APPLICATION NOTE

Common Misconceptions of FTIR in Field Operations

RedWave TECHNOLOGY

Myth: FTIR cannot work in high humidity or carbon dioxide rich environments.

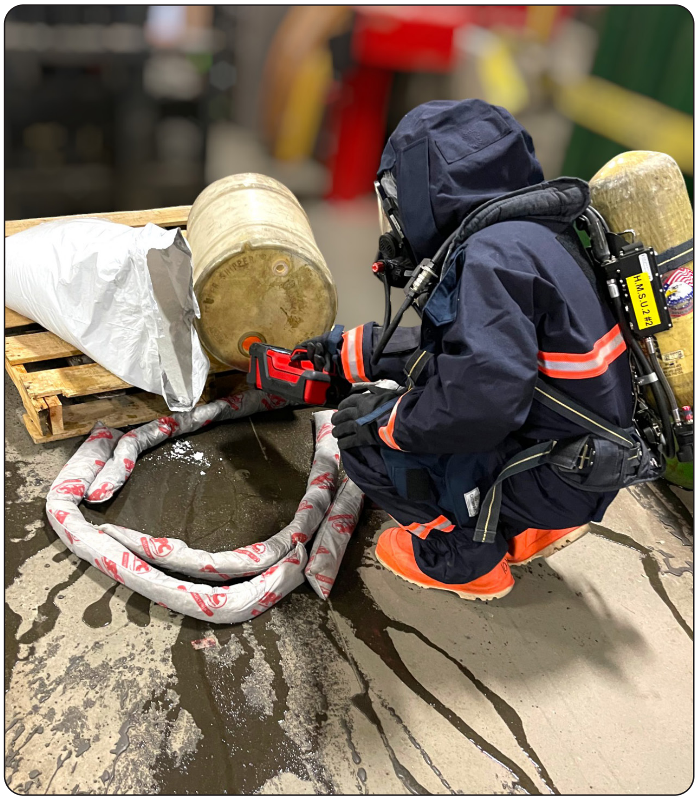
The RedWave Technology team solves this by using a new concept known as Adaptive Atmospheric Correction to not only remove water vapor and CO2 from the sample spectrum, but extract any underlying sample peaks, which is done by utilizing another technique known as Intelligent Subspace Scaling. Using these two approaches, water vapor and CO2 no longer have a significant influence on whether a correct identification is achieved.

Myth: Gas Phase FTIR cannot see threat materials at operationally relevant concentrations.

In HazMat/CBRN response, gases and vapors present the greatest danger as they can be toxic at low concentrations and flammable, corrosive, and/or reactive at higher concentrations. Therefore, it is critical to not only detect and quantify the threat, but also to uniquely identify it.

While gas phase FTIR systems have been available for field operations for the past decade, the data was often not operationally relevant due to environmental interferences and high limits of detection. The optimum detection system for either detect-to-warn or detect-to-protect operations uses continuous sampling to find the source and estimate its concentration in less than a minute. These systems must be able to measure in the low ppm range to ensure that they can detect at the appropriate protective action criteria or workplace exposure standards.

In the USA, OSHA sets enforceable permissible exposure limits (PELs) which are airborne concentrations of hazardous chemicals over which a worker must be provided protection.



These numbers are derived over an 8-hour time weighted average to accommodate the workday and may also include ceiling and peak values. In addition to the OSHA PELs, there are State-based systems (e.g., California PELs), federal recommendations (e.g., National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limits (RELs)), and non-Governmental (e.g., ACGIH Threshold Limit Values) that should be taken into consideration.

The RedWave Technology team has addressed environmental issues using a combination of Adaptive Atmospheric Correction and Intelligent Subspace Scaling. The limits of detection, and more importantly the limits of identification, were greatly reduced by increasing the length of the gas cell to 2 meters (multi-pass) while maintaining a small overall system size.

Like all gas measurement technologies, the XplorIR has a minimum concentration required for measurement. This limit of identification (LOI) varies by chemical. When using the XplorIR to evaluate 47 highly toxic gases identified in threat lists, 72% were found to have an estimated LOI less than 25 ppm and 45% have an estimated LOI less than 10 ppm. Therefore, the XplorIR provides unique identification at toxicologically relevant levels (workplace exposure limits and immediately dangerous to life and health levels).

Myth: FTIR sample preparation is too complex and time consuming.

There is very little sample preparation required with the current commercially available products. There are techniques available for sample clean up and preparation, but those are generally relegated to lab samples.

For solids and liquids, a sample does need to be taken and transferred to the FTIR sample interface. Gathering a representative sample is the most important and time-consuming part of the process; this step is inherent to all sampling strategies, not just those associated with FTIR.

For gas phase samples, it will depend upon the system that you are using. For example, the RedWave XplorIR allows you to bring the instrument to the area of interest and run either a continuous monitoring or point source sample, neither of which require any special sampling protocols. If using the RedWave ThreatID with the gas interface, you have the option to bring the instrument to the area of interest and running the samples inline with a photoionization detector (or another suitable detector with an inline pump) or you can take a sample and bring it to the instrument.

In fact, the RedWave XplorIR is the only system commercially available which can provide continuous monitoring at operationally relevant concentrations while also uniquely identifying the threat. The system will continuously monitor to find the threat material and will automatically apply the advanced data analytics when sufficient signal is present allowing for a hands-off approach from the operator between detection and identification. The RedWave XplorIR identifies over 5600 different gas phase chemicals in seconds; it is lightweight and handheld, allowing for positive gas identification with no sample preparation or pre-concentration.

Myth: FTIR can only see threat materials that are greater than 10% of the entire sample matrix.

Multi-component mixtures, especially solids, have increasingly become common in hazmat/CBRN operations. White powder calls have changed over the years from the biological threats that prevailed in the early 2000s to the narcotic threats today. However, the commonality is that these white powders are generally mixtures. There are two approaches which must be balanced when evaluating FTIR spectra of mixtures – spatial and spectral.

Spatial analysis focuses on taking representative samples while spectral analysis addresses simultaneous absorption of the mixture constituents. Spectral analysis can be addressed using the advanced algorithms developed by RedWave, while spatial analysis must be addressed by the user with proper sampling protocols. From a spectral standpoint, this effect is far more relevant in solid and liquid samples as the absorption bands are broad. In fact, this is where the 10% comes from (although it really means a 10:1 ratio). This effect is most pronounced in liquid samples as liquids have a high degree of interaction between molecules.

Unlike solids and liquids, the FTIR bands in gases are sharp. The ratio in gas phase is more like 100:1 (versus 10:1 in solids and liquids), so not as important. In addition, gases have molecules that are far apart and therefore do not have as many interactions that affect the spectra.

Spatial analysis affects solid samples more than anything else as mixing is more homogenous in liquids and gases. When sampling the mixtures, representative samples must be taken to ensure that the different parts of the non-uniform mixture are proportionally represented. The most common signs of non-uniformity include variations in color and crystallinity. This issue became more apparent to many operators when dealing with narcotics mixed with adulterants, cutting agents, and binder materials. All attempts should be made to capture samples representative of each of the mixture components. With good sampling techniques, the percentage of threat materials required in a sample matrix drops dramatically; it can further drop with advanced mixture algorithms like those present in RedWave instruments.

Myth: FTIR is too complicated to use in field operations.

Currently fielded FTIR systems have software protocols in place to automate the data collection process, making the systems simple to employ in the field. From calibration and system checks to spectral analysis, the entire system is automated to provide ease of use in field operations.

Continuous monitoring is a true survey mode where it detects the threat when sufficient material is available then identifies that threat when the signal-to-noise ratio is suitable. One of the things that makes this possible is the adaptive atmospheric correction process.

However, it is prudent to always view the spectra manually in comparison to the library spectra to make sure that there are no obvious anomalies. These anomalies may be indicators of multi-component mixtures.

Myth: FTIR is a new analysis technique.

Coblentz demonstrated that functional groups that make up a molecule exhibit very specific vibrations and characteristic absorptions in the infrared spectrum in the early 1900s. However, this process was slow due to the inability to analyze each wavelength concurrently. The first successful application of FTIR was in 1949 by Felgett. Felgett build upon Fourier's mathematics work in the 1800s to develop a scanning system capable of simultaneously scanning absorption and interference across the spectrum and then transforming the data into the frequency domain that we use today. Fast FTIR, which is still in use today, was developed by Cooley and Turkey in 1965.

Since 1965, significant work has been performed on the development of spectral libraries, miniaturization and hardening of system components, algorithms to remove interferences, and more. SensIR Technology sold the first TravelIR in 2002 and the first HazMat ID in 2003.

For the last 20 years, manufacturers of portable FTIR instrumentation have focused on developing robust, vibration and shock resistant systems with enhanced ergonomics and system usability. In parallel, considerable work is ongoing on sample preparation and automation.

Myth: FTIR is too expensive.

While FTIR systems are far more expensive than traditional detect-to-warn and detect-to-protect systems like electrochemical cells and photoionization detectors ($3K - $5K), they are also able to uniquely identify threat materials. In comparison to most detect-to-identify systems (mass spectrometry ($110K – $125K)), FTIR is a far less expensive approach ($45K - $75K).

More importantly, the inclusion of the RedWave XplorIR into your detection toolbox greatly reduces the time required to uniquely identify a product, decreases the training burden by automating the analysis, and replaces several technologies (colorimetric, electrochemical, and others) which are fraught with false positives.

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