Exploring the relationship between ergonomics and measurement quality in handheld FTIR spectrometers

Application note

Materials testing

Authors

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Introduction

The differences in spectrometers designed for use in the lab from those that are deployed at-site, in field locations are rather profound. As an example, laboratory instruments are designed to work on a planar horizontal surface — the bench top — whereas handheld spectrometers are often called upon to operate in virtually every physical position. Interferometers used in lab FTIR spectrometers perform quite well in the aforementioned horizontal position, but many cannot even scan if the measurement requires vertical positioning. For this reason, Agilent handheld FTIR systems have an innovative interferometer design that affords the same quality of data in any physical position that the application demands.

As important as optomechanical design, ergonomic considerations play a critical role in optimizing performance of handheld FTIR spectrometers. The mechanics of holding an object at arm's length are well understood; the force that bicep muscles must exert to hold one's forearm with a handheld object is many times greater than just the weight of the object. For this reason, holding even seemingly light objects over a period of time becomes tiresome. This can, in turn, affect the quality of data acquired by a handheld FTIR spectrometer, since typically a number of interferograms are co-added over a period of time (typically 10–30 s) to improve signal-to-noise. Data quality in all spectroscopic measurements is strongly affected by the position of the sample relative to the focus on the light beam; when the sample is at the optimum focus of the infrared light, the highest quality results are obtained. In the case of handheld FTIR, the user holds the spectrometer up to the sample. The user's ability to hold the system stable at focus will result in the best quality data, but physical stability may be hindered if the user's arm becomes tired or strained.

Of course, this implies that a lighter weight system is preferred over a heavier one, but that is only part of the issue. The center of gravity of the system must be optimized as well. If the spectrometer's center of gravity is located above the hand that is holding it, muscles will tire even more rapidly, resulting in unwanted movement that affects data quality. In contrast, a system with a properly positioned center of gravity causes less strain and less potential for movement during data acquisition.

For these reasons, the Agilent 4300 Handheld FTIR is designed to be as light as possible as well as perfectly balanced for handheld use. These ergonomic considerations, combined with the performance advantages offered by an ultra-short internal optical path, highly stable optomechanics and low noise electronics, ensures that the user will obtain the best possible spectral data and most accurate results.

In this application note, we will show the advantage in measurement quality offered by the 4300 Handheld FTIR, an ergonomically superior spectrometer for at-site, field use.

Ergonomic considerations in the design of the 4300 Handheld FTIR

- Weight — At 1.95 kg (4.8 lbs), the 4300 is the lightest handheld FTIR system currently available. The measured weight includes two Li ion batteries, the internal computer and the sampling interface.
- Center of Gravity — The center of gravity of the 4300 Handheld FTIR is exactly in the middle of the handle and at the trigger (Figure 1). This mean less torque acting on the user's wrist and greater overall physical stability.

Figure 1. Agilent 4300 Handheld FTIR. The center of gravity is located in the center of the handle as shown by the black dot. This balances the instrument in the users hand, providing superior ergonomics for consistent data collection.

- Control Trigger — The single control trigger is located where the index finger naturally falls when holding the system.
- User screen — The screen is articulated and is easily read regardless of the position of the 4300 Handheld FTIR or amount of ambient light present.
- Sample interface selection — Changing the sample interface is a simple one hand operation that takes seconds to accomplish.

Method and measurements

To show the advantages of ergonomic design on data quality, we will employ a model experiment to contrast the performance of the new 4300 Handheld FTIR with that of the older generation Agilent 4100 Exoscan system. The Exoscan system weighs 1 kg (2.2 lbs) more than the 4300 Handheld FTIR system and the center of gravity of the older system is located approximately 10 cm (2.5 in) above the supporting handle.

The data set for this study was collected from a series of coatings used in a composite aerospace application. The coating was comprised of six distinct samples: epoxy resin, primer, basecoat, topcoat 1, topcoat 2, and topcoat 3. Handheld measurements were made on this sample set with the samples mounted on a wall approximately 2.1 m (7 ft) from the ground. An experienced technician made all the measurements; the height of the samples required measurement with an outstretched arm. All measurements were made using the external reflectance sample interface, collecting 32 scans at 8 cm^{-1} resolution for both the background and the sample, resulting in an 8 second measurement time. Even at these short collection times, the positive effects of greater ergonomics can be observed.

Handheld spectra collected from both the 4100 ExoScan and the new 4300 Handheld FTIR were compared in several ways. First, a library of several materials in a composite coating system was created for each system; during the data collection for the library, each instrument was placed in its desktop stand to allow for the sample to be placed precisely at sample focus and held steady throughout the data collection. The desktop library was correlated to the handheld measurement and the correlation factors were compared. Secondly, the baseline noise in the region from 2750–2550 cm^{-1} was compared for each measurement. Baseline noise in this non-absorbing region can be due to variation in focus throughout the measurement.

Results and discussion

Differences can be observed between handheld spectra collected on the 4300 Handheld FTIR versus the 4100 ExoScan (Figure 2). Both systems exhibit typical specular reflectance data on the sample of epoxy resin shown. The 4100 ExoScan data shows considerably more noise, primarily in the baseline region; however, it can be seen to affect the band shape near 1700, 1480, and 1325 cm^{-1}. These small changes in the band shape can affect the ability to measure small changes in the coating due to additives or oxidative damage.

The library comparison also shows superior performance for the 4300 Handheld FTIR. Since the libraries used in this comparison were developed individually on each instrument, correlation values less than ideal (R^{-1}=1.0) are due to instability in sample focus. The results of the library experiment are tabulated in Table 1. In 14 out of 18 samples, the handheld data collected on the 4300 Handheld FTIR had a higher correlation than data for the same sample collected on the 4100 ExoScan. Additionally, the average correlation value for the 4300 Handheld FTIR was higher than the average value for the 4100 ExoScan. Most interestingly, though, the standard deviation in correlation values for the 4300 Handheld FTIR was half that of the 4100 ExoScan. The standard deviation demonstrates that the increased ergonomics of the 4300 handheld FTIR allows for more consistent, reproducible measurement.

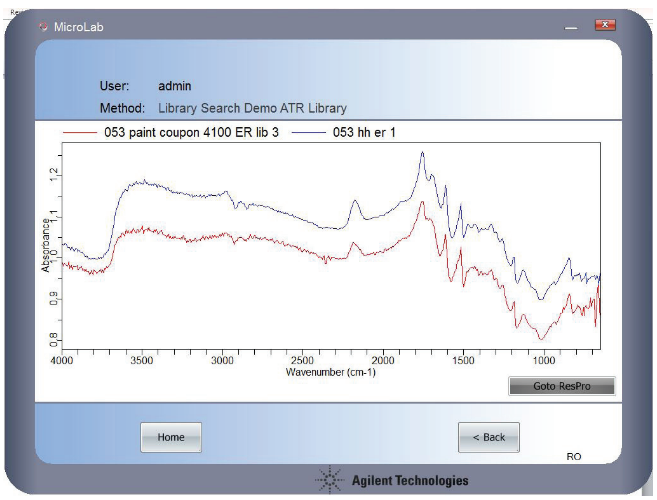

Figure 2. Comparison between handheld data of an epoxy resin sample collected on the 4100 ExoScan (red) and the new 4300 Handheld FTIR (blue) with improved ergonomics. The 4300 Handheld FTIR spectrum has less baseline noise and greater band definition due to the user's ability to hold the instrument steady, even during an overhead measurement.

Table 1. Results of library test comparing correlation of handheld measurements to the top match of library data collected on a stationary instrument. The increased average correlation and the decreased standard deviation in correlation measurements show the positive effect of the more ergonomic 4300 Handheld FTIR system.

Sample	4100 ExoScan correlation	4300 Handheld FTIR correlation
Epoxy resin	0.981	0.991
	0.980	0.996
	0.987	0.995
Primer	0.912	0.980
	0.936	0.977
	0.931	0.989
Basecoat	0.994	0.992
	0.994	0.997
	0.993	0.998
Topcoat 1	0.987	0.957
	0.988	0.986
	0.973	0.960
Topcoat 2	0.985	0.998
	0.990	0.999
	0.990	0.992
Topcoat 3	0.989	0.990
	0.985	0.998
	0.989	0.982
Average	0.977	0.988
Standard deviation	0.024	0.012

Another comparison was made by measuring the baseline noise from each of the above sample measurements. The RMS noise was measured in the region from 2750–2550 cm^{-1}. This region contains no spectral bands. Baseline noise increases as the intensity of light falling on the detector decreases. Using the external reflectance sample interface, the amount of light falling on the detector (and therefore the baseline noise) is directly correlated to accuracy of sample focus. When the instrument is held steady to the sample at a consistent sample focus, the baseline noise is minimized. A summary of results is shown in Table 2. While both instruments show impressive performance, the average baseline noise in the 4300 Handheld FTIR measurements is 35% lower than that of the 4100 ExoScan measurements.

Table 2. RMS noise measured from 2750–2550 cm^{-1} on the coating samples for both the 4100 ExoScan and 4300 Handheld FTIR systems. The 4300 Handheld FTIR shows less baseline noise for handheld measurements due to improved ergonomics.

Sample	4100 ExoScan baseline noise	4300 Handheld FTIR baseline noise
Epoxy resin	0.00197	0.00133
	0.00316	0.00165
	0.00240	0.00145
Primer	0.00196	0.00084
	0.00199	0.00063
	0.00157	0.00066
Basecoat	0.00252	0.00281
	0.00297	0.00269
	0.00242	0.00262
Topcoat 1	0.00160	0.00080
	0.00155	0.00080
	0.00165	0.00099
Topcoat 2	0.00150	0.00093
	0.00155	0.00097
	0.00155	0.00081
Topcoat 3	0.00183	0.00097
	0.00164	0.00063
	0.00137	0.00119
Average noise	0.00196	0.00126

Conclusion

Portable and handheld spectrometers must be designed and engineered for the environment in which they perform. These considerations extend to the optomechanics, electronics, software, user interface and serviceability perspective. Of equal importance is user comfort since we have shown that higher quality data can be generated by an ergonomically superior handheld spectrometer. This factor results from the need for the spectrometer to be physically stable while acquiring data in an environment or orientation. Moreover, because of ergonomic design, the 4300 Handheld FTIR will cause less strain on the user’s body.

Superior ergonomic design was one of the major product development goals for the Agilent 4300 Handheld FTIR and has been achieved, thus enhancing both the user experience and the resultant acquired information. For applications where at-site, field measurements are frequent, the 4300 Handheld FTIR is the system of choice.

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