

Tobias Schripp, Tobias Grein, Julia Zinsmeister, Patrick Oßwald, Markus Köhler, Franziska Müller-Langer¹, Stephanie Hauschild¹, Christian Marquardt², Sebastian Scheuermann², Alexander Zschocke³, and Dietmar Posselt⁴, Technical Application of a Ternary Alternative Jet Fuel Blend – Chemical Characterization and Impact on Jet Engine Particle Emission, *Fuel*, 288 (2021) 119606.

¹ Deutsches Biomasseforschungszentrum (DBFZ), Biorefineries, Leipzig, Germany

² Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe (WIWeB), Erding, Germany

³ Deutsche Lufthansa AG, Köln, Germany

⁴ Aviation Fuel Projects Consulting, Prien am Chiemsee, Germany

The original publication is available at

<https://www.sciencedirect.com/science/article/abs/pii/S0016236120326028>

<https://doi.org/10.1016/j.fuel.2020.119606>

© 2021. This manuscript version is made available under the CC-BY-NC-ND 4.0 license <http://creativecommons.org/licenses/by-nc-nd/4.0/>

1 **Technical Application of a Ternary Alternative Jet Fuel Blend – Chemical** 2 **Characterization and Impact on Jet Engine Particle Emission**

3 Tobias Schripp^{1*)}, Tobias Grein¹⁾, Julia Zinsmeister¹⁾, Patrick Oßwald¹⁾, Markus Köhler¹⁾,
4 Franziska Müller-Langer²⁾, Stephanie Hauschild²⁾, Christian Marquardt³⁾, Sebastian
5 Scheuermann³⁾, Alexander Zschocke^{4),*} and Dietmar Posselt⁵⁾

6 ¹⁾ German Aerospace Center (DLR), Institute of Combustion Technology, Stuttgart, Germany

7 ²⁾ Deutsches Biomasseforschungszentrum (DBFZ), Biorefineries, Leipzig, Germany

8 ³⁾ Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe (WIWeB), Erding, Germany

9 ⁴⁾ Deutsche Lufthansa AG, Köln, Germany

10 ⁵⁾ Aviation Fuel Projects Consulting, Prien am Chiemsee, Germany

11 * Current affiliation: Centre of Competence for Climate, Environment and Noise Protection in
12 Aviation, Frankfurt am Main, Germany

13 Keywords: HEFA, alcohol-to-jet, soot, storage stability

14 **Abstract**

15 The use of alternative fuels is an essential element in future aviation. There are currently
16 different approaches with regard to fuel production processes and feedstock materials. This
17 requires flexible handling of available fuel quantities. The production of fuel mixtures (blends)
18 is inevitable for an effective usage of commercially available fuel components. Within the
19 framework of the project DEMO-SPK approx. 600 t of a ternary mixture (multiblend) of
20 alternative jet fuels was produced and used in a real airport infrastructure at the airport
21 Leipzig/Halle. Production and application were accompanied with extensive R&D activities to
22 show, that on-spec, semi-synthetic multiblends can be produced from several different
23 synthetic fuels. One important aspect is the emission of soot particles from aircraft engines.
24 The Multiblend Jet A-1 has been analyzed in a flow reactor setup regarding the formation of
25 soot precursor compounds in comparison to a reference Jet A-1. The experiment revealed a
26 lower formation of relevant soot precursors which also corresponds to the higher hydrogen
27 content of the Multiblend Jet A-1 compared to the reference fuel. The lower soot formation in
28 a real aircraft engine has been proven during ground runs of an A300-600 aircraft with PW4158
29 engines. The Multiblend Jet A-1 showed lower particle number and particle mass emission
30 than the reference fuel. The difference to the reference fuel decreased with increasing power
31 settings. In summary, the emission of particle mass is reduced by ~29% and the number of
32 emitted particles is reduced by ~37% if the ICAO landing-and-take-off cycle is used for
33 evaluation.

34 **Introduction**

35 The aviation sector is facing particular challenges surrounding climate protection targets in
36 light of the Paris Climate Agreement. Prior to the worldwide COVID-19 pandemic, the aviation
37 industry showed growth rates between 3 % and 6 % (2015 – 2019) [1]. Despite the strong
38 decrease in flight movements in 2020, the aviation industry will also require high amounts of
39 jet fuel in the future. The use of sustainable aviation fuels (SAF) as a substitute for fossil fuels
40 will play an important role in reducing CO₂ emissions in aviation and fulfilling future regulations
41 on greenhouse gas emissions. A further driver for the increased application of alternative jet
42 fuels is the increasing relevance of airports as an emission source of ultra-fine particles (UFP).
43 Several studies worldwide showed the release of UFP into the environment that could be
44 attributed to jet engine emissions [2-5]. Aircraft jet engines release volatile and non-volatile
45 particles which feature different aerosol dynamics, airborne transport range and exposure
46 potential [6, 7]. Lab and field studies with alternative jet fuel blends have demonstrated that jet
47 fuels with an elevated hydrogen content (low amount of unsaturated hydrocarbons) show lower
48 soot emissions than a regular reference Jet A-1 for the same engine [8-12]. However, in order
49 to use SAF in aviation, compliance with sustainability criteria have to be monitored along the
50 entire supply chain. Furthermore, it must be ensured that fuel mixtures containing different
51 alternative fuel components do not deviate from current fuel specifications for Jet A-1 (“drop-
52 in fuel”).

53 The primary goal of the research and demonstration project on the use of renewable kerosene
54 at Leipzig/Halle Airport (short: DEMO-SPK) was to examine and verify the behavior of blends
55 of several renewable SAF with fossil Jet A-1 under realistic conditions in the supply
56 infrastructure of a major airport. Another aim was to successfully demonstrate the use of
57 Multiblend Jet A-1 in the general fuel supply infrastructure, from procurement to aircraft fueling
58 operations, on the international level for the first time. The key results are promising [13]. The
59 project demonstrated that the supply chain for Multiblend Jet A-1 was technically feasible and
60 that the fuel could be used without making any changes in normal operating procedures. The
61 project also verified that the use of Multiblend Jet A-1 resulted in a reduction of about 35 % in

62 CO₂ equivalents compared with pure fossil Jet A-1. A number of solutions and
63 recommendations to facilitate practical use were developed as well [13].

64 This study aims to summarize the findings with regard to the emission of ultra-fine particles
65 from the use of the Multiblend Jet A-1 produced within the framework of DEMO-SPK. Two
66 types of alternative jet fuel mixtures have been analyzed in a flow reactor experiment regarding
67 their expected soot formation potential. Due to limitations in the availability of certain fuel
68 components only one mixture has been tested on the engines of an A300 regarding the soot
69 emission in comparison to a reference Jet A-1. In order to use multiblends, they have to comply
70 with the fuel specification ASTM D7655 and have to possess sufficient storage stability. This
71 has been evaluated prior to the campaign to avoid biases of the experiment. The results of this
72 study demonstrate the positive impacts of SAF application in a real airport environment.

73 **Materials and Methods**

74 **Fuels** One reference Jet A-1 and two alternative jet fuel blends were tested on a lab-scale
75 basis. Multiblend Jet A-1 was a ternary mixture of 30 %v/v HEFA (hydroprocessed esters and
76 fatty acids) fuel, 8 %v/v ATJ (alcohol-to-jet) fuel and 62 %v/v reference Jet A-1. The second
77 blend (Multiblend Jet A-1 + SIP) consisted of 17 %v/v HEFA, 3 %v/v ATJ, 75 %v/v Jet A-1 and
78 5 %v/v SIP (synthesized iso-paraffins). All fuels comply with the requirements of ASTM D7566-
79 20b. The reference fuel used for blending and for the on-site emission test originated from the
80 same refinery (Lingen) but not necessarily from the same batch. It should be noted that the
81 Lingen refinery was selected for the DEMO-SPK project because of its stable properties across
82 batches. The engine ground runs were performed with one of the alternative jet fuel blends
83 (Multiblend Jet A-1) and the reference fuel (Reference Jet A-1). Minor changes in some fuel
84 parameters can be expected due to residues in storage tanks, fuel trucks and piping (see Table
85 SI1). Therefore, fuel samples were taken from the aircraft fuel tank after each ground run for
86 analysis. The relevant parameters are summarized in Table 1 (see Supporting Information for
87 test methods).

88 **Fuel Characterization and Stability** 900 L of Multiblend Jet A-1 + SIP and 400 L of Multiblend
 89 Jet A-1, respectively, were prepared and stored in tanks of the type TA 950 (Rietbergwerke
 90 GmbH & Co KG, material steel S355J2 with a hot-dip galvanized surface). The tanks were
 91 kept outdoors under a roof, exposed to the ambient climatic conditions during the storage
 92 period from April to October 2018 in Erding, Germany. However, they were protected from rain
 93 and sunlight. Samples were taken from both fuel blends at the beginning and at the end of the
 94 storage period and were subjected to a full analysis to determine possible alterations in fuel
 95 quality (see SI for test methods). The relevant fuel parameters are shown in Table 4.

96 Table 1: Selected physico-chemical parameters for the three different fuels of the lab-scale
 97 experiments (lab) and from the aircraft (A/C).

Parameter	Reference Jet A-1	Multiblend Jet A-1	Multiblend Jet A-1 + SIP	ASTM D 7566 Requirement
Components	Jet A-1	Jet A-1/ HEFA/ATJ	Jet A-1/HEFA/ ATJ/SIP	
Sample	A/C ^a	A/C ^a	Lab	
Aromatics [%v/v]	15.5	9.9	12.0	8–25
Density (15°C) [kg/m ³]	808.8	787.2	797.9	775–840
Freezing point [°C]	-72.6	-58.2	-63.4	< -47
Flash point [°C]	42.0	42.0	48.0	> 38
Viscosity (-20°C) [mm ² /s]	3.872	3.753	4.365	< 8
Viscosity (-40°C) [mm ² /s]	7.302	7.099	8.753	< 12
Net Heat of Combustion [MJ/kg]	43.187	43.527	43.400	> 42.8
Smoke point [mm]	24.0	30.0	26.8	> 25.0
Naphthalenes [%v/v]	0.28	n.d.	0.18 ^b	< 3.0
Sulfur, total [%m/m]	0.0027	0.0099	0.0018	< 0.30
Lubricity [mm]	0.65	0.68	0.62	< 0.85
Hydrogen content [%m/m]	13.72	14.30	n.d.	-
	13.788	14.319	14.138	
Distillation				
Initial boiling point [°C]	152.1	152.3	161.3	reported
10% vol. recovered [°C]	170.7	168.6	178.1	< 205
50% vol. recovered [°C]	193.7	192.2	202.3	reported
90% vol. recovered [°C]	225.9	231.4	233.0	reported
Final boiling point [°C]	257.8	256.0	248.6	< 300

98 ^aThe fuel parameters were determined from a sample taken from the aircraft fuel tank after the
 99 ground run; ^bcalculated; n.d.: not determined.

100 **Lab-scale flow reactor measurement** The oxidation of jet fuels was investigated at DLR's
 101 high-temperature flow reactor with coupled molecular-beam mass spectrometry (MBMS) to
 102 estimate the influence of the kerosene composition on the kinetic reaction process during

103 combustion. In previous studies detailed description of the atmospheric MBMS flow reactor
104 system [14-16] as well as the signal evaluation [17-19] is given and only a brief summary is
105 provided in the following.

106 The reactor setup consists of a ceramic flow tube (40 mm inner diameter, 1000 mm heated
107 length) placed in a high-temperature oven with temperature-controlled gas inlet to avoid
108 condensation effects of the pre-evaporated fuel. Detection takes place at the reactor outlet
109 using a time-of-flight mass spectrometer (TOF-MS) with electron ionization (nominal electron
110 energy of 13.5 eV). The in-situ gas sampling is carried out at ambient pressure (~980 mbar)
111 with a handmade quartz nozzle (25° internal angle, 1-2 mm wall thickness, 80 mm total length).
112 The extracted gas sample is expanded into a high vacuum and thus converted into a molecular
113 beam. A nickel skimmer transfers the molecular beam into the ionization chamber where the
114 neutral molecules are ionized. Species identification is performed on the basis of the exact
115 mass (mass resolution $R = 3000$) [15].

116 The fuels' oxidation was performed under lean ($\Phi = 0.8$) and slightly rich ($\Phi = 1.2$) combustion
117 conditions within a temperature range of 800 - 1200 K by applying a continuous decreasing
118 temperature ramp (-200 K/h), starting with complete oxidation and ending with non-reactive
119 state. Premixed gases are fed to the flow reactor highly diluted within the argon carrier gas (Ar
120 $> 99\% \text{v/v}$), whereby a self-sustaining combustion reaction is suppressed. Reaction
121 temperatures are known for any condition [19]. The liquid fuels were pre-evaporated before
122 entering the reactor. Table 2 presents the specific gas flow rates for the respective fuels and
123 oxidizer (O_2) at consistent argon flow (17.64 g/min). The fuels' hydrogen content was
124 determined using pulsed nuclear magnetic resonance (NMR) according to ASTM D7171
125 (Table 1) to calculate the respective stoichiometry conditions. Heteroatoms were neglected.
126 For both stoichiometry series a constant carbon flow was taken into account and the oxidizer
127 amount was adjusted accordingly. The resulting differences in the total volume flow are
128 negligible. The flow rates are controlled by mass flow controllers (Bronkhorst, Mini CORI-
129 FLOW™) with high accuracy and repeatability.

130 Table 2: Gas flow rates [mg/min] for examined combustion conditions of the fuels' oxidation at
 131 consistent argon flow (17.64 g/min).

Fuel	Abbreviation	Fuel [mg/min]	Oxidizer O ₂ [mg/min]	
		$\Phi=0.8$ $\Phi=1.2$	$\Phi=0.8$	$\Phi=1.2$
Reference Jet A-1	Ref	31.08	131.7	87.8
Multiblend Jet A-1	MB	31.27	133.6	89.1
Multiblend Jet A-1 + SIP	MB SIP	31.20	133.0	88.7

132

133 Signal quantification is performed by use of cold-gas-mixtures (“direct”) and via the empirical
 134 approximation method of relative ionization cross sections (RICS) after the signals were
 135 adjusted for background and fragmentation contributors. The uncertainty of the quantification
 136 reaches a maximum of 20 % if using direct calibration. In case of the RICS-method the
 137 uncertainty may increase by a factor of 2 to 4 [15] if ionization properties of the target species
 138 are unknown. It is important to note that signal contribution of isomers cannot be separated by
 139 use of electron ionization (EI) and therefore no differentiation of the molecular structure is
 140 possible. Assignment of chemical structure is solely based on experience gained by isomer-
 141 specific methods such as photoelectron photo ion coincidence spectroscopy (PEPICO) [19-
 142 21] that are typically applied to investigate combustion reactions of neat substances.

143 **Engine emission measurement** Two ground runs (“reference run” / “multiblend run”) were
 144 performed with an A300-600 (freight version) equipped with two Pratt & Whitney PW4158
 145 engines. The engine runs were performed in a noise protection hangar at Leipzig/Halle airport
 146 on the 30th September 2018. The air inlets of the hangar are designed to provide a laminar
 147 flow along the aircraft and the engines. Therefore, side-winds do not affect the measurement.
 148 The probe sampling was performed at the edge of the hangar at 2.5 m height and aligned to
 149 engine 1. The setup is visualized in the project video of DEMO-SPK [22] and the Supporting
 150 Information. The distance between sampling inlet and engine exhaust plane was 20 m. For
 151 each fuel, 7 different engine power settings were tested (see Table 3). The ambient
 152 temperature rose from 6 – 10°C (reference run) to 16°C (multiblend run) over the day. In case
 153 of the highest power setting (85 % N1), the relative uncertainty of the fuel flow is higher than
 154 in the other cases. This is caused from the manual operation of the thrust which led to a small

155 delay in reaching the target level and the shorter operating time. The time-resolved
 156 development of the parameters is illustrated in Figure SI2.

157 Table 3: Operation parameters and test matrix of the ground runs (in the order of execution).

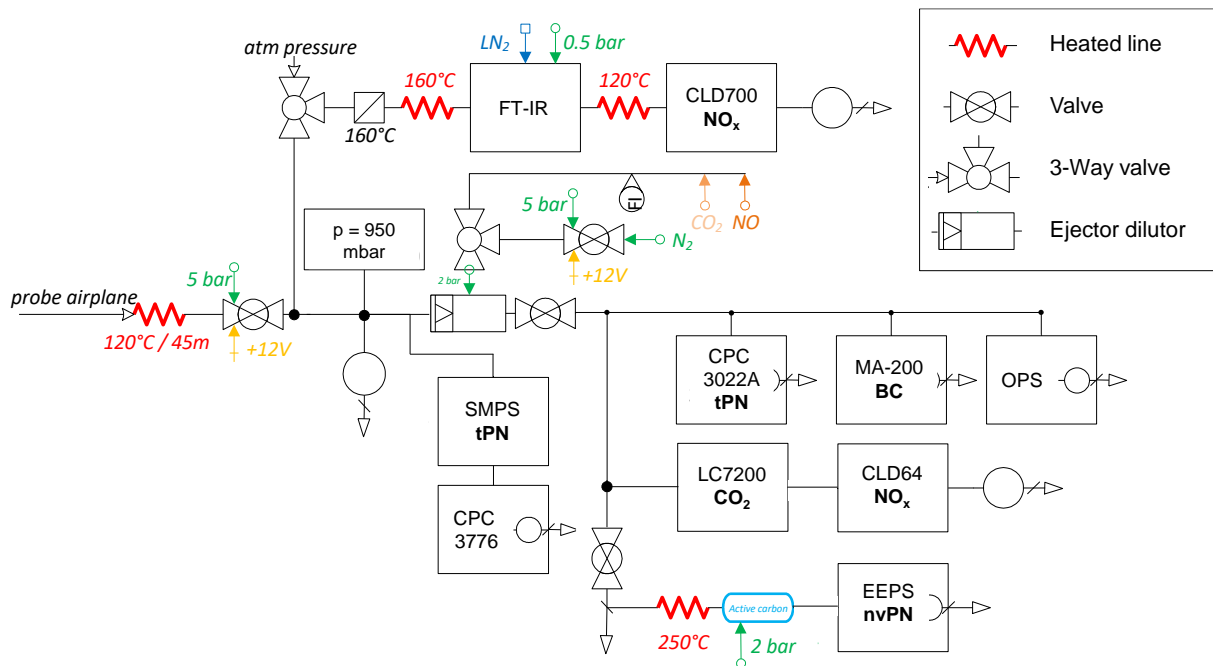
ID	%N1 ^a	t [min]	Reference run			Multiblend run		
			FF ^b [kg/h]	T25 ^c [°C]	EGT ^d [°C]	FF ^b [kg/h]	T25 ^c [°C]	EGT ^d [°C]
Start	23	8	699 ± 6	12.2 ± 0.2	354 ± 1	632 ± 6	20.5 ± 0.4	331 ± 4
1	40	8	1286 ± 11	22.5 ± 0.2	326 ± 1	1254 ± 24	31.3 ± 0.7	328 ± 9
2	60	5	2609 ± 15	45.6 ± 0.5	358 ± 1	2631 ± 15	55 ± 0.4	376 ± 1
3	50	8	1868 ± 11	33.4 ± 0.5	335 ± 1	1840 ± 10	41.6 ± 0.5	351 ± 1
4	30	8	880 ± 12	16.5 ± 0.5	335 ± 2	900 ± 20	24.7 ± 0.4	351 ± 2
5	85	1.5	6173 ± 370	88.1 ± 4.0	457 ± 11	6175 ± 16	99.1 ± 0.7	475 ± 2
Cool	23	8	691 ± 8	13.3 ± 0.9	366 ± 7	695 ± 6	20.5 ± 0.8	384 ± 12
6	75	5	4382 ± 27	71.6 ± 1.2	414 ± 2	4310 ± 12	78.9 ± 0.4	428 ± 1
7	23	8	690 ± 7	14.2 ± 0.5	364 ± 1	691 ± 6	20.7 ± 0.5	377 ± 1

158 ^aFan speed of the low pressure turbine; ^bEngine fuel flow; ^cInlet temperature of the high pressure turbine;
 159 ^dExhaust gas temperature of the combustion chamber.

160 The sampled aerosol was transferred via a heated 45 m sampling line (ID = 5.6 mm, 120°C)
 161 to the measuring container. The undiluted aerosol was measured via an Engine Exhaust
 162 Particle Sizer (EEPS, TSI Inc.) equipped with a thermal denuder (300°C, Dekati Ltd.). The
 163 EEPS measures particles in the range between 5.6 nm and 560 nm in 32 channels at 10 Hz.
 164 Further measurements on the diluted aerosol were performed with a 3022A CPC (TSI Inc.), a
 165 MA-200 Aethalometer (AethLabs) and a Scanning Mobility Particle Sizer (SMPS, TSI Inc.).
 166 The MA-200 recorded the data in a 5 s interval. The SMPS consisted of a 3082 Classifier, a
 167 3081 Long-DMA, 3088 Aerosol Neutralizer and a 3776 CPC. The SMPS measured a particle
 168 size distribution between 8 nm and 279 nm every 60 s. The aerosol was diluted with a DI-1000
 169 diluter (Dekati Ltd.) by factor 20.7 ± 0.9 . The inlet pressure of the diluter was kept stable at 950
 170 mbar with a pressure controller (Burkert Fluid Control Systems). Nitrogen oxides were
 171 measured via chemiluminescence using a CLD700 (Ecophysics, undiluted) and a CLD64
 172 (Ecophysics, diluted). The diluted carbon dioxide concentration was monitored with a LI-
 173 7200RS Enclosed Path CO₂/H₂O Analyzer (LI-COR). General combustion products (e.g. CO,
 174 NO_x, total hydrocarbons) were monitored with a MKS 2030 FT-IR instrument (undiluted). The
 175 full setup is summarized in Figure 1.

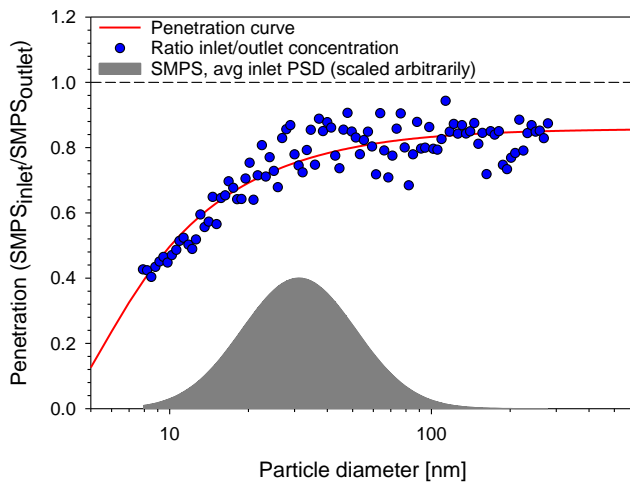
176 **Data analysis** The measured particle concentrations were converted into emission indices
177 using the CO₂ concentration recorded by the LI-7200RS. The calculation follows the
178 recommendation in AIR6241. The non-volatile particle number (nvPN) is derived from the data
179 of the EEPS and the non-volatile particle mass (nvPM) is derived from the MA-200
180 aethalometer. Since the particle number concentration of the CPC could not be corrected for
181 the particle loss in the sampling system, the data was used for orientation purposes only and
182 are not presented in the manuscript. The OPS data is also not included in this manuscript due
183 to the low number of particles with $d > 300$ nm. The results of the SMPS featured insufficient
184 statistics in the present experiment which not allowed measuring the total number of emitted
185 particles. Therefore, the SMPS was used for the loss correction analysis only.

186 **Loss correction** The loss of particles in the sampling system is a vital parameter that must be
187 considered for jet engine emission experiments [23]. In the present case, the particle loss rate
188 is determined experimentally using a portable aerosol generator. A sodium chloride test
189 aerosol with a count mode diameter of 42 nm is introduced into the probe inlet and the
190 concentration is recorded for 5 min by the SMPS. The procedure is repeated at the inlet of
191 SMPS afterwards. The ratio between the inlet concentration and outlet concentration for each
192 channel of the SMPS is calculated and the penetration curve is fitted from the obtained results
193 (Figure 2). The test aerosol features a broad particle size distribution (PSD) which covers the
194 range of the engine exhaust target aerosol. The experimental data from the SMPS and the
195 EEPS have been corrected for particle losses using the fitted penetration curve function. The
196 high particle loss is expected to be caused by the high residence time of ~10 s even though
197 the flow in the sampling tube is laminar ($Re = 997$).



198

199 Figure 1: Experimental setup of the engine emission measurement



200

201 Figure 2: Experimental loss correction function of the sampling system based on the ratio
 202 between the particle size distribution at inlet and outlet.

203

204 Results and Discussion

205 Fuel Characterization and Stability

206 Analysis results of Multiblend Jet A-1 and Multiblend Jet A-1 + SIP before and after storage
 207 are summarized in Table 4. The analysis of both Multiblend mixtures confirmed that ASTM
 208 D7566-compliant fuels had been obtained. This demonstrates that on-spec, semi-synthetic
 209 fuel mixtures can readily be produced from several different synthetic fuels. The comparison

210 of physico-chemical parameters before and after storage shows only variations within the
 211 range of the uncertainty of the applied test methods. Therefore, no deterioration of fuel quality
 212 was found after the storage period.

213 Table 4: Physico-chemical parameters of two alternative jet fuel mixtures before and after
 214 storage

Parameter	Multiblend Jet A-1 + SIP		Multiblend Jet A-1		Unit	ASTM D 7566 Requirement
	Before storage	After storage	Before storage	After storage		
Acidity, total	0.002	0.002	0.002	0.002	mg KOH/g	< 0.10
Aromatics	12.0 ^a		9.9 ^a		%v/v	8–25
Distillation						
Initial Boiling Point	161.3	160.5	159.0	159.1	°C	reported
10 %v/v recovered (T10)	178.1	177.8	174.2	174.7	°C	< 205
50 %v/v recovered (T50)	202.3	202.6	198.8	199.0	°C	reported
T50–T10	24.2	24.8	24.6	24.3	°C	> 15
90 %v/v recovered (T90)	233.0	233.4	232.2	232.6	°C	reported
T90–T10	54.9	55.6	58.0	57.9	°C	> 40
Final Boiling Point	248.6	252.7	251.2	253.0	°C	< 300
Distillation residue	1.2	1.2	1.2	1.2	%v/v	< 1.5
Distillation loss	1.1	1.0	1.0	1.0	%v/v	< 1.5
Flash point	48.0	47.0	45.5	45.5	°C	> 38
Density at 15 °C	797.9	798.0	789.0	789.0	kg/m ³	775–840
Freezing point	-63.4	-63.4	-57.0	-57.0	°C	< -47
Lubricity	0.618	0.616	0.655	0.665	mm	< 0.85
Viscosity (-20 °C)	4.365	4.355	4.198	4.112	mm ² /s	< 8
Viscosity (-40 °C)	8.753	8.862	8.142	8.149	mm ² /s	< 12
Existent gum	<1	<1	1.2	<1	mg/100ml	< 7
Deposit rating	1	1	1	1	-	<3
Pres. Drop	0	0	0	0	mmHg	< 25
Net Heat of Combustion	43.400	43.400	43.525	43.527	MJ/kg	> 42.8
Corrosion copper strip	1a	1a	1a	1a	-	< 1
Smoke Point	26.8 ^b	27.5 ^b	28.7 ^b	28.3 ^b	mm	> 25.0
Naphthalenes	0.18		0.15		%v/v	< 3.0
Sulfur, total	0.0018	0.0019	0.0016	0.0016	%m/m	< 0.30

215 ^aaromatics and naphthalene content was calculated and is only given once; ^b<25.0 mm or >18.0 mm
 216 and Naphthalenes <3.0 %v/v

217 *Flow Reactor Experiment*

218 The flow reactor experiment provides a basis for the estimation and explanation of pollutant
219 emission patterns, especially soot formation, in technical combustion systems. However, it
220 should be noted that this data set reflects homogeneous gas phase reactions only and thus is
221 focused on the chemical pollutant formation potential of the fuel. For technical combustion
222 systems, like turbofan engines, the combustion reaction is accompanied by complex
223 interactions of fuel atomization, fuel vaporization, fluid dynamics and the chemical reaction
224 network. All of these sub-processes can influence the final pollutant emissions of the engine.
225 Therefore, the combination of flow reactor measurements and full-scale engine experiments is
226 useful to illustrate and explore the impact of alternative jet fuels on engine exhaust emissions.

227 Major species (stable products and oxidizer) for the three tested fuels are shown in Figure 3
228 as a function of the oven temperature. The temperature can be considered as an indicator of
229 the reaction progress. At relatively cold oven temperatures, no reaction takes place and the
230 reactants (kerosene and oxygen) pass through the reaction zone unchanged. Starting at a
231 temperature of approx. 800 K, degradation of the fuel components begins, which is
232 accompanied by moderate oxygen consumption and formation of first intermediates. With
233 increasing temperature, carbon oxide and elemental hydrogen are formed. Chain-branching
234 reactions lead to an exponential increase in the radical pool and thus to a rapid increase in
235 reaction rate. This leads to significant oxygen consumption and carbon monoxide is oxidized
236 to carbon dioxide. Subsequently, only reaction products can be detected at the reactor outlet
237 beyond 1050 K. For lean condition ($\Phi = 0.8$) CO_2 , H_2O , and a corresponding excess of O_2 is
238 present as product, while for slightly-rich conditions ($\Phi = 1.2$) CO and H_2 are added as
239 products. The major species profiles of the three investigated jet fuels are qualitatively and
240 quantitatively very similar (same plot pattern) and are in line with previous findings for certified
241 kerosene [16, 24, 25]. Thus, the ternary fuel blending with alternative kerosene does not lead
242 to significant changes in the global reaction behavior under the examined conditions.

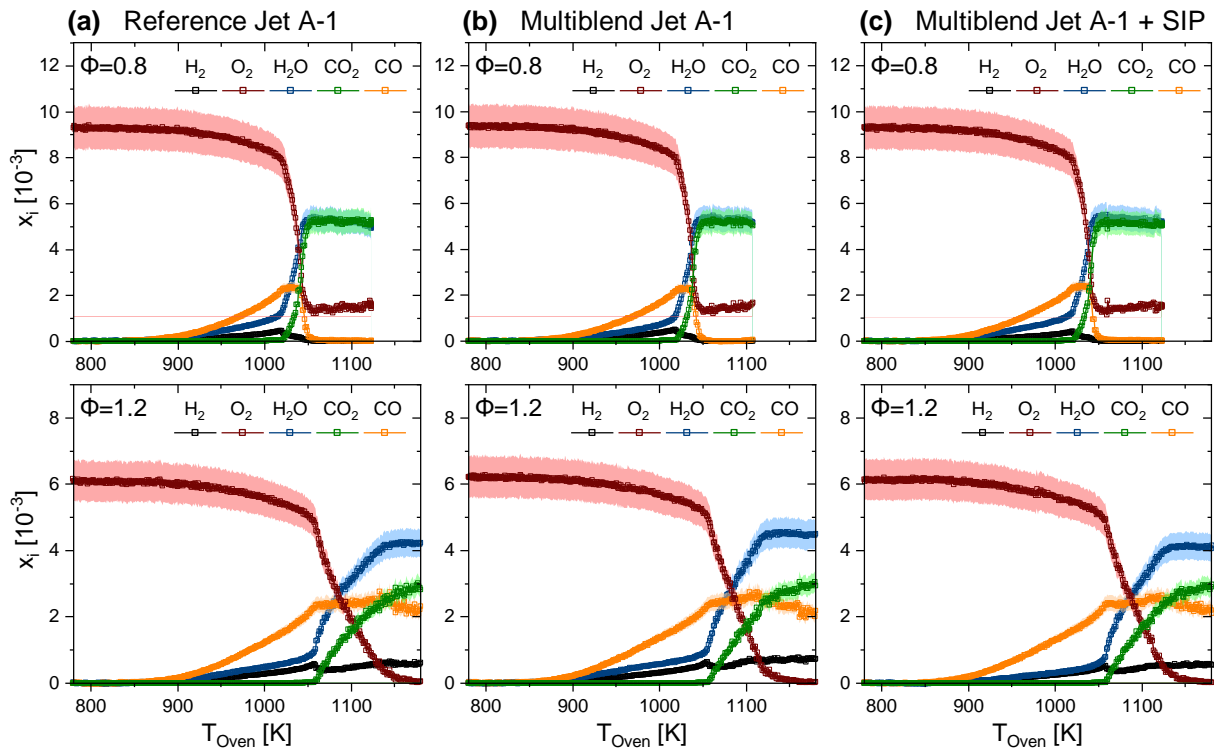


Figure 3: Mole fraction with uncertainty bars of major species (H_2 , H_2O , O_2 , CO_2 , CO) from oxidation of the technical jet fuels under lean ($\Phi = 0.8$) and slightly-rich ($\Phi = 1.2$) conditions.

243 Figure 4 shows selected main stable intermediates, including small hydrocarbons (a), like
 244 methane (CH_4) and ethylene (C_2H_4) as well as formaldehyde (CH_2O) as representatives of
 245 carbonyl compounds (b) for slightly-rich conditions ($\Phi = 1.2$). These species occur in
 246 combustion reactions of almost all hydrocarbons and their concentration shows only a slight
 247 dependence on the fuel composition. This is given in the inserts of Figure 4, where the fuels'
 248 hydrogen content is used to represent the molecular structure of the fuels. Due to higher
 249 proportion of aliphatic components, the alternative blends (MB and MB SIP) have higher
 250 hydrogen content than the fossil reference kerosene (Ref). For methane, no fuel dependency
 251 can be determined considering the experimental scatter. The ethylene concentration increases
 252 slightly with the addition of alternative components and higher hydrogen content of the fuels,
 253 respectively. This can be attributed to the methyl branching of the open-chain aliphatic
 254 compounds present in HEFA and SIP which tends to favor the formation of C3 fragments. A
 255 slight but detectable increase can also be observed for formaldehyde.

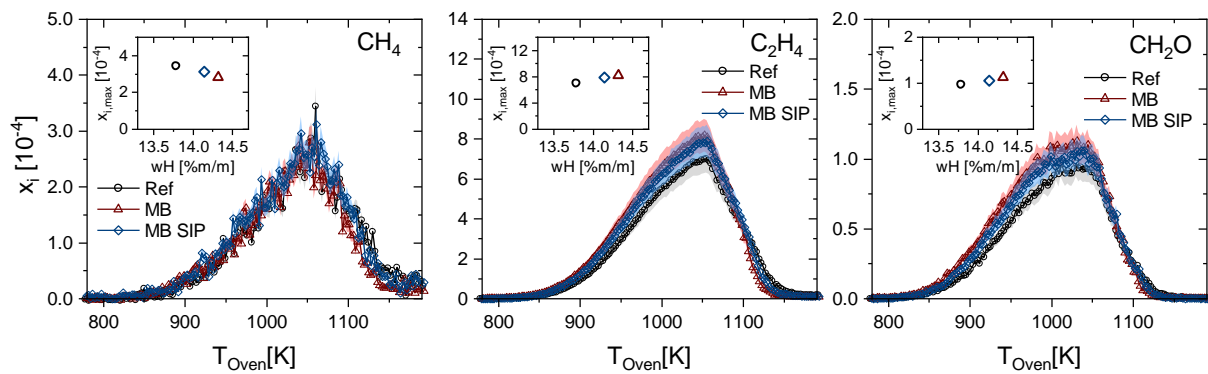


Figure 4: Mole fraction with uncertainty bars of selected small intermediates: Methane (CH_4), ethylene (C_2H_4), and formaldehyde (CH_2O) from the oxidation of the technical jet fuels under slightly-rich conditions ($\Phi = 1.2$). Insert: Maximum mole fraction as a function of the fuels' hydrogen content (wH) [%m/m].

256

257 In contrast to the previous mentioned intermediates, the maximum mole fractions of aromatic
 258 soot precursors show a clear correlation with the hydrogen content of the kerosene. This is
 259 illustrated for slightly-rich ($\Phi = 1.2$) combustion conditions in Figure 5. Here, the development
 260 of important soot precursor species, such as, benzene (C_6H_6), styrene (C_8H_8), indene (C_9H_8),
 261 naphthalene ($C_{10}H_8$), acenaphthylene ($C_{12}H_8$), and anthracene ($C_{14}H_{10}$) is summarized. The
 262 concentration of these soot precursor species decreases according to the following
 263 sequence: Reference Jet A-1 (Ref) > Multiblend Jet A-1 + SIP (MB SIP) > Multiblend Jet A-1
 264 (MB). Beside the dependence on the fuel composition, a decrease in the concentrations with
 265 increasing molecule size of the soot precursors can be recorded in accordance with previous
 266 findings [25-27]. Thus, a reduction in the concentration of soot precursor species by about one
 267 third for oxidation of the multiblends compared to the fossil reference kerosene can be
 268 observed. For example, the reduction of benzene in the case of the Multiblend Jet A-1 is almost
 269 33 % for both stoichiometries.

270 On the basis of the flow reactor experiment, a significant reduction of the soot emission can
 271 be expected in a real engine when changing from the reference kerosene to the Multiblend Jet
 272 A-1. It is very important to note that the observed reduction of the soot precursor species
 273 cannot be transferred into a real combustion system quantitatively. However, the trends in both
 274 parts of the experiment should be in alignment.

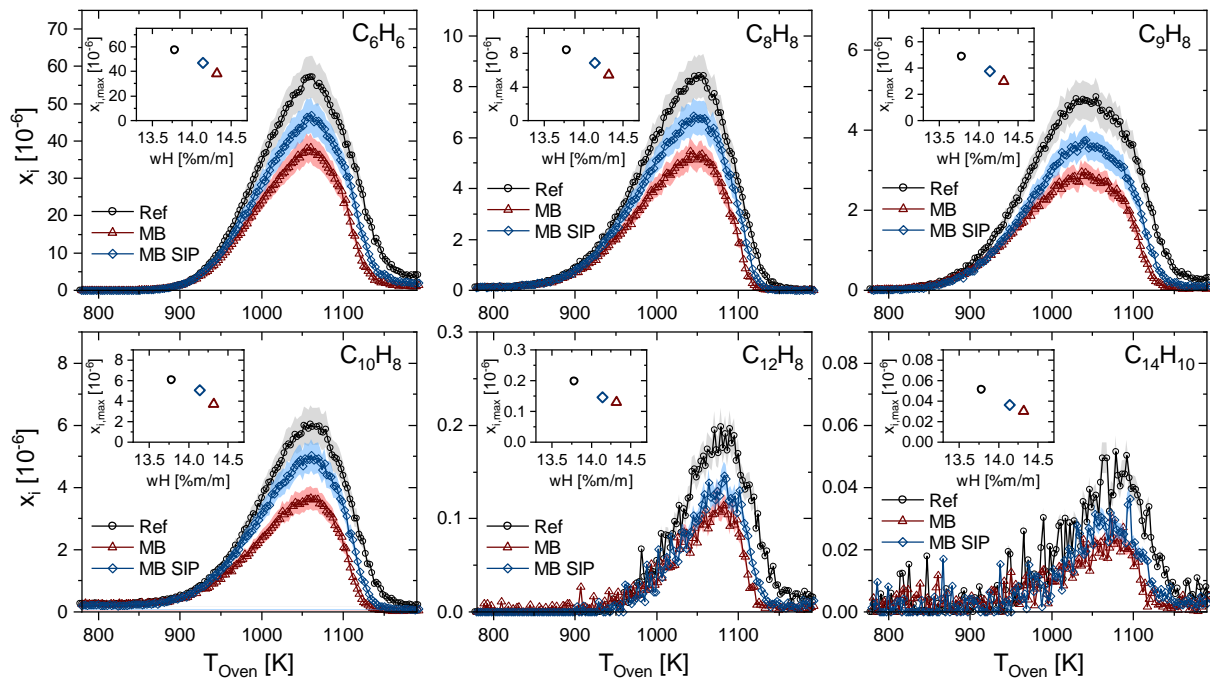


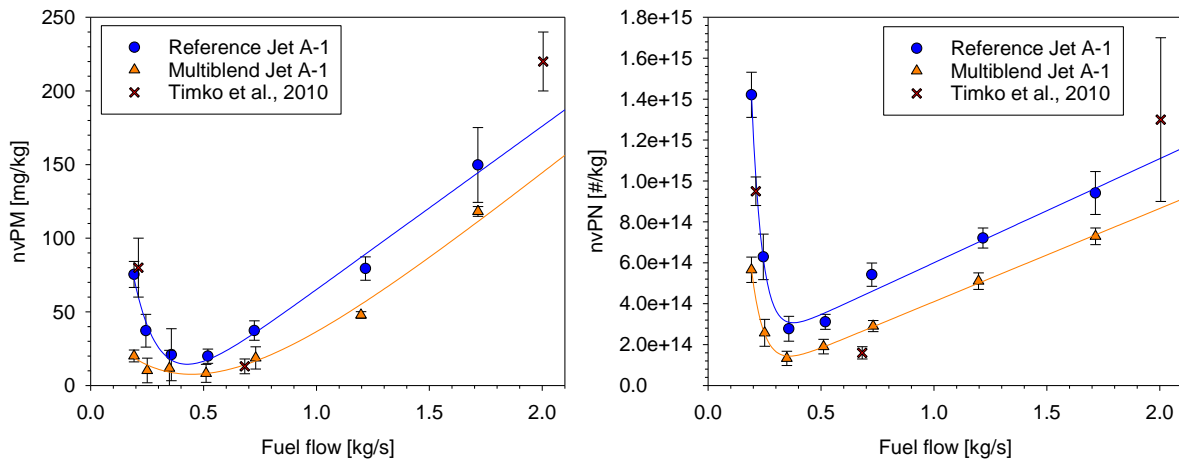
Figure 5: Mole fraction with uncertainty bars of selected soot precursors: benzene (C_6H_6), styrene (C_8H_8), indene (C_9H_8), naphthalene ($C_{10}H_8$), acenaphthylene ($C_{12}H_8$), and anthracene ($C_{14}H_{10}$) from the oxidation of the technical aviation fuels under rich conditions ($\Phi = 1.2$). Insert: Maximum mole as a function of the fuels' hydrogen content (wH) [%m/m].

275

276 *Jet Engine Experiment*

277 As expected from the lab-scale experiment, the application of the alternative jet fuel blend led
 278 to a reduction in particle number emission and particle mass emission for all power settings in
 279 the full-scale engine experiment (Figure 6). The engine particle emission profile of the PW4158
 280 engine showed a minimum at approx. 30 % - 40 % N1. In case of the non-volatile particle
 281 number emission index, the highest emission was observed for the lowest power setting.
 282 Published information on the particle emission characteristics of the PW4158 engine is limited.
 283 The ICAO database reports a smoke number of 8.1 for the highest power setting (T/O). Timko
 284 et al. [28] provide emission data for engine runs using a fuel with 600 ppm sulfur and 16.2 %
 285 aromatics. However, the reported particle emission indices (shown in Figure 6) are an average
 286 of several sampling distances (1, 15, 30, 43 and 50 m behind the engine). Therefore, additional
 287 uncertainties can be expected due to the evolution of the plume. The correlation between the
 288 results of the reference run and the published values is best for the highest and lowest power
 289 setting. Based on the aromatic content of the fuel, the values are expected to be between the
 290 reference Jet A-1 and the Multiblend Jet A-1. It must be noted, however, that the nvPM

291 emission correlates with fuel hydrogen content [29] which does not necessarily correlate with
292 aromatic content [10]. Considering the fuel uncertainty and the different instruments used (PM:
293 MA-200 / MAAP; PN: EEPS/CPC), the overall correlation is acceptable.



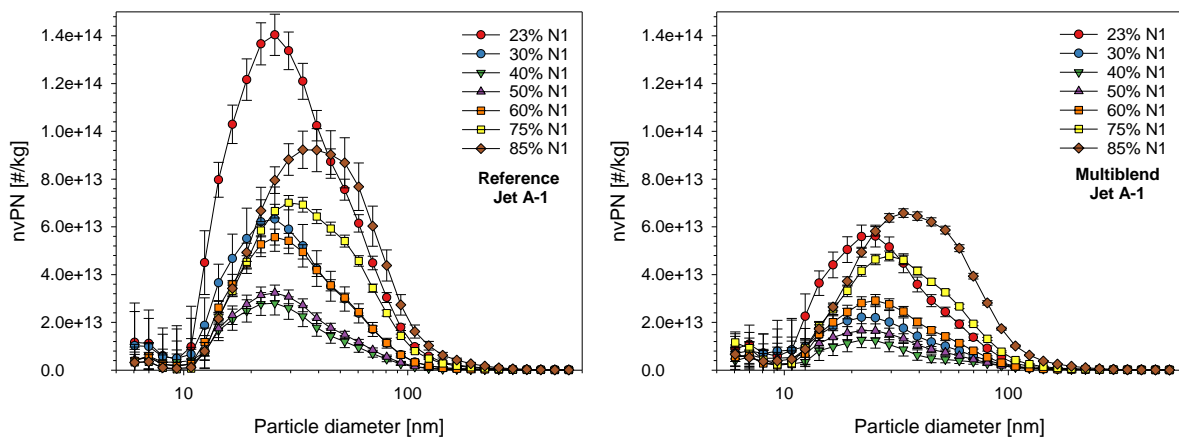
294

295 Figure 6: Particle mass emission index (left, MA-200) and particle number emission index
296 (right, EEPS) for the reference fuel and the alternative jet fuel blend. Emission indices for the
297 PW4158 engine from Timko et al. [28] are shown for comparison.

298 Regarding the size of the emitted particles no significant shift in the particle size distribution
299 can be observed for the two different fuels (Figure 7) at the same power setting. The main
300 fraction of non-volatile particles features diameters below 30 nm which is typical for turbofan
301 engine aerosols [9, 30]. The highest count mode diameter is observed for the highest power
302 setting tested in both cases. This may be attributed to the fact that the highest particle number
303 concentration is observed for this setting and coagulation occurs in this slightly aged aerosol.
304 Changing the fuel from the reference Jet A-1 to the Multiblend Jet A-1 had the highest impact
305 on the lowest two power settings (23 % N1 and 30 % N1). The emission of particle mass is
306 reduced by ~73 % and the emission of particle number is reduced by ~60 % for these cases
307 (Figure 8). The effect decreases with increasing power setting. In order to evaluate the overall
308 impact of the fuel change on the released amount of particles, the emission during the ICAO
309 landing-and-take-off cycle (LTO) has been calculated on the basis of the measured engine
310 emission profile (Figure 6). The measured power settings have been adjusted on the target
311 power settings of the LTO cycle (7 % thrust for 26 min, 30 % thrust for 4 min, 85 % thrust for
312 2.2 min, 100 % thrust for 0.7 min) based on the fuel flow of the engine. In the present

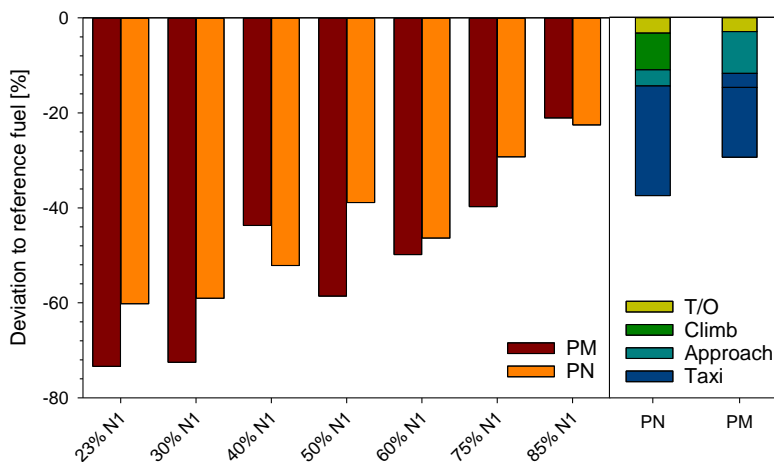
313 experiment, the application of the Multiblend Jet A-1 led to a 37 % reduction in the released
314 particle number and a 29 % reduction in released particle mass. It must be noted that the 100
315 % thrust setting has been extrapolated from the obtained data. Despite the correlation with
316 published values (Figure 6) a large uncertainty may be expected for this power setting.
317 However, the impact of this elevated uncertainty is insignificant considering the fact that only
318 9 % of the total reduction is caused from changes at the T/O power setting (Figure 8).

319 Considering the results of both experiments, the observed effect of soot reduction by using the
320 alternative kerosene can be directly attributed to the chemical combustion reactions and
321 therefore to the chemical composition of the multiblend itself. A beneficial effect of alternative
322 fuel components, such as HEFA, ATJ, and SIP, on particulate emissions can be expected over
323 a wide range of different combustion conditions. It is promising that the results from the actual
324 full-scale gas turbine combustor is consistent with earlier fundamental work performed in the
325 flow reactor and laminar diffusion flames. For instance, the observations are in line with
326 Saffaripour et al. [31] who observed a significant reduction in soot emissions by investigation
327 of laminar diffusion flames of Jet A-1 and different synthetic jet fuels based on Fischer-Tropsch
328 processes. Furthermore, a correlation between the soot precursor species benzene and soot
329 volume fractions on the centerline of the flame was stated. The qualitative trend is observed
330 by several studies [8, 11, 24] in which an alternative Fischer-Tropsch-component has shown
331 lower sooting propensity compared to conventional Jet A-1. A lower sooting tendency,
332 represented by a higher Smoke Point (SP) for alternative jet fuel blends and their neat
333 alternative components, like synthetic- and iso-paraffinic kerosene (SPK and IPK), HEFA, and
334 ATJ compared to petroleum-derived kerosene (JP-8) was also determined by Won et al. [32].



335

336 Figure 7: Non-volatile particle number size distribution (EEPS) for the engine ground runs with
 337 reference Jet A-1 (left) and Multiblend Jet A-1 (right).



338

339 Figure 8: Particle number emission and particle mass emission reduction by the Multiblend Jet
 340 A-1 compared to the reference fuel for the tested power settings (left) and for the LTO cycle
 341 (right). The value for take-off (T/O) has been estimated from the interpolation in Figure 6.

342 Conclusions

343 The experiment demonstrated the successful application of a ternary alternative jet fuel
 344 blending practice. On-spec, semi-synthetic fuel mixtures can be produced from several
 345 different synthetic fuels and be stored over the period of 6 months without the deterioration of
 346 fuel quality. The tendency to form soot from the different fuels was predicted in a flow reactor
 347 experiment on lab-scale basis. The trend in soot emission, which follows the hydrogen content
 348 of the fuels, could be demonstrated by engine runs at ground level. A change in other emission
 349 parameters was not observed in this context and the development of intermediates showed no
 350 significant deviation in the oxidation process. The emission of particle mass is reduced by ~29

351 % and the number of emitted particles is reduced by ~37 % if the ICAO landing-and-take-off
352 cycle is used for evaluation. The experiment demonstrated the flexible use of alternative jet
353 fuel components within the safety margins of the fuel specifications and their positive impact
354 on the jet engine particle emission. Further investigations are necessary to provide a
355 correlation between lab-scale experiments and real world engines to accelerate the
356 development and optimization of alternative jet fuel blends with minimized particle emission.

357 **Acknowledgements**

358 The research and demonstration project on the use of renewable kerosene at Leipzig/Halle
359 Airport (in short: DEMO-SPK) involved the collaboration of more than 20 international partners
360 from industry and science. It was initiated as a model project of the Mobility and Fuel Strategy
361 (MFS) and financed by the Federal Ministry of Transport and Digital Infrastructure (BMVI). In
362 addition to thanks to the whole project team, the authors are especially grateful for the support
363 and effort of European Air Transport Leipzig (EAT) and DHL which provided the A300 and
364 made the ground run experiments possible. The authors especially thank Nico Tenius and Lars
365 Remmers for their personal commitment to make this campaign successful.

366 **References**

- 367 [1] Berster P, Gelhausen M, Pabst H, Wilken D. DLR-Global Aviation Monitor March 2020 - Analysis
368 and Short Term Outlook of Global, European and German Air Transport. Cologne: German
369 Aerospace Center; 2020.
- 370 [2] Hudda N, Gould T, Hartin K, Larson TV, Fruin SA. Emissions from an International Airport
371 Increase Particle Number Concentrations 4-fold at 10 km Downwind. *Environmental Science
372 & Technology* 2014;48(12):6628-35, <https://doi.org/10.1021/es5001566>.
- 373 [3] Ren JL, Liu JJ, Li F, Cao XD, Ren SX, Xu B, et al. A study of ambient fine particles at Tianjin
374 International Airport, China. *Science of the Total Environment* 2016;556:126-35,
375 <https://doi.org/10.1016/j.scitotenv.2016.02.186>.
- 376 [4] Pirhadi M, Mousavi A, Sowlat MH, Janssen NAH, Cassee FR, Sioutas C. Relative contributions
377 of a major international airport activities and other urban sources to the particle number
378 concentrations (PNCs) at a nearby monitoring site. *Environmental Pollution* 2020;260:10,
379 <https://doi.org/10.1016/j.envpol.2020.114027>.
- 380 [5] Stacey B, Harrison RM, Pope F. Evaluation of ultrafine particle concentrations and size
381 distributions at London Heathrow Airport. *Atmospheric Environment* 2020;222:12,
382 <https://doi.org/10.1016/j.atmosenv.2019.117148>.
- 383 [6] Yu ZH, Timko MT, Herndon SC, Richard CML, Beyersdorf AJ, Ziemba LD, et al. Mode-specific,
384 semi-volatile chemical composition of particulate matter emissions from a commercial gas
385 turbine aircraft engine. *Atmospheric Environment* 2019;218:8,
386 <https://doi.org/10.1016/j.atmosenv.2019.116974>.

- 387 [7] He RW, Gerlofs-Nijland ME, Boere J, Fokkens P, Leseman D, Janssen NAH, et al. Comparative
388 toxicity of ultrafine particles around a major airport in human bronchial epithelial (Calu-3) cell
389 model at the air-liquid interface. *Toxicol Vitro* 2020;68:10,
390 <https://doi.org/10.1016/j.tiv.2020.104950>.
- 391 [8] Lobo P, Condevaux J, Yu ZH, Kuhlmann J, Hagen DE, Miake-Lye RC, et al. Demonstration of a
392 Regulatory Method for Aircraft Engine Nonvolatile PM Emissions Measurements with
393 Conventional and Isoparaffinic Kerosene fuels. *Energy & Fuels* 2016;30(9):7770-7,
394 <https://doi.org/10.1021/acs.energyfuels.6b01581>.
- 395 [9] Moore RH, Thornhill KL, Weinzierl B, Sauer D, D'Ascoli E, Kim J, et al. Biofuel blending reduces
396 particle emissions from aircraft engines at cruise conditions. *Nature* 2017;543(7645):411-5,
397 <https://doi.org/10.1038/nature21420>.
- 398 [10] Schripp T, Anderson B, Crosbie EC, Moore RH, Herrmann F, Osswald P, et al. Impact of
399 Alternative Jet Fuels on Engine Exhaust Composition During the 2015 ECLIF Ground-Based
400 Measurements Campaign. *Environmental Science & Technology* 2018;52(8):4969-78,
401 <https://doi.org/10.1021/acs.est.7b06244>.
- 402 [11] Kinsey JS, Squier W, Timko M, Dong YJ, Logan R. Characterization of the Fine Particle Emissions
403 from the Use of Two Fischer-Tropsch Fuels in a CFM56-2C1 Commercial Aircraft Engine. *Energy*
404 *& Fuels* 2019;33(9):8821-34, <https://doi.org/10.1021/acs.energyfuels.9b00780>.
- 405 [12] Schripp T, Herrmann F, Oßwald P, Köhler M, Zschocke A, Weigelt D, et al. Particle emissions of
406 two unblended alternative jet fuels in a full scale jet engine. *Fuel* 2019;256:115903,
407 <https://doi.org/10.1016/j.fuel.2019.115903>.
- 408 [13] Müller-Langer F, Dögnitz N, Marquardt C, Zschocke A, Schripp T, Oehmichen K, et al.
409 Multiblend JET A-1 in Practice: Results of an R&D Project on Synthetic Paraffinic Kerosenes.
410 *Chem Eng Technol* 2020;43(8):1514-21, <https://doi.org/10.1002/ceat.202000024>.
- 411 [14] Köhler M, Osswald P, Xu HB, Kathrotia T, Hasse C, Riedel U. Speciation data for fuel-rich
412 methane oxy-combustion and reforming under prototypical partial oxidation conditions.
413 *Chemical Engineering Science* 2016;139:249-60, <https://doi.org/10.1016/j.ces.2015.09.033>.
- 414 [15] Oßwald P, Köhler M. An atmospheric pressure high-temperature laminar flow reactor for
415 investigation of combustion and related gas phase reaction systems. *Review of Scientific*
416 *Instruments* 2015;86(10):105-9, <http://dx.doi.org/10.1063/1.4932608>.
- 417 [16] Köhler M, Osswald P, Krüger D, Whitside R. Combustion Chemistry of Fuels: Quantitative
418 Speciation Data Obtained from an Atmospheric High-temperature Flow Reactor with Coupled
419 Molecular-beam Mass Spectrometer. *J Vis Exp* 2018(132):10, <https://doi.org/10.3791/56965>.
- 420 [17] Herrmann F, Jochim B, Osswald P, Cai LM, Pitsch H, Kohse-Höinghaus K. Experimental and
421 numerical low-temperature oxidation study of ethanol and dimethyl ether. *Combustion and*
422 *Flame* 2014;161(2):384-97, <https://doi.org/10.1016/j.combustflame.2013.09.014>.
- 423 [18] Herrmann F, Osswald P, Kohse-Höinghaus K. Mass spectrometric investigation of the low-
424 temperature dimethyl ether oxidation in an atmospheric pressure laminar flow reactor.
425 *Proceedings of the Combustion Institute* 2013;34:771-8,
426 <https://doi.org/10.1016/j.proci.2012.06.136>.
- 427 [19] Osswald P, Hemberger P, Bierkandt T, Akyildiz E, Köhler M, Bodi A, et al. In situ flame chemistry
428 tracing by imaging photoelectron photoion coincidence spectroscopy. *Review of Scientific*
429 *Instruments* 2014;85(2):11, <https://doi.org/10.1063/1.4861175>.
- 430 [20] Bierkandt T, Hemberger P, Osswald P, Krüger D, Köhler M, Kasper T. Flame structure of laminar
431 premixed anisole flames investigated by photoionization mass spectrometry and
432 photoelectron spectroscopy. *Proceedings of the Combustion Institute* 2019;37(2):1579-87,
433 <https://doi.org/10.1016/j.proci.2018.07.037>.
- 434 [21] Krüger D, Osswald P, Köhler M, Hemberger P, Bierkandt T, Karakaya Y, et al. Hydrogen
435 abstraction ratios: A systematic iPEPICO spectroscopic investigation in laminar flames.
436 *Combustion and Flame* 2018;191:343-52,
437 <https://doi.org/10.1016/j.combustflame.2017.12.025>.

- 438 [22] BMVI. Erneuerbares Kerosin: Forschungs- und Demonstrationsvorhaben (DEMO-SPK)
439 Flughafen Leipzig/Halle; 2019. Available from: [https://www.youtube.com/watch?v=Fj--](https://www.youtube.com/watch?v=Fj--omcYeVc)
440 [omcYeVc](https://www.youtube.com/watch?v=Fj--omcYeVc).
- 441 [23] Durand EF, Crayford AP, Johnson M. Experimental validation of thermophoretic and bend
442 nanoparticle loss for a regulatory prescribed aircraft nvPM sampling system. *Aerosol Science*
443 *and Technology*;15, <https://doi.org/10.1080/02786826.2020.1756212>.
- 444 [24] Jürgens S, Osswald P, Selinsek M, Piermartini P, Schwab J, Pfeifer P, et al. Assessment of
445 combustion properties of non-hydroprocessed Fischer-Tropsch fuels for aviation. *Fuel Process*
446 *Technol* 2019;193:232-43, <https://doi.org/10.1016/j.fuproc.2019.05.015>.
- 447 [25] Oßwald P, Whitside R, Schäffer J, Köhler M. An experimental flow reactor study of the
448 combustion kinetics of terpenoid jet fuel compounds: Farnesane, p-menthane and p-cymene.
449 *Fuel* 2017;187:43-50, <https://doi.org/10.1016/j.fuel.2016.09.035>.
- 450 [26] Chu TC, Buras ZJ, Oßwald P, Liu MJ, Goldman MJ, Green WH. Modeling of aromatics formation
451 in fuel-rich methane oxy-combustion with an automatically generated pressure-dependent
452 mechanism. *Physical Chemistry Chemical Physics* 2019;21(2):813-32,
453 <https://doi.org/10.1039/c8cp06097e>.
- 454 [27] Kathrotia T, Oßwald P, Köhler M, Slavinskaya N, Riedel U. Experimental and mechanistic
455 investigation of benzene formation during atmospheric pressure flow reactor oxidation of n-
456 hexane, n-nonane, and n-dodecane below 1200 K. *Combustion and Flame* 2018;194:426-38,
457 <https://doi.org/10.1016/j.combustflame.2018.05.027>.
- 458 [28] Timko MT, Onasch TB, Northway MJ, Jayne JT, Canagaratna MR, Herndon SC, et al. Gas Turbine
459 Engine Emissions-Part II: Chemical Properties of Particulate Matter. *J Eng Gas Turbines Power-*
460 *Trans ASME* 2010;132(6):15, <https://doi.org/10.1115/1.4000132>.
- 461 [29] Moore RH, Shook M, Beyersdorf A, Corr C, Herndon S, Knighton WB, et al. Influence of Jet Fuel
462 Composition on Aircraft Engine Emissions: A Synthesis of Aerosol Emissions Data from the
463 NASA APEX, AAFEX, and ACCESS Missions. *Energy & Fuels* 2015;29(4):2591-600,
464 <https://doi.org/10.1021/ef502618w>.
- 465 [30] Lobo P, Christie S, Khandelwal B, Blakey SG, Raper DW. Evaluation of Non-volatile Particulate
466 Matter Emission Characteristics of an Aircraft Auxiliary Power Unit with Varying Alternative Jet
467 Fuel Blend Ratios. *Energy & Fuels* 2015;29(11):7705-11,
468 <https://doi.org/10.1021/acs.energyfuels.5b01758>.
- 469 [31] Saffaripour M, Zabeti P, Kholghy M, Thomson MJ. An Experimental Comparison of the Sooting
470 Behavior of Synthetic Jet Fuels. *Energy & Fuels* 2011;25(12):5584-93,
471 <https://doi.org/10.1021/ef201219v>.
- 472 [32] Won SH, Veloo PS, Dooley S, Santner J, Haas FM, Ju YG, et al. Predicting the global combustion
473 behaviors of petroleum-derived and alternative jet fuels by simple fuel property
474 measurements. *Fuel* 2016;168:34-46, <https://doi.org/10.1016/j.fuel.2015.11.026>.

475

476