SafetyNews No. 35:

Today's ***SafetyNews*** focuses on gas phase analysis and provides a range of interesting information on **gas and vapor identification** using gas FT-IR and **continuous monitoring of highly toxic vapors/gas and aerosols** in critical event security, building protection and other applications.

In the section on **gas FT-IR**, you will find information on dynamic adaptive background correction (why it is important, how to automate analysis even at low concentrations, etc.) and a range of practical information on fast and reliable quantitative analysis using FT-IR and PID detectors and the benefits of using PID and continuous gas FT-IR detectors together in real-life situations. You will also find a link to an interesting webinar dedicated to practical issues in the use of gas FT-IR and more.

In the section dedicated to **continuous monitoring of highly toxic gases and aerosols**, we will show how the **BEACON** novelty can be used to turn the MX908 handheld HPMS detector into a continuous monitor that monitors both the gas phase and aerosols in the air, and how multiple units can be easily networked to secure, for example, a stadium or a large area during large meetings or sporting events.

In both sections you will also find links to **interesting webinars**, we recommend watching them.

Hardware *news*

A new attachment is available that allows you to "convert" the Stand OFF Raman spectrometer Pendar X10 into a small mobile laboratory for the analysis of different types of samples (vials, tablets, bags, bottles, ...) including very small samples.

Thanks to the automatic focusing on the sample and the use of a class 3R laser (no need for goggles), just place the sample on the window of the attachment and an automatic and very fast analysis is performed. This is similar to FT-IR spectrometers with ATR, but in this case no pressure on the sample is required. Thus, even pressure-sensitive materials can be safely measured. Of course, one of the main advantages of the Pendar X10 spectrometer remains, the safe measurement of dark samples as well as any type of energetic material, including primary materials such as azides or fulminates. It is also possible to measure the internal content of double-walled vials (vial within a vial), which are used for extremely toxic materials. The spectrometer focuses itself on the contents of the inner vial and performs the analysis. When connected to a PC (via USB-C or wirelessly via WiFi), you can then use the Windows software to use the Pendar X10 as a powerful tool for field forensic analysis or as a laboratory Raman spectrometer.

The second short piece of hardware news concerns the launch of the new generation of affordable identiFINDER R225 handheld gamma spectrometers. The R225 replaces the previous R200 model and is a personal radiation monitor with the ability to track radiation sources and identify them immediately. The identification capabilities of the R225 are on par with the "large" identiFINDER R425. It has become the world's best-selling handheld gamma spectrometer, similar to its predecessor identiFINDER R400. Compared to the R425, the sensitivity is of course lower, a smaller crystal is used). However, the sensitivity is still at a significantly higher level than other handheld devices of this type, as an 18x18x18 mm cubic crystal coupled to a SiPIM photomultiplier plate is used. In addition to the standard CsI(Tl) crystal material**, a version with a LaBr(Ce) detector** of the same size **is also available**, which already offers a spectral resolution better than 3.5% (FWHM at 662 keV). This is the first time that a "pocket-sized" device with this resolution and high sensitivity, certified to both IP67 and MIL STD 810G (Salt Fog), is available on the market.

For more information click here: https://www.flir.com/products/identifinder-r225/?vertical=radiation&segment=detection

Short video here: https://youtu.be/oyMgSW4KBYQ

Continuous gas analysis with the XplorIR mobile FT-IR spectrometer.

We have already informed you about the launch of the XplorIR mobile FT-IR spectrometer for instant identification of vapours and gases directly in the hot zone

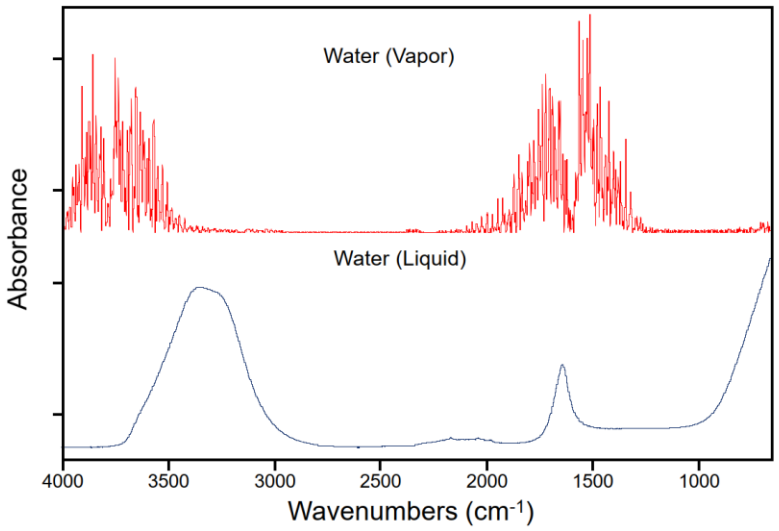
in our Safety News 32 (download here: Safety News 32). One year has passed since then and we have not only been able to follow the development of this device, but also to test the new products in our company. This year we have seen two major innovations. The first was the launch of a new version of the spectrometer with a **12x** more powerful internal computer (and thus massive computing power for data-intensive operations). This allowed virtually instantaneous simultaneous identification of all 5500 compounds in the library in a spot measurement.

The second new feature was Dynamic Adaptive Atmospheric Background Correction, which also requires massive computing power. This brought the capability of instantaneous simultaneous identification of all 5500 well into continuous monitoring. This is a new algorithmic technology that has opened the way to fully automatic monitoring/identification of substances using gas FT-IR, even in situations where the background spectrum changes dynamically during monitoring (i.e., for example, when the handheld analyzer moves in the hot zone). **In our opinion, this technology represents a major breakthrough in the possibility of using gas FT-IR for continuous monitoring in the hot zone by ordinary workers without special knowledge**, and we therefore also discuss it in more detail in this issue of Safety News. Essentially, the **same "breakthrough" that Ahura First Defender Raman spectrometers once brought to solid and liquid identification has been made. That is to say, simple push-button operation, with intelligent**

algorithms running in the background to make reliable identifications for the operator, providing immediate and unambiguous results.

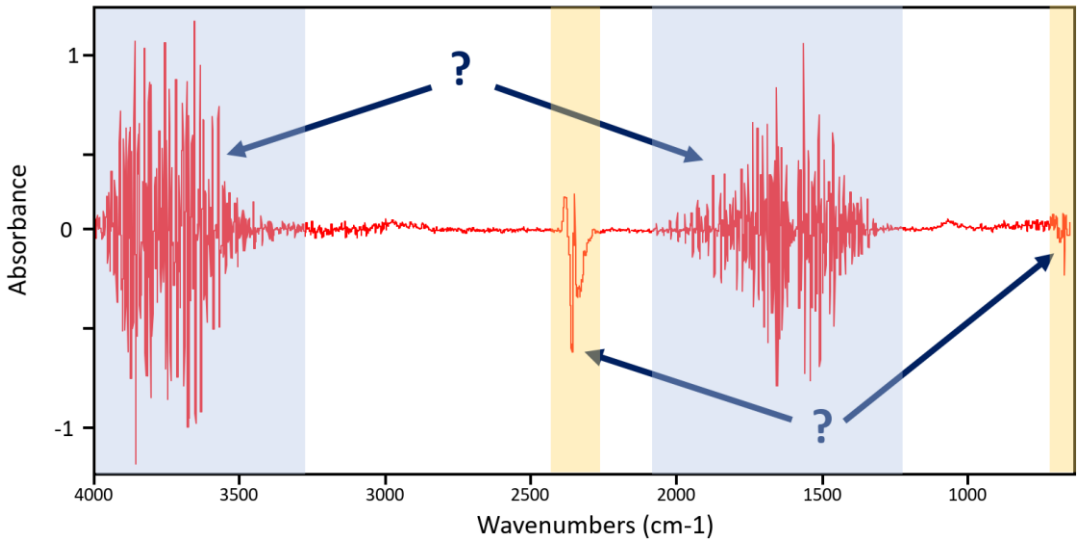
Gas phase analysis with FT-IR spectrometers - influence of the atmosphere on the analysis itself.

Infrared spectrometry is an ideal technique for the identification of substances in the gas phase. As in the case of the identification of unknown solid or liquid samples using FT-IR spectrometers (which has been widely used for years in the identification of hazardous substances), the spectra in the case of gases and vapours are substance-specific (they represent the chemical fingerprint of the substance). However, the spectra contain a larger number of sharp peaks (a rotational vibrational structure that can only be seen in gaseous substances - the molecules can also rotate and so the spectra often show a fine rotational structure). The figure below compares the spectra of water in the liquid and gas phases. On the one hand, this places greater demands on the spectral data processing and the spectrometers themselves, which should achieve a spectral resolution of at least 4 cm^{-1} .

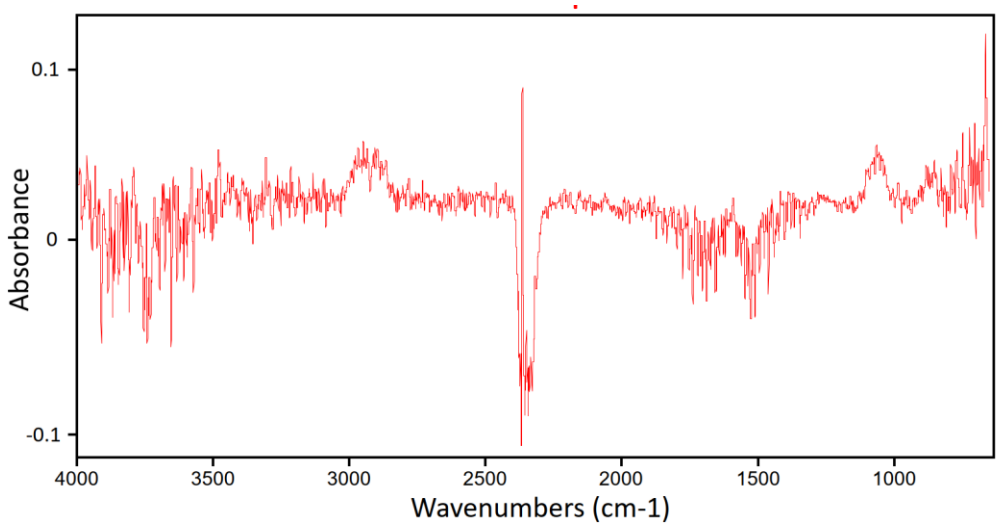


On the other hand, however, the identification performance is considerably higher, especially in the case of mixtures, where it is quite common to be able to reliably identify up to six components in the spectrum.

The actual analysis is further complicated by the fact that the normal atmospheric components exhibit very intense infrared spectra. We have already shown the spectrum of water above, the other major absorber is CO_2 , two common components found in the air in high concentrations. At a humidity of 80% and a temperature of 20°C, the concentration of water vapor in the air is about 14,000 ppm, and the average concentration of CO2 in the air is about 500 ppm. The IDLH limits, which are important for the immediate use of protective equipment, are at much lower concentration levels for a large part of the pollutants. Thus, for correct identification, it is necessary to compensate for/remove background that is due to atmospheric components. Since the concentrations of these constituents vary over time and the concentration response is not linear, performing this compensation is challenging even for point measurements and is a source of "residual" spectra in the water and CO2 spectral regions, typically showing negative peaks. The lower the concentration/absorbance we need to measure, the greater this problem becomes and in many cases is the main cause of poor identification performance (ability to identify an unknown substance) when present at low concentrations (see below). The figure below shows a typical "residual" spectrum after subtracting the atmospheric components using the convective correction method, and the next shows a spectrum of a sample of a lower concentration of an unknown substance in a real air sample after conventional background correction.



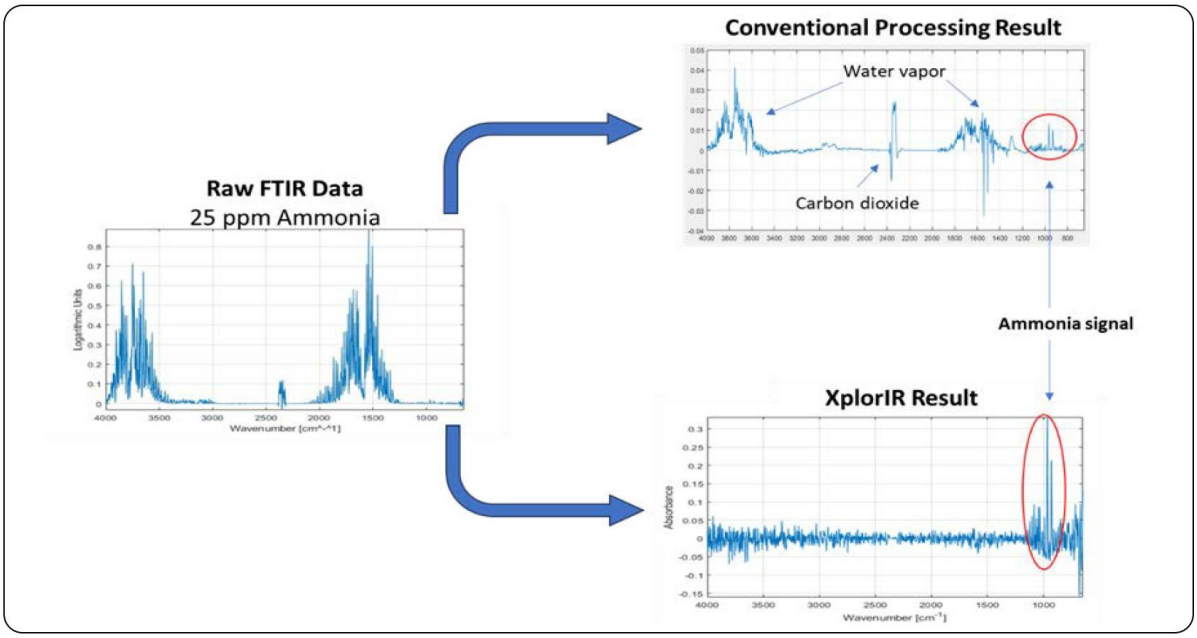
Residual spectrum after convective compensation of atmospheric components. The blue bands correspond to water, the yellow bands to CO2, identification of unknown substances that have characteristic bands in this region can be difficult, especially at low concentrations.



Spectrum of the unknown sample overlaid on the residual spectrum of water and CO2 after convective background correction.

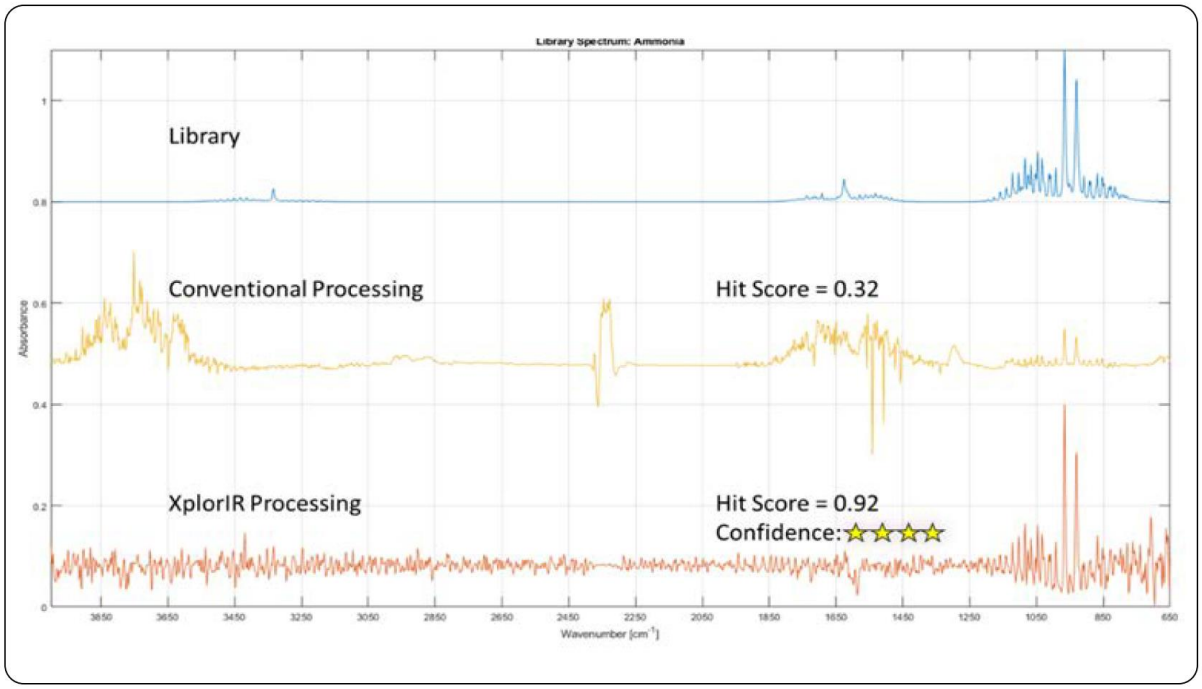
Dynamic adaptive atmospheric background correction - reliable identification in all conditions.

Dynamic adaptive correction uses modern nonlinear dynamic modelling calculations and is able to compensate very effectively for the spectrum of atmospheric constituents. The spectrum after dynamic adaptive correction contains virtually no residual spectrum and even low concentrations of substances can be reliably identified. The basic function can be illustrated in the following two figures, which show the identification of 25 ppm ammonia on the XplorIR spectrometer. In the figure below we see on the left the uncorrected (RAW) FT-IR spectrum of a 25 ppm ammonia sample in air, on the top right the spectrum after conventional background spectrum compensation (linear 1:1 reading) and on the bottom right the spectrum after dynamic adaptive correction. In the case of ammonia, the situation is still quite favourable, because the characteristic spectrum of ammonia is not significantly overlapped by the residual spectrum, so the identification of 25 ppm ammonia is a simple matter in manual mode.

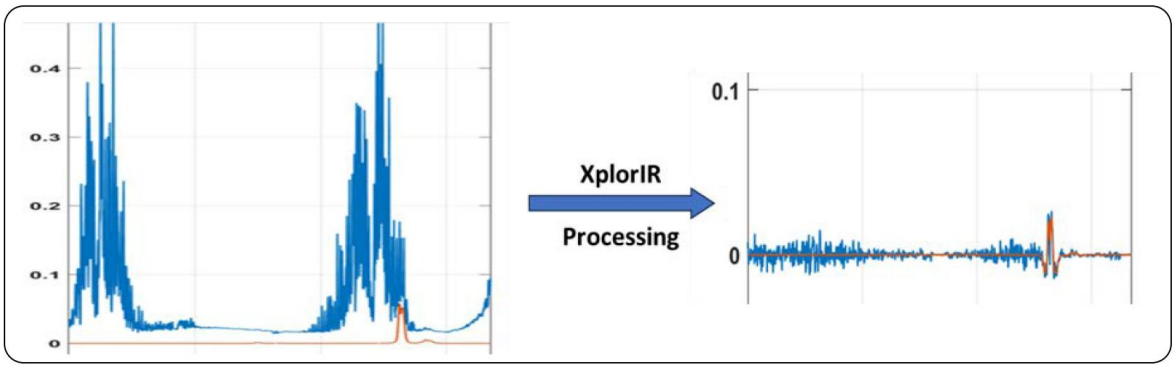


Infrared absorption spectrum of 25 ppm ammonia processed conventionally and in a new way in the XplorIR spectrometer showing the advantage of adaptive atmospheric correction.

However, the residual spectrum after conventional spectral modification is also the cause of low reliability of automatic identification - we obtain very low hit score values, the situation is fundamentally different from the situation when we evaluate spectra of liquid or solid substances. Thus, until now, it has been common that the confirmation of the identification match had to be verified by an operator with experience in spectral data processing. The figure below shows the spectrum of pure ammonia from the spectral library and the spectrum of a real sample of 25 ppm in air after conventional processing. The hit score is only 0.32! Then the next spectrum shows the same sample after dynamic adaptive correction, the hit score in this case is 0.92! Thus, a completely automatic and reliable identification of the substance is possible.



As mentioned above, in the case of ammonia there is not yet a direct overlap with the residual spectrum. However, let us now look at the less favorable case of SO_2 , where the characteristic spectrum is completely overlaid by the water spectrum. In the figure below, on the left hand side is the spectrum of 30 ppm SO_2 in a real air sample, the characteristic spectrum is completely "absorbed" by the residual spectrum. Then on the right hand side, the spectrum using dynamic adaptive correction, SO_2 can be reliably detected and identified.



Spectra of 30 ppm SO2 in a real air sample after convective correction of atmospheric components and using dynamic adaptive atmospheric correction.

It is also important to look at the effect of dynamic adaptive correction on the identification limits achieved (how low concentrations we are able to identify), especially under different atmospheric conditions. For this purpose, spectra of eight selected compounds were measured under different atmospheric conditions (relative humidity from 20 to 80%) in different concentration ranges from 1 to 300 ppm. For each substance, the concentrations were chosen such that approximately 20% of the concentrations lay below the expected instrumental detection limit. The results show that the use of dynamic adaptive correction achieves low detection limits at the level of theoretical instrumental values and that the influence of different atmospheric conditions is eliminated. Full results and further details can be found in the application note "***Infrared Gas Identification in Any Conditions: XplorIR's Adaptive Atmospheric Correction***", which can be downloaded here:

https://drive.google.com/file/d/163au5ZhI3vTfgIeTJB6ImpbuLS9oKqNO/view?usp=sharing

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For more quite detailed information, you can also find the recording of the webinar ***"RedWave & The Hazmat Guys On-Demand Webinar - Adaptive Atmospheric Correction"***, which was dedicated to Dynamic Adaptive Atmospheric Background Correction: the **webinar can be viewed at the following link:**

https://youtu.be/CDPHboMDXM0

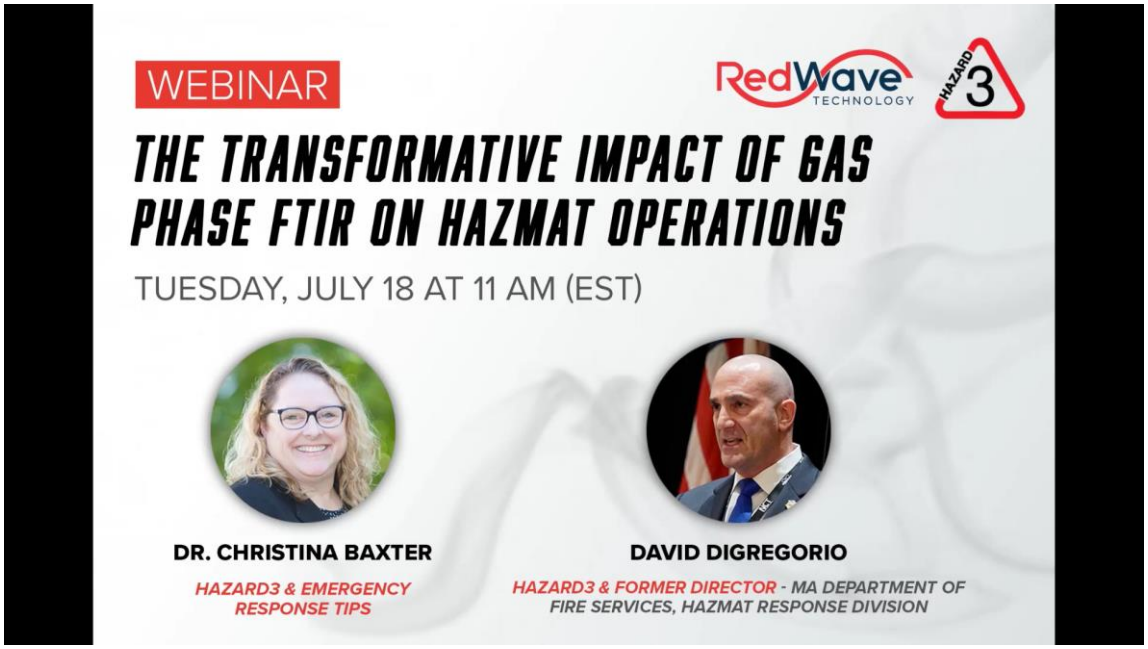
Expanding Your Toolbox: Pairing Your PID with FTIR.

This application note explains why the simultaneous use of PID detectors and XplorIR spectrometers is advantageous when dealing with real incidents. For example, it is possible to obtain immediate information about the concentration of a given substance - the value obtained from the PID must be multiplied by a factor that is valid for the substance in question. XplorIR identifies the substance and simultaneously displays the correction factor for the PID detectors on the display. Further examples can be found in the application note.

Download here: https://drive.google.com/file/d/1R_7lxA-Hsn7U52CeNZ6Kx_xYfkJQ_28e/view?usp=sharing

Webinar: The Transformative Impact of Gas Phase FTIR for Hazmat Operations

If you are interested in field analysis of hazardous gases, we recommend this webinar. There is a very nice discussion on the use of FT-IR for vapor and gas analysis, the position relative to colorimetric tests (typically Drager), gas multidetectors and PID. The second half is a very interesting discussion of the position of handheld mass analyzers (MX908) and mobile GC-MS in dealing with real world situations.

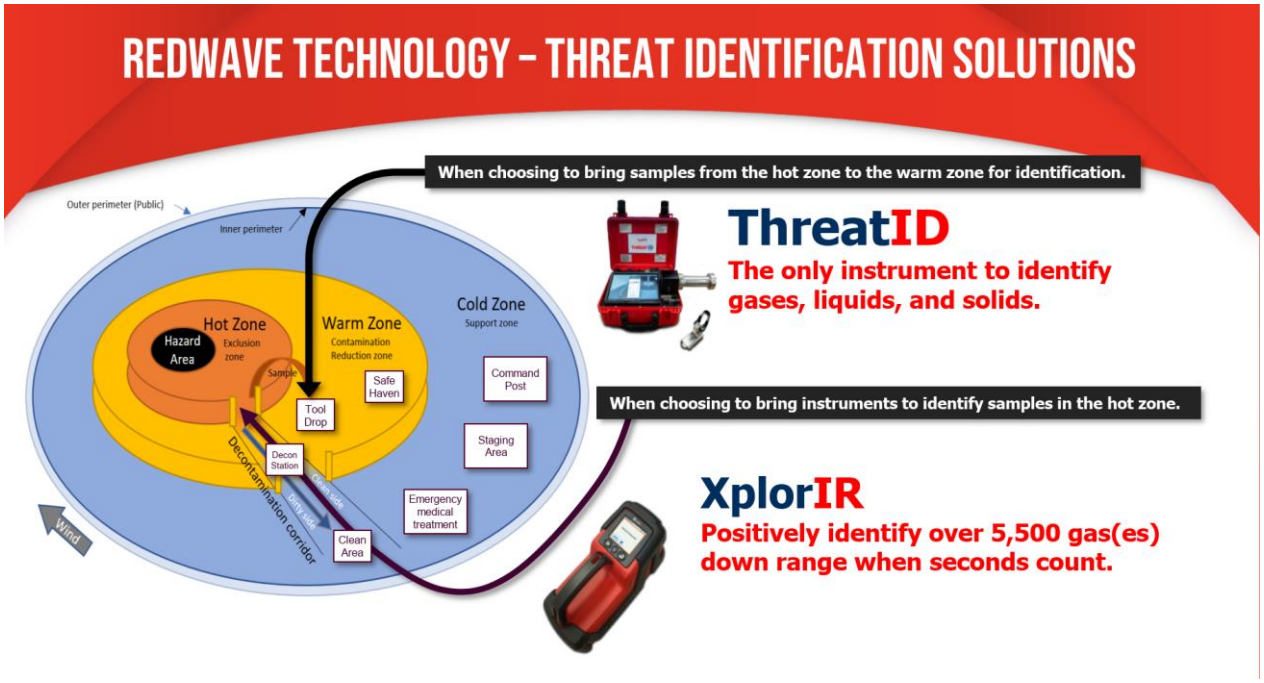


To be viewed here: https://www.youtube.com/watch?v=OGESb6teopk

We are also often asked what the difference is between **ThreatID** spectrometers (which can analyse liquid, solid and gaseous samples) and **XplorIR**. ThreatID spectrometers are more for mobile laboratories that operate at the boundary of the hot zone but do not operate directly in the hot zone. They require gaseous samples to be collected in the hot zone (Tedlar bags, syringes, etc.) and transported to the mobile laboratory. These spectrometers are also designed for more advanced analyses. XplorIR spectrometers are designed for direct deployment in the hot zone with minimal operator requirements and provide instant information or the ability to actively search for sources/leaks etc. The instrument is equipped with

communication that allows direct sharing of results to a cloud solution for instant control from outside the hot zone.

The picture below explains it nicely:



RedWave is a relatively "young" company, operating on the mobile FT-IR spectrometer market for about 7 years, last year it also entered the European market. Behind this company are the "matadors" of mobile FT-IR spectrometer development, who previously worked at Smiths Detection, Thermo and A2 (now part of Agilent). They offer the greatest cumulative knowledge in the field of mobile FT-IR spectrometers and their instruments always come with solutions that are "tailored" based on real customer requirements. At the same time, they also strive to fill gaps in the current market (offering new solutions that have been missing so far). No one is surprised by the speed with which these instruments have established themselves in the US market (where they are already the number one mobile FT-IR device). Although **RedWave** spectrometers have been officially available in Europe for about 1.5 years, there are already more than 100 spectrometers in the equipment of First Responders teams in many countries, including the Czech Republic. RMI is the exclusive representative and service center

for the Czech Republic, Slovakia, Hungary, Slovenia, Croatia and, if serviced, other countries. Our service centre is fully equipped and trained to service RedWave spectrometers including the new XplorIR. We are thus able to quickly and flexibly address any service requirements right here in the Czech Republic.

Continuous monitoring of highly toxic gases and aerosols with MX908/BEACON

All current equipment used for continuous monitoring of toxic substances in the air during security of important events, protection of mobile bases or protection of VIPs analyses only the gaseous phase. However, aerosols are also a significant threat. Aerosolized pharmaceutical substances of high toxicity are considered one of the greatest threats today because they are readily available in the drug scene in large quantities. However, aerosols are also encountered in the case of fourth generation chemical warfare agents (Novichok) or VX agents. This issue is well covered in "***Responding to Chemical Warfare and Pharmaceutical Based Agents".***

To be viewed here: https://908-devices-ls.wistia.com/medias/61t736ub4a

The first commercially available device that could simultaneously monitor both the gas phase and aerosol was the mobile HPMS (High Pressure Mass Spectrometer) detector **MX908** in conjunction with the **Aero** aerosol module. We have already written about this issue in our Safety News 27, which can be downloaded here.

http://www.rmi.cz/download.php?group=stranky3_soubory&id=2418

This equipment has become the "standard" in the field, but was primarily designed for mobile monitoring in the field. The spectrometer manufacturer has now come up with a new product - the **BEACON** module . It makes it possible to turn the MX908 handheld HPMS detector into a continuous monitor monitoring both gas phase and aerosols in the air. It is easy to connect multiple units to a network that can then secure, for example, a stadium or a larger area during large meetings or sporting events.

The actual set up is very simple and quick. The MX908 detector is inserted into the BEACON "case" and connected to the BEACON unit. This connects it to the internet and virtually any number of units can be monitored on mobile apps or PCs.

Also, during the protection of large events, there is often a situation where multiple government organizations or multiple different units are involved, each may have their own MX908 units. Any MX908 detector with an aerosol attachment can be inserted into any BEACON, it will automatically connect, a QR code and https address with the code will be generated on the MX908 display. Anyone who has the mobile app will read the QR code (it can be shared) and have access to track the unit on their mobile or tablet, likewise after entering the https address the app will open on the PC and anyone who knows the access code can track the unit (up to 8 units in one window). Security of large events becomes a simple and very fast operation, within minutes you have a fully functional secure monitoring network, even with the participation of multiple organizational units with their equipment.

MX908 Beacon

If you are interested in obtaining more detailed information, please contact us. You can also watch the podcast "**The New MX908 Beacon for Area Monitoring", available here:** [The New MX908 Beacon for Area Monitoring - 908 Devices]

Your RMI, s.r.o. team - we are here for you☺ .

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