a certified SPK containing jet fuel might be field blended again with 50% SPK resulting in a 75% SPK jet fuel – it simply would not meet the minimum density specification.

The only other limitation on the final blend would be the question of a minimum aromatic content.

8. SUMMARY AND CONCLUSIONS

Four new synthetic paraffinic kerosenes have been made available to make semi-synthetic jet fuels for comparison with the original Sasol semi-synthetic jet fuel that has been in continuous use in South Africa for 9 years. These four new SPKs were derived from synthesis gas using a Fischer-Tropsch process to produce a waxy syn-crude, a hydro-cracking step, and downstream refining. The resource used for the synthesis gas was natural gas rather than coal as used by

Sasol in producing IPK for their SSJF produced in South Africa. Also, the F-T process and the downstream processing for the four new fuels were different than that used for IPK.

Although all five SPKs, including the original Sasol IPK, were comprised almost entirely of saturated hydrocarbons, i.e., normal/iso-/cyclo-paraffins, there were distinct differences in the ratio of the three families and in the distribution of carbon numbers. Despite these differences, when blended at 50%(v) with conventional jet fuels these five SPK fuels produced semi-synthetic jet fuels that were very similar to each other and had fit-for-purpose properties and characteristics that were very typical of conventional jet fuel. It is important to realize there are no new chemical compositions are involved in these SSJF, just a change in the ratios of the aromatics to the saturates, i.e., the paraffin families.

It is believed that these five fuels represent as broad a range of composition and properties that are likely to occur in SPK, based on the ratios of the paraffin families and the variation in the range of carbon numbers. It is therefore concluded that semi-synthetic kerosenes containing up to 50% synthetic paraffinic kerosenes derived from synthesis gas, like those evaluated here, are fit-for-purpose as jet fuel. This conclusion has been validated by nine years of operation on one SSJF and in-depth flight-testing and experience in ground support systems on another two of the five SSJFs evaluated here.

Based on the property data of the five SPKs evaluated, it was possible to develop a definition of SPK produced from synthesis gas through an F-T and downstream processes that would assure that SSJF containing up to 50%(v) of such SPK will be fit-for-purpose as jet fuel and certifiable under major fuel specifications.

9. RECOMMENDATIONS

The data presented in this study support a recommendation that synthetic paraffinic kerosenes produced from synthesis gas using Fischer-Tropsch catalysis, hydrocracking or hydrotreating, and fractionation and meeting the requirements defined above in Section 7 be approved by the major fuel specifications for blending up to 50%(v), subject to the minimum density requirement. The resultant fuel will then be certified without special designation, i.e., as D1655, etc.

Other restrictions to consider are a minimum aromatic content of 8%(v) and a lubricity requirement.

- The restriction on aromatics is to alleviate concerns about seal swell until research determines the actual need and defines the lower limit if necessary.
- Lubricity may not be an issue with SSJF because the lubricity will be defined by the petroleum-derived component.

Finally there are many alternative sources and processing schemes that can result in synthesized paraffinic kerosenes of composition similar to those evaluated in this report. Important progress can be made in helping the aviation industry to reduce its carbon footprint by expanding these evaluations to include bio-derived materials. It is quite likely that those other paraffinic

kerosenes will have many, if not all, of the same properties and characteristics as the SPKs evaluated in this study, and will be fit-for-purpose. While it was not within the scope of this study to expand the conclusions to other SPK which have not been evaluated, it is believed that this study provides a roadmap for the evaluation and approval of SPK from other sources by defining of what is expected of an SPK that can be used to produce SSJF, including the tests to be conducted and the acceptable limits on the results.

10. RESEARCH NEEDS

There is a fundamental lack of understanding about aromatics in jet fuel – whether they are necessary and, if so, at what minimum level. Answering these questions is important for the use of paraffinic kerosenes in semi-synthetic fuels because the minimum aromatic content is one of the limiting factors on the concentration of SPK that can be blended with a given jet fuel.

The most urgent need is an understanding of the role of jet fuel and its aromatic content in the design and performance of seals, o-rings, self-sealing bladders, adhesives, etc. It is known that nitrile elastomers are affected by aromatics in the fuel. For example, nitrile o-rings swell in the presence of aromatics and the amount of swell is linear with the aromatic content. It is known that designers of fuel systems do not require any swell. The seal systems are designed to seal when initially assembled. It is thought that the presence of aromatics may be required to prevent shrinkage of older seals that may have taken some plastic set and which would leak upon shrinkage. Much of the evidence seems anecdotal and most of the existing data are on new materials. As difficult as it may be, test data are needed on aged materials that may have taken some plastic set.

Also, there is not a sufficient understanding of the role of trace materials, i.e, metals and organics, on the overall quality of jet fuel. An improved understanding should make it easier to expand the coverage to other SPKs, including those derived from bio-materials, and other synthetic fuels in general as well as the evaluation of additives and contaminants.

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APPENDICES

A1. Specification Properties of IPK and S-8

A2. Effect of 50/50 Blend of Sasol IPK on Specification Properties of Base Jet A-1 Fuel (Sasol)

A3. Effect of 50/50 Blend of S-8 on Specification Properties of Base JP-8 Fuel (Edwards AFB)

A4. Effect of 50/50 Blend of Shell GTL on Specification Properties of Base JP-8 Fuel (Dyess AFB)

A5. Effects of 50/50 Blends of Sasol GTL-1/-2 on Specification Properties of Base Jet A Fuel (SwRI)

Line No.	Property	Limits	IPK	S-8	Shell GTL	Sasol GTL-1	Sasol GTL-2	
COMP	COMPOSITION							
1	Acidity, mg KOH/g	0.015 (max)	0.004	0.004	0.003	0.002	0.003	
2	Aromatics, v%	25.0	0.5	0.0	0.2	0	0	
3	Mercaptan sulfur, m%	0.003 (max)	< 0.001	0.000	< 0.0003	0.0001	0.0001	
4	Total sulfur, m%	0.03 (max)	< 0.001	0.002	< 0.01	< 0.01	< 0.01	
5	Hydrogen content, m%	Report	15.1	15.4		15.2	14.7	
VOLA	FILITY	•						
6	Initial boiling point, °C	Report	174	144	154.1	144	179	
7	10% recovered, °C	205 (max)	181	167	160.8	153	196	
8	20% recovered, °C	Report	182	177	162.3	157	204	
9	50% recovered, °C	Report	188	206	168	170	226	
10	90% recovered, °C	Report	210	256	183.3	194	256	
11	Final boiling point, °C	300 (max)	232	275	195.2	208	266	
12	Residue, %	1.5 (max)	1.4	1.5	1	0.4	0.4	
13	Loss, %	1.5 (max)	0.4	0.9	1	1.0	0.6	
14	Flash point, °C	38 (min)	53	45	43	48	70	
15	Density @ 15°, kg/m ³	771 - 836	765*	756*	736*	735*	762*	
FLUID								
16	Freezing point, °C	-47 (max)	<-65	-51	-53.8	-52.5	-62	
17	Viscosity @ -20°C, cSt	8.0 (max)	3.23	4.9	2.49	2.43	6.09	
COMB	USTION							
18	Net heat of combustion, kJ/kg	42.8 (min)	44.0	43.9	44.2	44.3	44.2	
19	Smoke point, mm	25 (min)	42	42	>50	29	28	
20	Naphthalenes, v%	3.0 (max)	0	NR	0	NR	NR	
CORR	OSION							
21	Copper strip, 2hrs @ 100°C	1 (max)	1A	1A	1A	1A	1A	
22	Silver strip	2 (max)	0	NR	NR	NR	NR	
THER	MAL STABILITY							
23	Filter pressure drop, mm Hg	25 (max)	0	0	0	0	0	
24	Tube deposit rating @ 260°C	<3	<1	1	1	<1	<1	
CONT	AMINANTS							
25	Microseparometer wo SDA	70 (min)	NR	NR	NR		98	
26	Microseparometer w SDA	85 (min)	95	NR	99	97		
27	Existent gum, mg/100mL	7 (max)	0.6	0.6	4.2	0.9	0.6	
28	Particulate matter, mg/L	1.0	NR	1	NR	<0.1	<0.1	
29	Filtration time, minutes	15	NR	10	NR	NR	NR	
30	Water reaction	1B	1B	1	NR	NR	NR	
OTHE	OTHER TESTS							
31	Conductivity, pS/m	150 - 600	NR	456	180	292	<1*	
32	Lubricity, mm WSD	0.85 (max)	0.76	0.58	0.92	NR	NR	

A1. Table 1 Specification Properties of SPK Fuels

* does not meet specification requirement

Line No.	Property	Limits	Base Jet A	Jet A-1/Sasol IPK (50/50)			
COM	COMPOSITION						
1	Acidity, mg KOH/g	0.015 (max)	0.003	0.002			
2	Aromatics, v%	22.0	18.7	11			
3	Mercaptan sulfur, m%	0.003 (max)	0.001	0.001			
4	Total sulfur, m%	0.03 (max)	0.21	0.11			
5	Hydrogen content, m%	Report	14.09	14.61			
VOLA	VOLATILITY						
6	Initial boiling point, °C	Report	160	170			
7	10% recovered, °C	205 (max)	180	183			
8	20% recovered, °C	Report	186	186			
9	50% recovered, °C	Report	203	197			
10	90% recovered, °C	Report	241	232			
11	Final boiling point, °C	300 (max)	268	257			
12	Residue, %	1.5 (max)	1.2	1.0			
13	Loss, %	1.5 (max)	0.7	0.5			
14	Flash point, °C	38 (min)	47	52			
15	Density @ 15° , kg/m ³	771 - 836	800.5	784.4			
FLUI	DITY						
16	Freezing point, °C	-47 (max)	-49	-54.6			
17	Viscosity @ -20°C, cSt	8.0 (max)	4.1	4.35			
COM	BUSTION						
18	Net heat of combustion, kJ/kg	42.8 (min)	43.4	43.6			
19	Smoke point, mm	25 (min)	26	27			
20	Naphthalenes, v%	3.0 (max)	na	1.63			
COR	ROSION						
21	Copper strip, 2hrs @ 100°C	1 (max)	1A	1A			
22	Silver strip	2 (max)	0	0			
THE	THERMAL STABILITY						
23	Filter pressure drop, mm Hg	25 (max)	0	0			
24	Tube deposit rating @ 260°C	<3	<1	<1			
CON	CONTAMINANTS						
25	Microseparometer wo SDA	70 (min)	74	88			
26	Microseparometer w SDA	85 (min) 90					
27	Existent gum, mg/100mL	7 (max)	0.5	0.7			
OTHER TESTS							
28	Lubricity, mm WSD	0.85 (max)	0.63	0.69			

A2. Effect of 50/50 Blend of Sasol IPK on Specification Properties of Base Jet A-1 Fuel (Sasol)

Line No.	Property	Limits	Base JP-8	JP-8/S-8 (50/50)			
COMPOSITION							
1	Acid number, mg KOH/g	0.10 (max)	0.004	0.005			
2	Aromatics, v%	25 (max)	16.5	8.3			
3	Mercaptan sulfur, m%	0.002 (max)	0.000	0.000			
4	Total sulfur, m%	0.30 (max)	0.060	0.029			
5	Hydrogen content, m%	13.4 (min)	13.8	14.5			
VOLA	ATILITY						
6	Initial boiling point, °C	Report	145	148			
7	10% recovered, °C	205 (max)	172	170			
8	20% recovered, °C	Report	181	179			
9	50% recovered, °C	Report	205	206			
10	90% recovered, °C	Report	252	253			
11	Final boiling point, °C	300 (max)	277	275			
12	Residue, %	1.5 (max)	1.3	1.3			
13	Loss, %	1.5 (max)	1.3	1.1			
14	Flash point, °C	38 (min)	48	48			
15	Density @ 15° , kg/m ³	775 - 840	807	782			
FLUI	DITY						
16	Freezing point, °C	-47 (max)	-52	-52			
17	Viscosity @ -20°C, cSt	8.0 (max)	4.8	4.6			
COM	BUSTION						
18	Net heat of combustion, kJ/kg	42.8	43.2	43.4			
19	Smoke point, mm	19 (min)	23	34			
20	Naphthalenes, v%	3.0 (max)	1.2	NR			
CORROSION							
21	Copper strip, 2hrs @ 100°C	1 (max)	1a	1a			
THE	RMAL STABILITY						
22	Filter pressure drop, mm Hg	25 (max)	0	5			
23	Tube deposit rating @ 260°C	<3	0	1			
CON	CONTAMINANTS						
24	Water reaction	1b (max)	1	1			
25	Existent gum, mg/100mL	7.0 (max)	0.8	0.6			
OTH	OTHER TESTS						
26	Conductivity, pS/m	150 - 600	177	305			
27	Lubricity, mm WSD	0.85 (max)	0.56	0.54			

A3. Effect of 50/50 Blend of S-8 on Specification Properties of Base JP-8 Fuel (Edwards AFB)

Line No.	Property	Limits	Base JP-8	JP-8/Shell GTL (50/50)				
COMPOSITION								
1	Acid number, mg KOH/g	0.015 (max)	0.004	0.003				
2	Aromatics, v%	25 (max)	19.1	8.7				
3	Mercaptan sulfur, m%	0.002 (max)	0.001	< 0.0003				
4	Total sulfur, m%	0.3 (max)	0.09	0.05				
5	Hydrogen content, m%	13.4	13.7	14.6				
VOLA	ATILITY							
6	Initial boiling point, °C	Report	182	160				
7	10% recovered, °C	205 (max)	196	171				
8	20% recovered, °C	Report	200	175				
9	50% recovered, °C	Report	209	188				
10	90% recovered, °C	Report	224	216				
11	Final boiling point, °C	300 (max)	244	236				
12	Residue, %	1.5 (max)	1.1	1.0				
13	Loss, %	1.5 (max)	0.6	0.3				
14	Flash point, °C	38 (min)	64	50				
15	Density (a) 15° , kg/m ³	775 - 840	808	773				
FLUI	DITY							
16	Freezing point, °C	-47 (max)	-52	-61				
17	Viscosity @ -20°C, cSt	8.0 (max)	4.9	3.6				
COM	COMBUSTION							
18	Net heat of combustion, kJ/kg	42.8 (min)	43.1	43.5				
19	Smoke point, mm	25.0 (min)	26.0	34.0				
20	Naphthalenes, v%	3.0 (max)	Not reported	Not reported				
CORROSION								
21	Copper strip, 2hrs @ 100°C	1 (max)	1A	1A				
THEF	RMAL STABILITY							
22	Filter pressure drop, mm Hg	25 (max)	0	0				
23	Tube deposit rating @ 260°C	<3	1	1				
CONTAMINANTS								
24	Water reaction interface rating	1b (max)	1	1				
25	Existent gum, mg/10mL	7 (max)	<1	<1				
OTHER TESTS								
26	Conductivity, pS/m	150 - 600	300	195				
27	Lubricity, mm WSD	0.85 (max)	0.53	0.54				

A4. Effect of 50/50 Blend of Shell GTL on Specification Properties of Base JP-8 Fuel (Dyess AFB)

Line No.	Property	Limits	Base Jet A	Jet A/Sasol GTL-1 (50/50)	Jet A/Sasol GTL-2 (50/50)		
COM	COMPOSITION						
1	Acid number, mg KOH/g	0.015 (max)	0.032	0.035	0.017		
2	Aromatics, v%	22.0	17.7	7.3	8.3		
3	Mercaptan sulfur, m%	0.003 (max)		0.0007	0.0006		
4	Total sulfur, m%	0.03 (max)	707	325	359		
5	Hydrogen content, m%	Report	13.58	14.87	14.43		
VOL	ATILITY	•					
6	Initial boiling point, °C	Report	155	137	166		
7	10% recovered, °C	205 (max)	171	160	183		
8	20% recovered, °C	Report	179	165	190		
9	50% recovered, °C	Report	201	182	215		
10	90% recovered, °C	Report	247	228	253		
11	Final boiling point, °C	300 (max)	264	257	265		
12	Residue, %	1.5 (max)	1.3	1.2	1.0		
13	Loss, %	1.5 (max)	0.7	0.2	0.2		
14	Flash point, °C	38 (min)		43.9	56.7		
15	Density @ 15°, kg/m ³	775 - 840	812	772	787		
FLUI	DITY						
16	Freezing point, °C	-40 (max)	-45	-50.2	-47		
17	Viscosity @ -20°C, cSt	8.0 (max)	4.5	3.2	5.4		
COM	BUSTION						
18	Net heat of combustion, kJ/kg	42.8	43.2	43.6	43.5		
19	Smoke point, mm	19 (min)	19	22	24		
20	Naphthalenes, v%	3.0 (max)	2.05	1.40	1.43		
CORROSION							
21	Copper strip, 2hrs @ 100°C	1 (max)	1A	1A	1A		
THERMAL STABILITY							
22	Filter pressure drop, mm Hg	25 (max)	0	0	0		
23	Tube deposit rating @ 260°C	<3	2	<1	<1		
24	JFTOT breakpoint, °C	260 (min)	260	285	295		
25	Deposit thickness, nm	Report	50	25	25		
CONTAMINANTS							
26	Microseparometer wo SDA		73	44	58		
27	Microseparometer w SDA						
28	Existent gum	7 (max)	0.3	0.3	<0.1		
OTHER TESTS							
29	Conductivity, pS/m	150 - 600	24	208	131		
30	Lubricity, mm WSD	0.85 (max)	0.52	0.75	0.69		

A5. Effect of 50/50 Blends of Sasol GTL-1/-2 on Specification Properties of Base Jet A Fuel (SwRI)