

# Thermal Stability Investigation using Ellipsometry

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# Outline

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- 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

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- 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

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- ASTM Standard D3241 “Standard Test Method for Thermal Oxidation Stability of Aviation Turbine Fuels”
  - 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



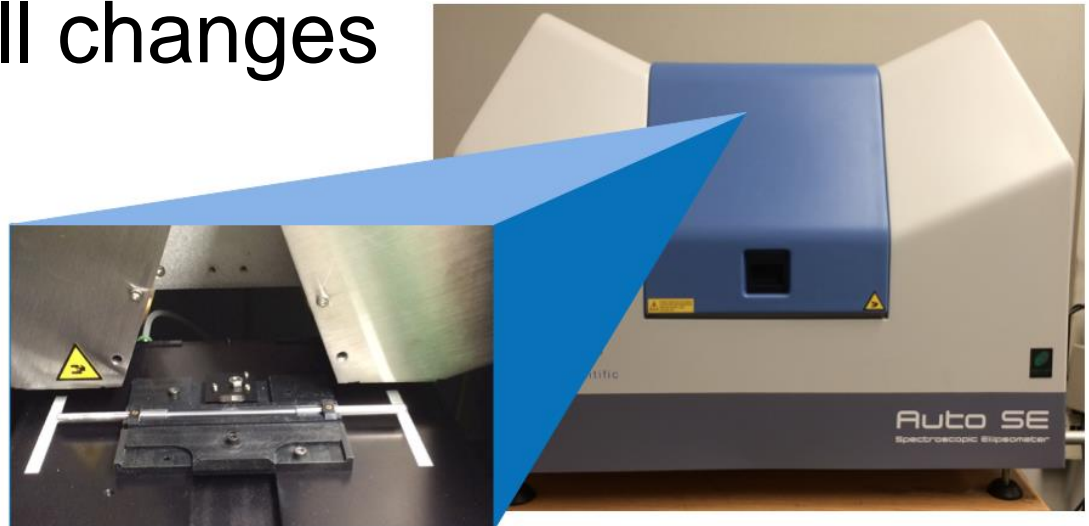
Browne, S. T., Wong, H., Hinderer, C. B., and Klettlinger, J. "Enhancement of Aviation Fuel Thermal Stability Characterization Through Application of Ellipsometry," 2012.

- 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

Fuel	Aromatics v%	Mercaptan Sulfur m%	Total Sulfur m%	Hydrogen Content m%
Sasol IPK	0.5	<0.001	<0.001	15.1
S-8	0.0	0.000	0.002	15.4
Jet A	18.7	0.001	0.21	14.09
JP-8	16.5	0.000	0.060	13.8

Moses, C. A. "Comparative evaluation of semi-synthetic jet fuels," *Contract* Vol. 33415, No. 02-D, 2008, p. 229



# Methods – Tube Preparation with HLPS

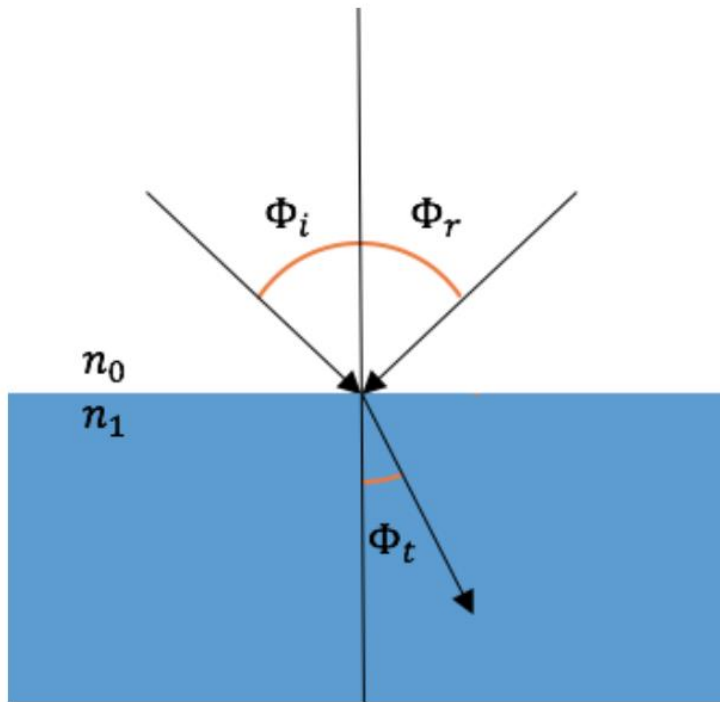
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- Tubes prepared with Hot Liquid Process Simulator
- Used JFTOT specifications except for tube substrate



# Methods – Principles of Ellipsometry

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

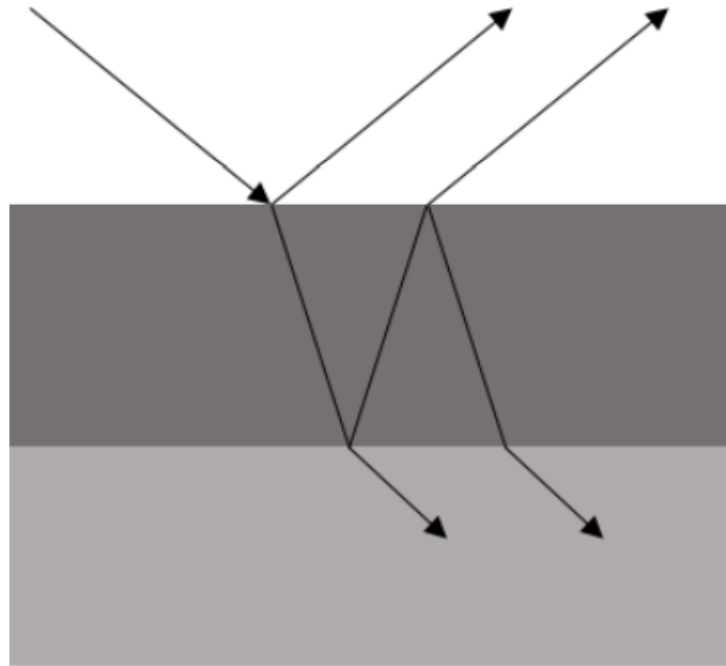


$$n_0 \sin(\phi_i) = n_1 \sin(\phi_1)$$



# 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

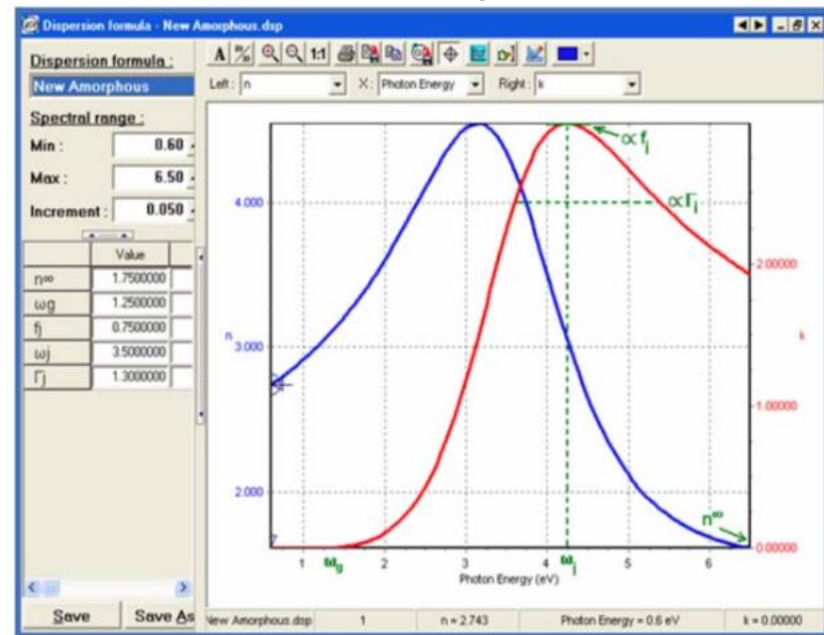
- New amorphous dispersion formula used to model n and k change with wavelength

$$k(\omega) = \sum_{j=1}^N \frac{f_j(\omega - \omega_g)^2}{(\omega - \omega_j)^2 + \Gamma_j^2} \text{ for } \omega > \omega_g \quad n(\omega) = n_{\infty} + \sum_{j=1}^N \frac{B_j(\omega - \omega_j) + C_j}{(\omega - \omega_j)^2 + \Gamma_j^2}$$

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

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

$$C_j = 2f_j\Gamma_j(\omega_j - \omega_g)$$



Horiba New Amorphous Dispersion Formula.



## Results – Repeatability

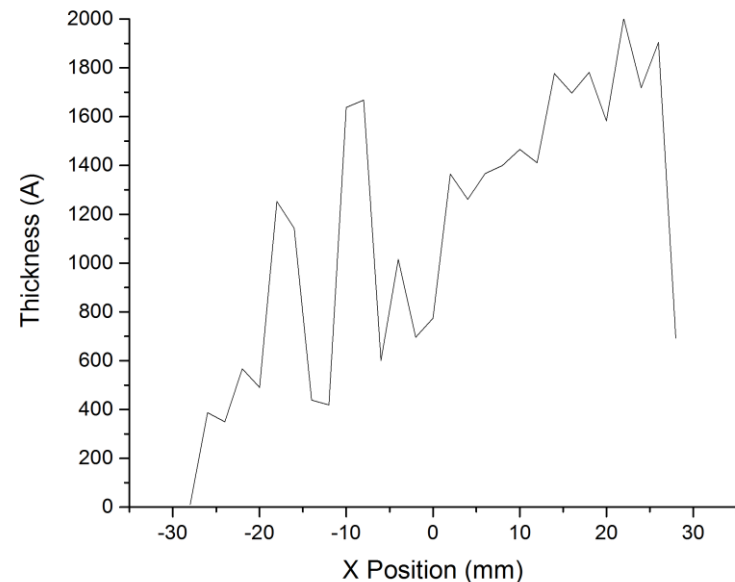
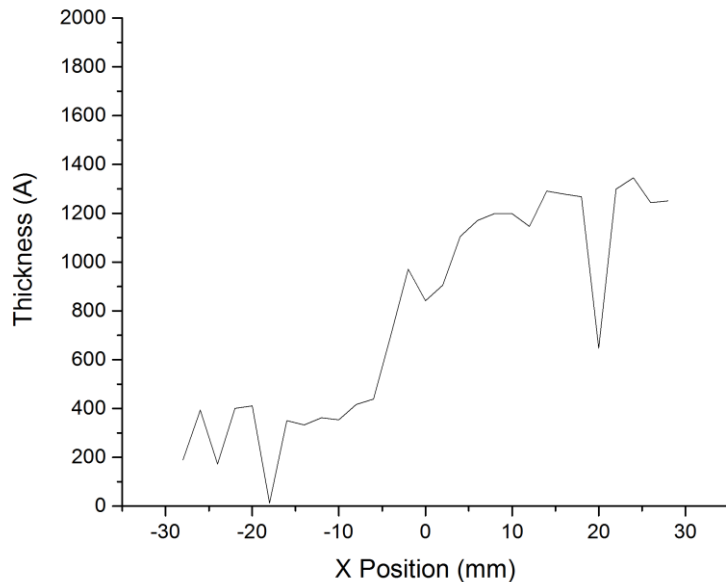
- Tubes 1311 and 1329
  - Sasol IPK with 99% naphthalene
  - 385 K
  - 1334.87 and 1278.22 Å (4.2% difference)





# Results – Increasing Temperature

- Deposit thickness increases with increasing temperature





## Results – Increasing Naphthalene Concentration

- Increasing naphthalene concentration increases deposit thickness

Tube Number	Temperature (K)	Percent Naphthalene	Average Deposit Thickness (Å)
1309	385	0	1037.438
1329	385	1	1278.222
1332	385	3	1307.806
1333	385	5	1796.44

- Opposite effect seen in aluminum tubes



## Future Work

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- 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

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- 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



# Acknowledgements

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- NASA Harriet G. Jenkins Fellowship
- Michelle Sestak and Celine Eypert from Horiba Scientific



# Questions?