SUPPLEMENTAL MATERIAL

to

Combustion Kinetics of Alternative Jet Fuels, Part-I: Experimental Flow Reactor Study

Patrick Oßwald¹, Julia Zinsmeister¹, Trupti Kathrotia¹, Maíra Alves-Fortunato², Victor Burger³, Rina van der Westhuizen³, Carl Viljoen³, Kalle Lehto⁴, Reetu Sallinen⁴, Kati Sandberg⁴, Manfred Aigner¹, Patrick Le Clercq¹, Markus Köhler¹

¹ Institute of Combustion Technology, German Aerospace Center (DLR), 70569 Stuttgart, Germany

² IFP Energies Nouvelles (IFPEN), 1 et 4 avenue de Bois-Préau, 92852 Reuil-Malmaison, Cedex, France

³ Sasol Energy, 1 Klasie Havenga Road, Sasolburg 1947, South Africa

⁴ Neste Corporation, Keilaranta 21, 02150 Espoo, Finland

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1 Inlet Flow conditions

In Table S1 the inlet flow conditions for the individual measurements at fuel-rich ($\Phi=1.2$) and fuel-lean ($\Phi=0.8$) conditions are shown. Stoichiometry Φ is calculated from the NMR (ASTM-D7171) results for Hydrogen content. Heteroatoms are neglected.

Table S1: Inlet Flow conditions for the individual measurements.

Fuel	Ar [g/min]	Fuel [mg/min]	O ₂ (Fuel-rich) [mg/min]	Φ	O ₂ (Fuel-lean) [mg/min]	Φ
ECLIF Ref 1	17.64	31.1	88.1	1.19	132.1	0.80
ECLIF Ref 2	17.64	31.1	88.1	1.20	132.1	0.80
ECLIF SSJF 1	17.64	31.4	89.7	1.20	134.5	0.80
ECLIF SSJF 2	17.64	31.4	89.9	1.20	134.8	0.80
ECLIF SSJF 3	17.64	31.2	88.5	1.20	132.8	0.80
ECLIF FSJF	17.64	31.3	88.9	1.20	133.4	0.80
SASOL IPK	17.64	31.67	91.77	1.20	137.65	0.80
SASOL IPK-A	17.64	31.3	89.2	1.20	133.8	0.80
SASOL Heavy Naphtha #1	17.64	31.5	90.4	1.20	135.6	0.80
SASOL Heavy Naphtha #2	17.64	30.7	84.94	1.20	127.4	0.80
SASOL Light Distillate #1	17.64	31.1	88.6	1.19	132.9	0.80
SASOL Light Distillate #2	17.64	30.78	85.83	1.20	128.74	0.80
ECLIF2/ND-MAX Ref 3	17.64	31.02	87.5	1.20	131.2	0.80
ECLIF2/ND-MAX Ref 4	17.64	31.19	88.6	1.20	132.9	0.80
ECLIF2/ND-MAX SAJF 1	17.64	31.3	89.3	1.20	133.9	0.80
ECLIF2/ND-MAX SAJF 2	17.64	31.34	89.6	1.20	134.4	0.80
ECLIF2/ND-MAX SAJF 3	17.64	31.17	88.4	1.20	132.6	0.80
ECLIF2/ND-MAX HEFA (JS-B2)	17.64	31.66	91.7	1.20	137.5	0.80
airegEM Ref	17.64	31.2	88.6	1.20	132.9	0.80
airegEM ReadJet™ (JS-B3)	17.64	31.1	87.7	1.20	131.5	0.80
airegEM ATJ (JS-B1)	17.64	31.7	92.1	1.19	138.2	0.80
ATJ-SKA	17.64	31.5	90.4	1.20	135.7	0.80
SIP (Farnesane)	17.64	31.6	91.2	1.20	136.8	0.80
FT-Light	17.64	31.7	92.0	1.19	138.0	0.80
DEMO-SPK Ref A/C	17.64	31.08	87.8	1.20	131.7	0.80
DEMO-SPK Ref Lab	17.64	31.13	88.1	1.20	132.2	0.80
DEMO-SPK MB A/C	17.64	31.27	89.1	1.20	133.6	0.80
DEMO-SPK MB SIP	17.64	31.2	88.7	1.20	133.0	0.80
JETSCREEN JS-A1	17.64	31.16	88.4	1.20	132.6	0.80
JETSCREEN JS-A1.3	17.64	31.31	89.4	1.20	134.0	0.80
JETSCREEN JS-B1	17.64	31.62	91.4	1.20	137.1	0.80
JETSCREEN JS-C1	17.64	30.69	85.2	1.20	127.9	0.80
JETSCREEN JS-C3	7.64	31.0	87.6	1.20	131.3	0.80
NJFCP A1 (JP-8: POSF 10264)	17.64	31.3	89.2	1.20	133.8	0.80
NJFCP A2 (Jet A: POSF 10325)	17.64	31.1	88.1	1.20	132.1	0.80
NJFCP A3 (JP 5: POSF 10289)	17.64	31.0	87.3	1.20	130.9	0.80
ACCESS2 Reference	17.64	31.1	87.9	1.20	131.8	0.80
ACCESS2 HEFA Blend (50:50)	17.64	31.4	90.0	1.19	135.0	0.80

Fuel	Ar [g/min]	Fuel [mg/min]	O ₂ (Fuel-rich) [mg/min]	Φ	O ₂ (Fuel-lean) [mg/min]	Φ
Neste Jet A-1 Ref	17.64	31.3	89.0	1.20	133.5	0.80
Neste HFP HEFA Blend 1	17.64	31.3	89.5	1.19	134.2	0.80
Neste HFP HEFA Blend 2	17.64	31.4	89.8	1.20	134.7	0.80
Neste HFP HEFA Neat	17.64	31.6	91.5	1.19	137.2	0.80

2 Fuel Composition and Decay

The detailed chemical composition as well as the fuel decay at fuel-lean ($\Phi=0.8$) conditions is shown on the next pages for one fuel per page. Use Table S2 and following description for identification of chemical classes.

Table S2: Definition of hydrocarbon classes

Formula	Hydrocarbon classes	IHD	W_H -range [mass-%]
C_nH_{2n+2}	n-Paraffins and iso-Paraffins	0	14.5-18.0
C_nH_{2n}	Mono-cyclic Paraffins (or Olefins)	1	14.0-15.0
C_nH_{2n-2}	Bicyclic Paraffins	2	12.5-14.0
C_nH_{2n-4}	Tricyclic Paraffins	3	11.5-13.0
C_nH_{2n-6}	Mono-cyclic Aromatics	4	7.5-12.5
C_nH_{2n-8}	Naphthenic-mono-Aromatics	5	8.5-12.0
C_nH_{2n-10}	Naphthenic-mono-Aromatics	6	7.5-11.0
C_nH_{2n-12}	Bicyclic Aromatics	7	6.0-11.5

Fuel Composition

The bar chart in the top left-hand corner of the page shows the detailed chemical fuel composition. Herein, each bar series show an individual hydrocarbon class (n-/iso-paraffins, mono-/bi-/tri-cyclic paraffins, mono-/bi-cyclic- and naphthenic-aromatics) with associated Index of Hydrogen Deficiency (IHD). Each HC-class is broken down to the number of carbon atoms in the molecule (z-axis: #C). Note, there is a differentiation between n- and iso-paraffins (first HC-class, IHD=0) shown as thinner (total paraffins) and thicker (n-paraffins) bars. The mass fractions (y-axis: y_i) of species i are plotted against their hydrogen content (x-axis: w_H). The color scale bar is used for better readability of the lower mass fraction values. The red lines reflect the average C-number and hydrogen content of the fuel.

Fuel Decay

The diagram in the top right-hand corner shows the mole fraction of the individual hydrocarbons within their HC-class at non-reactive inlet conditions. (Note, C_nH_{2n-4} and C_nH_{2n-10} are not shown.). The six figures below show in each case the fuel decay of a HC-class separated by the individual number of C-atoms at fuel-lean ($\Phi=0.8$) conditions.

ECLIF Ref 1

ECLIF Ref 2

ECLIF SSJF 1

ECLIF SSJF 2

ECLIF SSJF 3

ECLIF FSJF

SASOL IPK

SASOL IPK-A

SASOL Heavy Naphtha #1

SASOL Heavy Naphtha #2

SASOL Light Distillate #1

SASOL Light Distillate #2

ECLIF2/ND-MAX Ref 3

ECLIF2/ND-MAX Ref 4

ECLIF2/ND-MAX SAJF 1

ECLIF2/ND-MAX SAJF 2

ECLIF2/ND-MAX SAJF 3

ECLIF2/ND-MAX HEFA (JS-B2)

airegEM Ref

airegEM ReadiJet™ (JS-B3)

airegEM ATJ (JS-B1)

ATJ-SKA

SIP (Farnesane)

FT-Light

DEMO-SPK Ref A/C

DEMO-SPK Ref Lab

DEMO-SPK MB A/C

DEMO-SPK MB SIP

JETSCREEN JS-A1

JETSCREEN JS-A1.3

JETSCREEN JS-B1

JETSCREEN JS-C1

JETSCREEN JS-C3

NJFCP A1 (JP-8 POSF 10264)

NJFCP A2 (Jet-A POSF 10325)

NJFCP A3 (JP-5 POSF 10289)

ACCESS2 Reference

ACCESS2 HEFA Blend (50:50)

Neste Jet A-1 Ref

Neste HFP HEFA Blend 1

Neste HFP HEFA Blend 2

Neste HFP HEFA Neat