SUPPLEMENTAL MATERIAL

to

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

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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 $\Phi$ is calculated from the NMR (ASTM-D7171) results for Hydrogen content. Heteroatoms are neglected.

**Table S1: Inlet Flow conditions for the individual measurements.**

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Ar [g/min]</th>
<th>Fuel [mg/min]</th>
<th>$O_2$ (Fuel-rich) [mg/min]</th>
<th>$O_2$ (Fuel-lean) [mg/min]</th>
<th>$\Phi$</th>
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<tr>
<td>ECLIF Ref 1</td>
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<td>1.19</td>
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<td>90.0</td>
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<td>135.0</td>
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</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Formula</th>
<th>Hydrocarbon classes</th>
<th>IHD</th>
<th>(\text{W}_{\text{H}})-range [mass-%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(<em>n)H(</em>{2n+2})</td>
<td>n-Paraffins and iso-Paraffins</td>
<td>0</td>
<td>14.5-18.0</td>
</tr>
<tr>
<td>C(<em>n)H(</em>{2n})</td>
<td>Mono-cyclic Paraffins (or Olefins)</td>
<td>1</td>
<td>14.0-15.0</td>
</tr>
<tr>
<td>C(<em>n)H(</em>{2n-2})</td>
<td>Bicyclic Paraffins</td>
<td>2</td>
<td>12.5-14.0</td>
</tr>
<tr>
<td>C(<em>n)H(</em>{2n-4})</td>
<td>Tricyclic Paraffins</td>
<td>3</td>
<td>11.5-13.0</td>
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<tr>
<td>C(<em>n)H(</em>{2n-6})</td>
<td>Mono-cyclic Aromatics</td>
<td>4</td>
<td>7.5-12.5</td>
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<tr>
<td>C(<em>n)H(</em>{2n-8})</td>
<td>Naphthenic-mono-Aromatics</td>
<td>5</td>
<td>8.5-12.0</td>
</tr>
<tr>
<td>C(<em>n)H(</em>{2n-10})</td>
<td>Naphthenic-mono-Aromatics</td>
<td>6</td>
<td>7.5-11.0</td>
</tr>
<tr>
<td>C(<em>n)H(</em>{2n-12})</td>
<td>Bicyclic Aromatics</td>
<td>7</td>
<td>6.0-11.5</td>
</tr>
</tbody>
</table>

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\(_4\)H\(_{2n-4}\) and C\(_8\)H\(_{2n-10}\) 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.
SASOL Heavy Naphtha #2
ECLIF2/ND-MAX SAJF 2
airegEM ReadiJet™ (JS-B3)
DEMO-SPK Ref A/C

n/a
Neste HFP HEFA Blend 1

\[ \frac{x}{x_{\text{max}}} \]

\[ T/K \]

\[ C_8, C_9, C_{10}, C_{11}, C_{12}, C_{13}, C_{14}, C_{15} \]

\[ \phi = 0.8 \]

\[ C_{n=2}, C_{n=3}, C_{n=4}, C_{n=8}, C_{n=12} \]

\[ n/\text{a} \]