Application note

Using FTIR spectrometry for field analysis of unknown gases in firefighting

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Industry/application

Firefighting and hazardous gas detection

Products used

Thermo Scientific™ Nicolet™ Apex FTIR Spectrometer

Thermo Scientific™ Nicolet™ Gas Cell (2 m)

Thermo Scientific™ OMNIC™ Software

Thermo Scientific™ OMNIC™ Specta™ Software Libraries

Goals

Demonstrate the advantages of using an integrated FTIR spectrometer system in firefighting operations for the detection and identification of hazardous gaseous compounds under field conditions.

Key terms

FTIR spectroscopy, firefighting, gas analysis, OMNIC software, OMNIC Specta libraries

Key benefits

- Enables rapid, on-site identification of unknown gases.
- Enhances firefighter safety through remote sampling and chemical identification.
- Provides accurate results using advanced spectral analysis software.
- Integrates robust, field-ready sampling systems with laboratory-level precision.

Introduction

Firefighters often encounter situations where they must quickly analyze unknown products in the field: pollutants, industrial chemicals, warfare agents, or hazardous materials such as flammable, corrosive, oxidizing, explosive, or toxic compounds. Rapid identification of these gases is essential to determine the appropriate level of personal protection, establish secure intervention perimeters, and assess potential risks to both responders and the public. Traditional detection technologies, such as electrochemical sensors or photoionization detectors (PIDs), provide rapid alerts but lack molecular specificity. These instruments cannot distinguish structurally similar compounds or resolve mixtures, and their reading may be influenced by humidity, temperature, or interfering gases. In contrast, Fourier Transform Infrared (FTIR) spectroscopy provides a unique spectral fingerprint for a molecule based on its molecular vibrations, enabling precise identification of single compounds or complex gas mixtures. By integrating the Thermo Scientific™ Nicolet™ Apex FTIR Spectrometer into a Detection, Identification, and Sampling Vehicle (DIS), emergency response units gain access to laboratory-grade analytical capability directly at the intervention site. This eliminates the delays associated with submitting samples to off-site laboratories and supports rapid, informed decision-making during critical operations. The DIS Vehicle configuration enables remote sampling through hoses or probes, reducing exposure to hazardous zones. Rapid identification supports operational decisions like these:

- defining exclusion zones
- selecting optimal respiratory protection
- predicting the evolution of fire chemistry
- organizing ventilation strategies
- assessing environmental contamination

FTIR spectroscopy's specificity surpasses that of common detection devices, making it a valuable complement to traditional gas monitors.

Material and method

The analytical system employed here combines the Thermo Scientific Nicolet Apex FTIR Spectrometer with a 2-meter Thermo Scientific Nicolet gas cell equipped with chemically resistant BaF_2 windows (Figure 1). This configuration ensures compatibility with corrosive or acidic gases frequently encountered during industrial or chemical incidents. Gas sampling is achieved using a 2-liter evacuated stainless-steel cylinder, which follows three main steps:

1. Vacuum Preparation: The gas cylinder and the gas cell are initially evacuated using a vacuum pump. The vacuum ensures the removal of any residual gases or contaminants from the sampling system, minimizing interference with the analysis.
2. Field Sampling: Once the cylinder and gas cell are adequately evacuated, the cylinder can be transported to the field for gas sampling. The evacuated cylinder is opened near the emission source, drawing gas in naturally due to pressure differential. It is important to take appropriate safety measures during the sampling process to ensure the well-being of the firefighters and the accurate collection of the gas samples.
3. Transfer to Gas Cell: After the field sampling is complete, the gas cylinder, containing the sampled gas, is transferred back to the DIS vehicle for analysis. The cylinder is connected to the gas cell, and the gas sample is transferred into the gas cell for analysis.

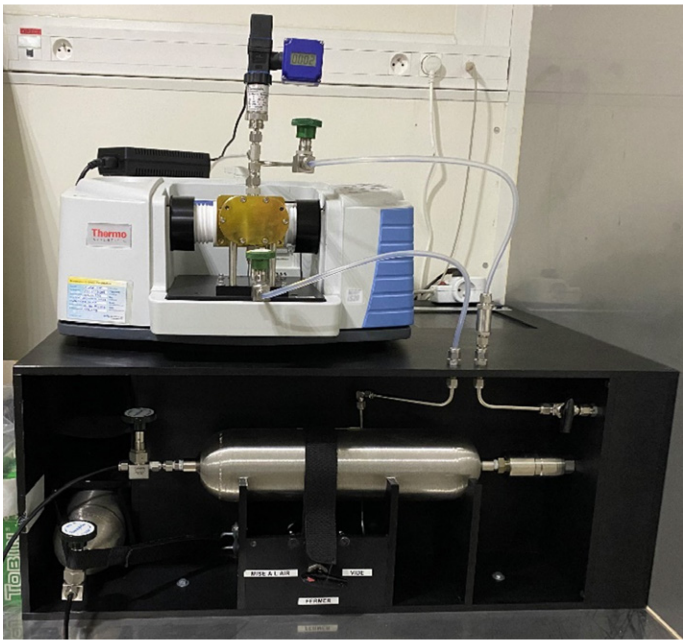

Figure 1. FTIR spectrometer and its sampling system in a Detection, Identification and Sampling vehicle.

Spectral acquisition and analysis

Spectral measurements are carried out using the Nicolet Apex FTIR spectrometer equipped with OMNIC software. Typical acquisition parameters include a resolution of 4 cm^{-1} and 10 scans, producing results within approximately 15 seconds. In this configuration—2-meter gas cell, DTGS detector, and no heating—the minimum detectable levels typically fall within the low-ppm range, depending on the intrinsic absorption strength of each analyte. While this setup is not designed for trace quantification, it provides more than sufficient sensitivity for qualitative identification of most gases encountered during firefighting operations. For higher selectivity or quantitative analysis, resolutions up to 0.5 cm^{-1} can be applied.

The modular design allows integration of accessories such as ATR modules for identifying liquid or solid residues.

Software and spectral libraries

OMNIC software supports a full suite of data preprocessing tools, including baseline correction, noise smoothing, atmospheric compensation, and water vapor subtraction. These corrections are critical in firefighting environments where humidity and variable temperature conditions may mask weaker analyte signals. The software's real-time visualization capabilities also assist operators in validating spectral quality before performing identification.

Identification of unknown gases is performed using OMNIC Specta software, a powerful platform that integrates multiple curated reference libraries. These include spectra for industrial chemicals, volatile organic compounds (VOCs), toxic gases, combustion by-products, fuel additives, and common environmental pollutants.

OMNIC Specta software offers three complementary identification workflows, all of which can be performed either over the full spectral range or on user-defined regions to isolate specific diagnostic peaks or to avoid saturated portions of the spectrum:

- **Library search:** This workflow compares the acquired spectrum to reference library entries to identify the most likely matching compounds. This mode is well suited for single-component samples or cases where one compound is expected to dominate.
- **Multi-component search:** This deconvolutes mixtures by mathematically reconstructing the measured spectrum from multiple library spectra. This workflow is essential when several species contribute simultaneously to the spectral signature.
- **Contaminant search:** This feature helps identify minor constituents by analyzing the residual differences between the measured spectrum and a user-defined major component. Although this mode is not illustrated in the current application note, it is valuable when a dominant compound is known and the analytical objective is to detect unknown impurities or secondary gases.

The multi-component algorithm is particularly advantageous in fireground atmospheres where water vapor, hydrocarbons, acids, and nitrogen-containing gases frequently coexist. The algorithm reconstructs a composite spectrum based on library matches and compares it to the acquired spectrum, enabling robust identification even in highly congested spectral conditions.

Although the search algorithms provide highly valuable guidance for identifying unknown gases, their output must be evaluated critically by the operator. The approach highlights the most plausible spectral contributors, but it does not guarantee exhaustive identification of all components in heavily congested mixtures, nor does it replace quantitative analysis. For accurate concentration measurements, dedicated calibration models remain necessary.

Results and discussion

The following examples illustrate the performance of the Apex FTIR spectrometer for analyzing gases encountered in firefighting scenarios.

Unknown gas sample no. 1

The first unknown gas sample presented a relatively simple spectral profile, with well-defined absorption bands and limited overlap from other species. For this reason, the identification was performed using the standard Spectral Search mode applied over the entire spectral range, without the need to restrict the analysis to specific vibrational regions. This whole-spectrum approach enables direct comparison of all characteristic bands with the reference library. The spectrum displayed canonical alcohol features, including a broad O–H stretch and characteristic C–O stretching vibrations. OMNIC Specta software identified methanol with a strong 85.42% match, fully consistent with the relatively simple spectral profile observed (Figure 2). Methanol is a frequent by-product of synthetic material combustion and can originate from solvents, fuels, or industrial intermediates. Rapid identification of methanol helps responders evaluate toxic exposure risks and determine whether specialized personal protective equipment is required.

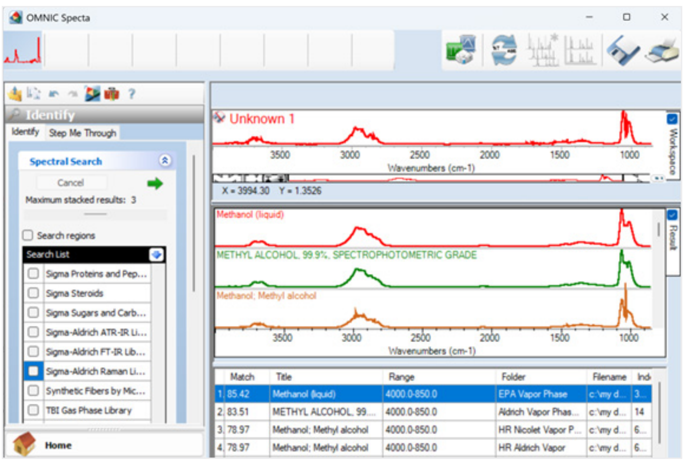

Figure 2. Result of spectral search for unknown gas sample No.1 (methanol).

Unknown gas sample no. 2

The second unknown gas sample displayed a much more complex spectral profile than the first one. In addition to the characteristic absorption features of organic vapors, the spectrum was heavily dominated by water vapor, whose strong rotational–vibrational bands can obscure weaker signals. Because of this interference, a simple full-spectrum search was not sufficient to achieve an accurate identification. To overcome this challenge, the analysis was carried out using two separate region-specific spectral searches, each targeting spectral windows less affected by water vapor. A first search in the 1000–1300 cm^{-1} region, where C–O deformation and C–O–H bending modes are prominent, yielded a strong 92.05% match with acetic acid (Figure 3). A second search in the 850-1000 and 2800–3000 cm^{-1} regions, dominated by C–H stretching vibrations, identified heptanol with a 90.66% match (Figure 4). The combined interpretation of these targeted regions, selected specifically to minimize water vapor interference, indicates the presence of a mixture of acetic acid and heptanol. This example illustrates how regional analysis can successfully resolve multi-component samples when strong atmospheric contributions are present.

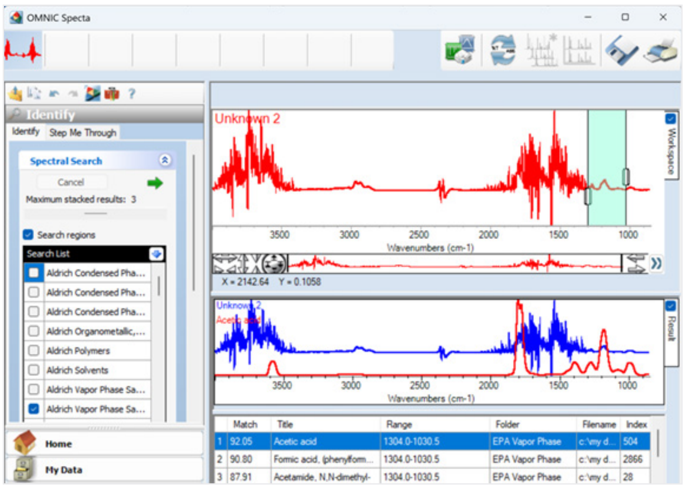

Figure 3. Result of spectral search in the 1000–1300 cm^{-1} region (acetic acid).

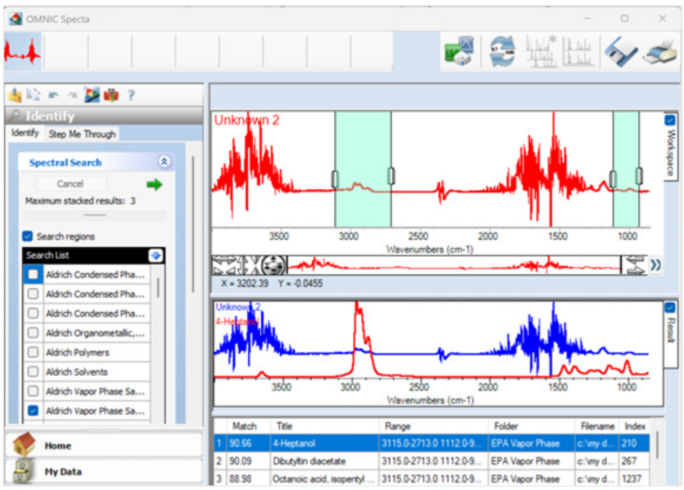

Figure 4. Result of spectral search in the 850-1100 and 2800–3000 cm^{-1} region (heptanol).

Unknown gas sample no. 3

The third unknown sample exhibited a highly congested spectrum strongly dominated by water vapor, whose broad rotational–vibrational bands obscured many of the other spectral features. To overcome this challenge, the identification was performed using the Multi-Component Search mode, applied exclusively to selected spectral regions outside the most intense water vapor absorption zones. This approach is necessary when atmospheric water vapor saturates large parts of the spectral range. Based on initial inspection, the algorithm was configured to identify three components, with water vapor being explicitly included due to its clear presence in the spectrum. Under these constraints, the multi-component search identified water vapor (57.19% match), acetone (31.20% match), and ammonia (11.61% match) as the three contributors, resulting in a global match value of 66.46% (Figure 5). Importantly, the composite spectrum generated by the algorithm overlaps almost perfectly with the experimental spectrum, apart from slight differences attributable to spectral resolution. This excellent agreement demonstrates the robustness and reliability of the multi-component approach for resolving complex mixtures, particularly in real firefighting scenarios where atmospheric interference is unavoidable.

Figure 5. Result of the multi-component search in region mode for unknown sample No.3.

Conclusion

Integration of the Thermo Scientific Nicolet Apex FTIR Spectrometer into a mobile DIS platform provides firefighters with an advanced analytical capability that significantly enhances situational awareness during hazardous incidents. The system offers rapid, reliable identification of unknown gases, including mixtures of volatile and semi-volatile compounds, directly at the intervention site. This helps reduce operational uncertainty and improve responder safety. The 2-meter Thermo Scientific Nicolet gas cell, combined with high-resolution FTIR analysis and powerful spectral interpretation software, enables detection of complex gas profiles that traditional sensors cannot resolve. This capability is essential for modern firefighting environments where synthetic materials, industrial chemicals, and diverse combustion products are increasingly present. Looking ahead, further enhancements such as automated quantification workflows, expanded fire-specific spectral libraries, integration with atmospheric modeling tools, and real-time wireless transmission to command centers could strengthen decision-making during emergencies even further. Together, these innovations establish FTIR spectroscopy as a cornerstone technology for chemical hazard assessment in firefighting and emergency response operations.

