

Measuring Total Naphthalene Hydrocarbons in Aviation Fuels by UV-Vis Spectroscopy

Optimizing photometric accuracy and streamlining data handling with the Agilent Cary 3500 UV-Vis



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Abstract

This study explores the application of UV-Vis spectroscopy as an efficient and straightforward method for the qualitative and quantitative analysis of naphthalene hydrocarbons in aviation fuels. Using the Agilent Cary 3500 UV-Vis spectrophotometer and Agilent Cary UV Workstation UV-Vis software, a simple workflow was developed to measure the total concentration of naphthalenes in three Jet A-1 fuel samples. Excellent method precision data are presented, confirming the potential of this technique in evaluating the quality, combustion properties, and potential environmental impact of fuels.

Introduction

UV-Vis spectroscopy can be used to provide a simple and quick qualitative analysis of aviation engine performance by measuring the concentration of component hydrocarbons in turbine fuel samples.

One method of evaluating aviation engine performance includes characterizing fuel combustion. Naphthalene, a hydrocarbon composed of two aromatic rings and classified as a polycyclic aromatic hydrocarbon¹, is commonly used as a fuel additive in kerosene. Low levels of acenaphthene and alkylated derivatives of these hydrocarbons may also be present in jet fuels. Although these naphthalenes constitute only a small percentage of a fuel sample's volume, they disproportionately contribute to the level of particulate matter in engine exhaust.² They also contribute soot, smoke, and thermal radiation as a result of incomplete combustion.³ Since these combustion properties indicate lower fuel efficiency and a higher risk of pollutant emissions⁴, it is essential to calculate the total concentration of naphthalene hydrocarbons in aviation fuel.

Through qualitative absorbance measurements and quantitative calculations, the total concentration of naphthalene in a jet fuel sample can be determined by UV-Vis spectroscopy. This application note demonstrates the benefits of the Agilent Cary 3500 UV-Vis spectrophotometer and Agilent Cary UV Workstation v1.6 for determining the total concentration of naphthalene hydrocarbons in three Jet A-1 fuel samples.

Experimental

Sample preparation

Solvent control: Spectroscopic grade isooctane (2,2,4-trimethylpentane, Sigma-Aldrich, part number 1047182500, CAS No. 540-84-1). Three milliliters of isooctane was transferred into a standard 3.5 mL, 10 mm optical pathlength, quartz cuvette (Agilent Technologies, part number 5061-3387). Three solvent controls were prepared and used as a blank for the samples.

Samples 1 to 3: 0.075 mL aliquots of three Jet A-1 fuel samples (bought locally) were pipetted into clean, dry, tared 100 mL volumetric flasks. The mass of each sample was recorded to the nearest 0.0001 g (64.1, 63.4, and 65.5 mg, respectively), then diluted with spectroscopic-grade isooctane to the mark, stoppered, and mixed thoroughly. Three milliliters of the solution was then transferred into a 10 mm quartz cuvette, ready for analysis.

Instrumentation

Once the solvent control and sample cells had been prepared, the absorbance was measured using an Agilent Cary 3500 Multicell UV-Vis (Figure 1), using the parameters listed in Table 1. The Multicell module enables a user to measure up to seven samples and a reference simultaneously. In this experiment, the three fuel samples were measured altogether, and absorbance spectra were collected on one graph. The absorbance measurements of the samples were then compared to the spectroscopic isooctane (solvent control) at 285 nm.



Figure 1. The Agilent Cary 3500 Multicell UV-Vis spectrophotometer.

Table 1. Agilent Cary 3500 Multicell UV-Vis data collection parameters.

Parameter	Value
Spectral Range	240 to 350 nm
Signal Averaging Time	0.1 s
Data Interval	1 nm
Spectral Bandwidth	1 nm

Results and discussion

Qualitative and quantitative analysis of samples

The Cary UV Workstation v1.6 includes functional tools that help users produce and analyze results within a single program, simplifying the analysis. Both the operating parameters and calculation methods were set up using a new batch within the Scan application program. Users can choose to collect absorbance over a wavelength range or at a specified wavelength or wavelengths. In this study, the 240 to 350 nm wavelength region was scanned so that the shape of the absorbance spectrum could be analyzed.

To evaluate the concentration of total naphthalene present within the jet fuel samples, three calculations were input into the "end of sequence analysis" feature, as shown in Figure 2.

Analysis 1 was used to calculate the volume percentage (volume %) of naphthalenes in the samples, using mass percentage (mass %), and relative density values of the naphthalenes (1) and fuel (0.8).⁵

Analysis 2 was used to calculate the mass percentage (mass %) of naphthalenes in the jet fuel samples using the absorbance value at 285 nm (A), mass of respective sample in grams (W), and two constants, 0.10 (K) and the average absorptivity of the C₁₀ to C₁₃ naphthalenes at 285 nm, 33.7 L/g·cm.³ Weight was added into the sequence analysis setup, using the customizable parameters feature, which allows the user to tailor the variable and unit to their choice (Figure 2).

Analysis 3 was used to find the absorbance (Abs) at 285 nm, using the "value at (285)" equation.

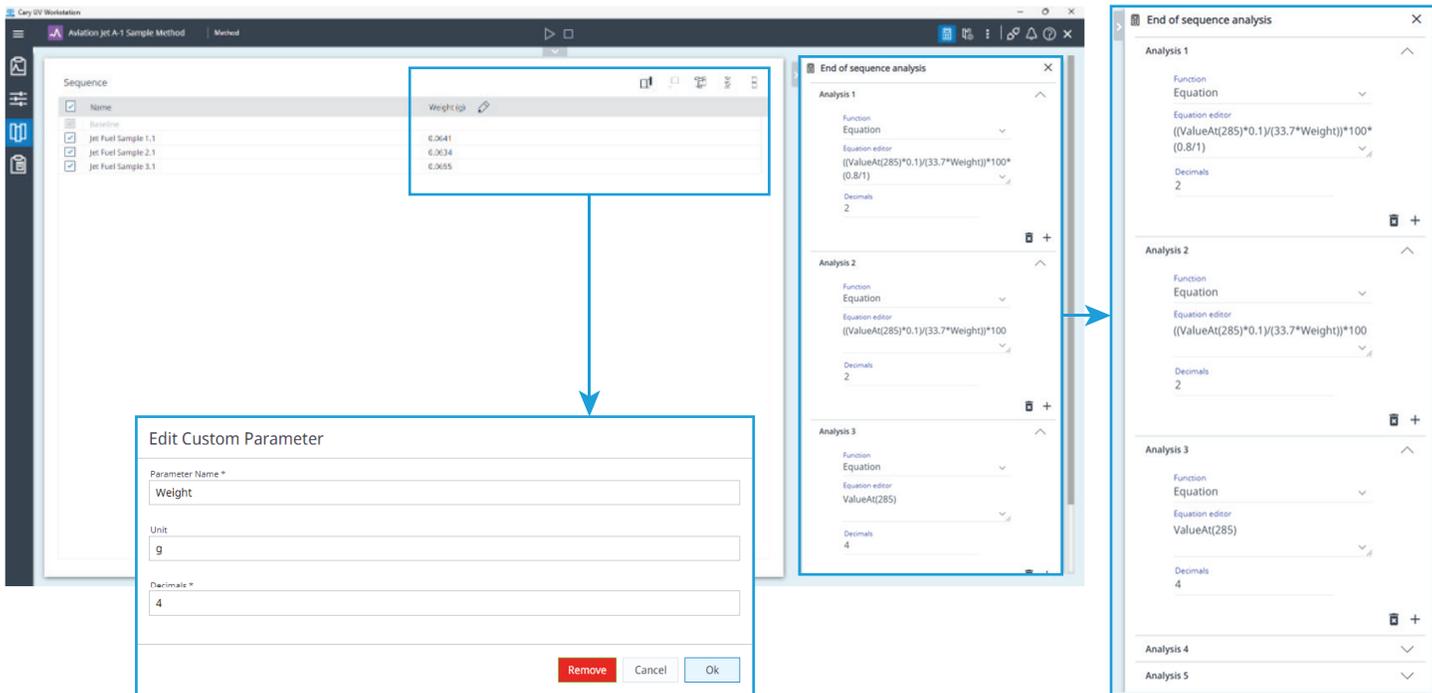


Figure 2. The sequence setup page in Agilent Cary UV Workstation v1.6, which allows users to create the test and calculation methods. Sample weight was added as a custom parameter (bottom) and three calculations (right) were input into the end of sequence analysis section of the page.

Once the measurement of the samples was complete, the Cary UV Workstation v1.6 produced a scalable graph of the specified wavelength region, as shown in Figure 3. All three of the end of sequence analysis calculations returned easy-to-read tables of values. Decimal places were set up to four for Abs and two for mass and volume %. The volume % of naphthalene hydrocarbons in each respective jet fuel sample was then reported to the nearest 0.01 %, as shown in Table 2.

The Cary UV Workstation v1.6 determined the volume % of naphthalenes in the jet fuel samples without needing to perform any calculations offline or to export data to another program. Both the data collection parameters and data analysis method were saved as a test method to streamline the setup of future experiments. Creating a test method for the analysis of naphthalenes eliminates the need to re-enter analysis settings, enabling a faster, more efficient workflow and allowing users to focus on their analysis rather than on method setup.

Table 2. Volume percentage of naphthalenes in each jet fuel sample, reported to two decimal places.

	Sample 1	Sample 2	Sample 3
Volume % of Naphthalene in Jet Fuel Sample	1.00	1.08	1.36

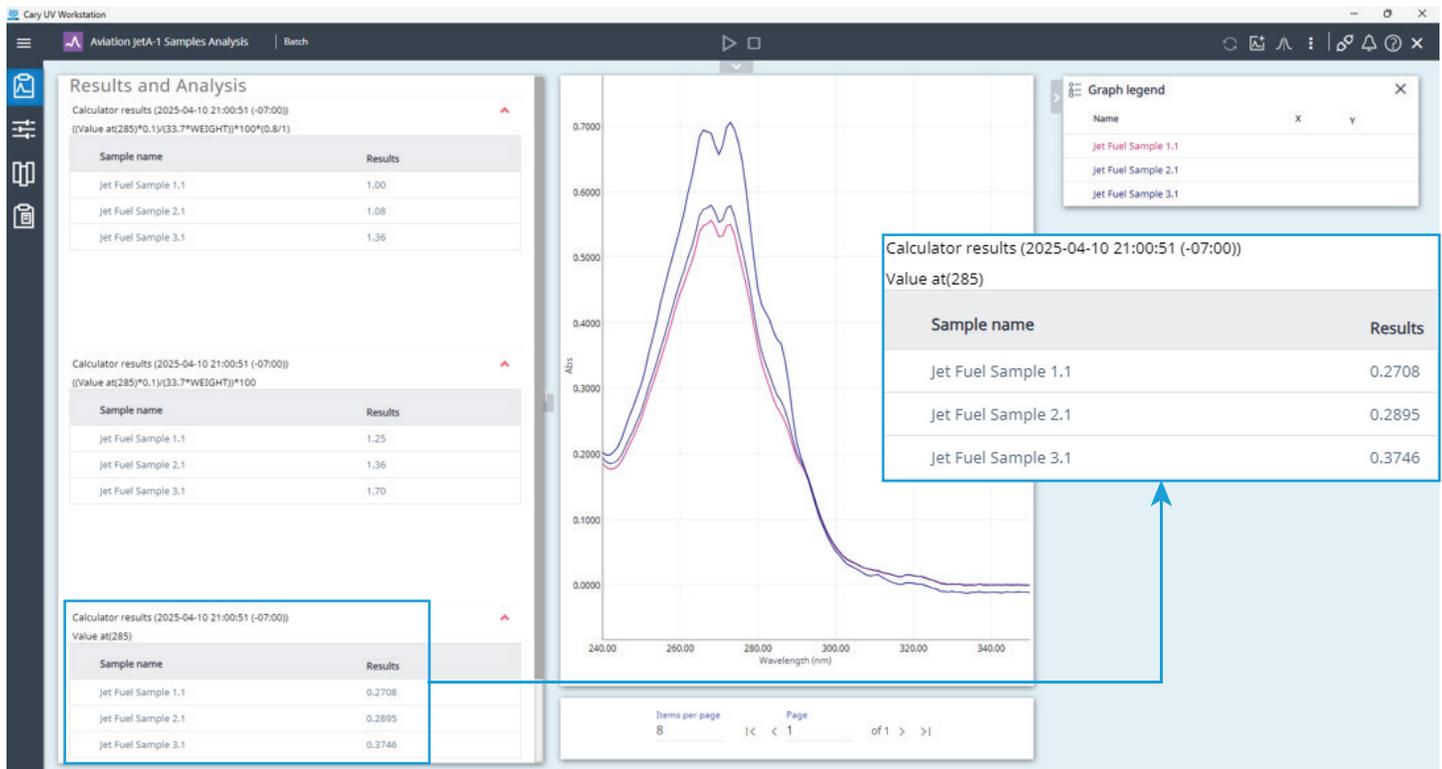


Figure 3. The Agilent Cary UV Workstation v1.6 returns data in a simple table of values format, allowing users to conduct relevant quantitative analysis upon measurement.

Report generation

The Cary UV Workstation v1.6 consolidates the qualitative and quantitative results into a report. As shown in Figure 4, the report for this study was customized to include content such as data calculations with table of values, a scaled graph to show the 285 nm region, plus other options. Report content preferences can also be saved as part of the test method. The report for the three jet fuel samples was then generated as a PDF.

Method precision

The precision of the Cary 3500 UV-Vis method was evaluated through repeatability and reproducibility tests.

Repeatability: To assess repeatability, 20 successive measurements were performed on each sample under constant operating conditions. As shown in Table 3, the low calculated standard deviation values for the respective measurements highlights the consistency of the absorbance readings. This level of stability is important for photometric accuracy.

Table 3. Average and variation of 20 absorbance measurements of each jet fuel sample.

	Sample 1	Sample 2	Sample 3
Average of Absorbance at 285 nm (Abs)	0.2691	0.2933	0.3748
Standard Deviation (Abs)	0.0004	0.0004	0.0005

Figure 4. The Agilent Cary UV Workstation v1.6 enables users to automatically export reports in PDF or CSV formats at the end of sequence acquisition. Users can define a custom export location for these reports, customize the report content by selecting or deselecting specific elements based on their preferences, and scale graphs to highlight the region of interest.

Scan report
File name: Aviation JetA-1 Samples Analysis

W mode	F mode	Averaging time (s)	Scanned bandwidth (nm)
nm	Absorbance	0.100	1.00

Data interval (nm)	Scan range start (nm)	Scan range stop (nm)
1.00	350.00	240.00

Detector module: Multiple experiments
 MultiCell Peltier UV-VIS
 Equilibrium temperature (°C): 1 zone
 Zone 1: N/A

Status: On

End of sequence analysis

Analysis 1	Equation ((ValueAt(285)*(3.14159*(33.7*Wavelength)^100)^0.81)); Decimals: 2
Analysis 2	Equation ((ValueAt(285)^0.1)*(33.7*Wavelength)^100); Decimals: 2
Analysis 3	Equation (ValueAt(285)); Decimals: 4

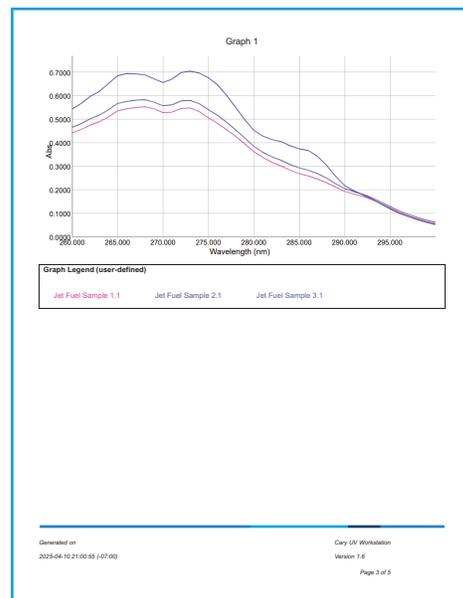
Engine name	Engine serial number	Module serial number
MP23162A05	MP23162A05	MP2320203

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Sample information

Jet Fuel Sample 1.1	Weight (g)	0.0641
Jet Fuel Sample 2.1	Weight (g)	0.0634
Jet Fuel Sample 3.1	Weight (g)	0.0655

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Analysis 1 results (2025-04-22 21:30:47 (-07:00))
 ((Value at(285)^0.1)*(33.7*WEIGHT)^100)^0.81)

Sample name	Results
Jet Fuel Sample 1.1	1.00
Jet Fuel Sample 2.1	1.00
Jet Fuel Sample 3.1	1.30

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Report preferences

Export locations

Report (.pdf) - C:\Users\test\Desktop\Naphthalene Jet A-1 Fuel
 Report (.csv) - C:\Users\test\Desktop\Naphthalene Jet A-1 Fuel

Report contents

- Method Setup
- Sample Information
 - Weight (g)
- Graphs
 - Graph 1
- Results and Analysis
 - Analysis 3 results (2025-04-22 21:30:47 (-07:00))
 - Analysis 2 results (2025-04-22 21:30:47 (-07:00))
 - Analysis 1 results (2025-04-22 21:30:47 (-07:00))
- Hidden Traces
- Report Preferences

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Figure 5. The generated scan report for the three jet fuel samples.

An acceptance range was calculated based on average volume % of naphthalene measured in the respective jet fuel sample across the 20 runs under consistent conditions.³ As shown in Table 4, the acceptance values for the samples were calculated as $\pm 0.18\%$ for Sample 1, $\pm 0.19\%$ for Sample 2, and $\pm 0.21\%$ for Sample 3. The variation (standard deviation) in volume % naphthalene across the runs was also calculated for each sample to assess how individual measurements deviated from the mean.

The Cary 3500 Multicell UV-Vis provided consistent and repeatable measurements, as demonstrated by the calculated variation values of $\pm 1.42 \times 10^{-3}\%$ for Sample 1, $\pm 1.61 \times 10^{-3}\%$ for Sample 2, and $\pm 1.96 \times 10^{-3}\%$ for Sample 3. As shown in Table 4, the observed variation in volume % naphthalene for each sample was well within the accepted repeatability range, confirming the instrument's ability to perform precise measurements.

Table 4. Repeatability test results for measurements of three jet fuel samples, n = 20.

	Sample 1	Sample 2	Sample 3
Average (Vol % of Naphthalene)	1.00	1.10	1.36
Repeatability Criteria (%)	± 0.18	± 0.19	± 0.21
Standard Deviation (Vol % of Naphthalene)	1.42×10^{-3}	1.61×10^{-3}	1.96×10^{-3}

Reproducibility: To establish precision and consistency in absorbance measurements between instruments, a second Agilent Cary 3500 was employed, and another 20 successive runs were performed using the same three sample test materials. The small standard deviation of the results obtained from the separate, independent sample analysis demonstrated excellent reproducibility of the method and instruments (Table 5).

Table 5. Average and variation across 20 absorbance measurements of each jet fuel sample, performed by a second operator.

	Sample 1	Sample 2	Sample 3
Average of Absorbance at 285 nm (Abs)	0.2715	0.2916	0.3755
Standard Deviation (Abs)	0.0002	0.0003	0.0002

An acceptance range for reproducibility was calculated based on variation in measurements between operators.³ The average volume % of naphthalene was calculated using the second Cary 3500 Multicell UV-Vis, and the acceptance values for the samples were calculated as $\pm 0.24\%$ for Sample 1, $\pm 0.26\%$ for Sample 2, and $\pm 0.29\%$ for Sample 3 (Table 6). By comparing the variation in results obtained by different operators, measurement precision across instruments could be established.

Table 6. Reproducibility test results for measurements of three jet fuel samples performed by a second operator, n = 20.

	Sample 1	Sample 2	Sample 3
Average (Vol % of Naphthalene)	1.01	1.09	1.36
Reproducibility Criteria (%)	± 0.24	± 0.26	± 0.29
Standard Deviation (Vol % of Naphthalene)	7.73×10^{-4}	1.18×10^{-3}	8.10×10^{-4}

The variation (standard deviation) values for the measurements of $\pm 7.73 \times 10^{-4}\%$ for Sample 1, $\pm 1.18 \times 10^{-3}\%$ for Sample 2, and $\pm 8.10 \times 10^{-4}\%$ for Sample 3 were well within the accepted reproducibility range.

As shown in the summary provided in Table 7, the absorbance values and calculated volume % of naphthalene of the samples were significantly similar between the two instruments, demonstrating consistency of the method. In addition, differences in standard deviations between the instruments indicated a low degree of operator-based variation. The calculated standard deviations illustrated the instruments' ability to provide repeatable, reproducible, and reliable absorbance measurements, across multiple runs.

Table 7. Comparison of variation of absorbance and volume % of naphthalene for the same three jet fuel samples measured by two instruments.

		Instrument 1	Instrument 2
Abs at 285 nm	Sample 1	0.2691 ± 0.0004 Abs	0.2715 ± 0.0002 Abs
	Sample 2	0.2933 ± 0.0004 Abs	0.2916 ± 0.0003 Abs
	Sample 3	0.3748 ± 0.0005 Abs	0.3755 ± 0.0002 Abs
Naphthalene, Volume %	Sample 1	$1.00 \pm 1.42 \times 10^{-3}\%$	$1.01 \pm 7.73 \times 10^{-4}\%$
	Sample 2	$1.10 \pm 1.61 \times 10^{-3}\%$	$1.09 \pm 1.18 \times 10^{-3}\%$
	Sample 3	$1.36 \pm 1.96 \times 10^{-3}\%$	$1.36 \pm 8.10 \times 10^{-4}\%$

Conclusion

The Agilent Cary 3500 Multicell UV-Vis spectrophotometer and Agilent Cary UV Workstation v1.6 software enabled an efficient and straightforward analysis of the total concentration of naphthalene hydrocarbons in jet turbine fuels. The reliability of the Cary 3500 was demonstrated through its precise and repeatable absorbance measurements.

Retrieving saved methods and using automated in-sequence calculations in the software streamlined data collection and analysis, eliminating the need for manual input, offline calculations, or external software. Also, the integrated reporting functionality within the software ensured efficient result consolidation and facilitated easy information review.

The Cary 3500 Multicell UV-Vis with Cary UV Workstation v1.6 provides a fast, reliable, robust, and user-friendly methodology for fuel quality assessment.

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DE-005997

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Printed in the USA, April 30, 2025
5994-8266EN