Thermal Stability Investigation using Ellipsometry

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Outline

• Introduction – Replacement of the JFTOT color standard

• Methods – Principles of Ellipsometry

• Results – Discussion of repeatability, increasing temperature, and increasing naphthalene concentration

• Conclusion
Introduction – Thermal Stability

• Defined as the degree to which a fuel breaks down when heated

• Poor thermal stability leads to engine component fouling and decreased fuel flow

• Important to understand to anticipate maintenance schedules and component wear
Introduction – Jet Fuel Thermal Oxidation Test

  – Resistively heat tubes to 260 °C
  – Flow fuel for 2.5 hours
  – Perform color and pressure tests
  – Increase temperature by 5 °C and repeat until failure
Introduction – Jet Fuel Thermal Oxidation Test

• Color standard


• 3 or greater is failing
Introduction – Implementation of Ellipsometry

• Ellipsometry added to ASTM D3241

• Benefits
  – Quantitative
  – Sensitive to small changes
  – Nondestructive
  – Versatile
Introduction – Sasol IPK and Naphthalene

• Sasol Iso-Paraffinic Kerosene: Fisher-Tropsch synthetic jet fuel
  – Mostly $C_{10}$ and $C_{12}$ isoparaffins (>95%)
  – Far fewer components than traditional jet fuels

• Naphthalene: 2 ringed aromatic additive
# Introduction – Fuel Composition

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Aromatics v%</th>
<th>Mercaptan Sulfur m%</th>
<th>Total Sulfur m%</th>
<th>Hydrogen Content m%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sasol IPK</td>
<td>0.5</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
<td>15.1</td>
</tr>
<tr>
<td>S-8</td>
<td>0.0</td>
<td>0.000</td>
<td>0.002</td>
<td>15.4</td>
</tr>
<tr>
<td>Jet A</td>
<td>18.7</td>
<td>0.001</td>
<td>0.21</td>
<td>14.09</td>
</tr>
<tr>
<td>JP-8</td>
<td>16.5</td>
<td>0.000</td>
<td>0.060</td>
<td>13.8</td>
</tr>
</tbody>
</table>

Methods – Tube Preparation with HLPS

• Tubes prepared with Hot Liquid Process Simulator

• Used JFTOT specifications except for tube substrate
Methods – Principles of Ellipsometry

- At an interface light reflects and refracts according to Snell’s Law

\[ n_0 \sin(\phi_i) = n_1 \sin(\phi_1) \]
Methods – Principles of Ellipsometry

• Reflection and refraction occurs at each interface
Methods – Principles of Ellipsometry

• Fresnel Relations used to track intensity and phase through each interface and calculates thickness

\[
R^p = \frac{r_{12}^p + r_{23}^p \exp(-j2\beta)}{1 + r_{12}^p r_{23}^p \exp(-j2\beta)}
\]

\[
R^s = \frac{r_{12}^s + r_{23}^s \exp(-j2\beta)}{1 + r_{12}^s r_{23}^s \exp(-j2\beta)}
\]
Methods – Modeling

• New amorphous dispersion formula used to model n and k change with wavelength

\[ k(\omega) = \sum_{j=1}^{N} \frac{f_j(\omega-\omega_g)^2}{(\omega-\omega_j)^2 + \Gamma_j^2} \text{ for } \omega > \omega_g \]

\[ n(\omega) = n_\infty + \sum_{j=1}^{N} \frac{B_j(\omega-\omega_j)}{(\omega-\omega_j)^2 + \Gamma_j^2} + C_j \]

\[ k(\omega) = 0 \text{ for } \omega \leq \omega_g \]

\[ B_j = \frac{f_j}{\Gamma_j^2} \left[ \Gamma_j^2 - (\omega_j-\omega_g)^2 \right] \]

\[ C_j = 2f_j \Gamma_j (\omega_j-\omega_g) \]

Horiba New Amorphous Dispersion Formula.
Results – Repeatability

- Tubes 1311 and 1329
  - Sasol IPK with 99% naphthalene
  - 385 K
  - 1334.87 and 1278.22 Å (4.2% difference)
Results – Increasing Temperature

- Deposit thickness increases with increasing temperature

![Graph 1](image1)

![Graph 2](image2)
### Results – Increasing Naphthalene Concentration

- Increasing naphthalene concentration increases deposit thickness

<table>
<thead>
<tr>
<th>Tube Number</th>
<th>Temperature (K)</th>
<th>Percent Naphthalene</th>
<th>Average Deposit Thickness (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1309</td>
<td>385</td>
<td>0</td>
<td>1037.438</td>
</tr>
<tr>
<td>1329</td>
<td>385</td>
<td>1</td>
<td>1278.222</td>
</tr>
<tr>
<td>1332</td>
<td>385</td>
<td>3</td>
<td>1307.806</td>
</tr>
<tr>
<td>1333</td>
<td>385</td>
<td>5</td>
<td>1796.44</td>
</tr>
</tbody>
</table>

- Opposite effect seen in aluminum tubes
Future Work

• Measure thermal stability of other fuels and additives using the same technique

• Perform more tests at identical conditions to better assess repeatability

• Create predictive model for deposit thickness
Conclusion

• Ellipsometry has been added to the thermal stability standard

• This method was shown to be repeatable

• Increasing temperature increases the deposit thickness

• Increasing naphthalene concentration increases deposit thickness
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Questions?