A guide to choosing sensor technologies for food safety and oil analysis spectrometry applications
Executive summary

Infrared (IR) sensing is widely used today in a broad range of detection and analysis applications, including flame and gas detection, fuel and oil analysis, food safety, and motion and gesture sensing. However, only recently has IR sensing technology for spectrometry applications developed sufficiently to facilitate truly portable analysers.

Today, instruments can be reliably taken to the field, rather than the traditional approach of bringing samples to the laboratory. Typical portable spectrometry applications currently include analysing oil in ships’ engines, while on the move; and in food safety, to identify additives, adulterants and contaminants in products such as milk, honey, fruit juice, spices and lavender oil.

The potential for portable IR sensor-based spectrometry is enormous across a huge variety of additional industry sectors, including pharmaceuticals, healthcare, IoT, process control and environmental monitoring. Yet portable systems are required to be highly responsive, making fast, accurate, repeatable and reproducible measurements, to detect a large number of diverse substances across a range of industries.

The technological challenge to meet the need for compact, low-power and robust equipment that requires minimal calibration demands an innovative approach from both the equipment designers and the suppliers of the core sensing technology.

This white paper covers some of the different IR sensing techniques available to developers of spectrometry equipment and focuses on the characteristics and advantages of mid-IR sensing, specifically for spectrometry applications in the food safety and oil analysis industries.

Introduction

In the electromagnetic spectrum, infrared radiation is found between visible light and microwaves. It is typically defined as spanning the region from 800nm to 1mm. See Figure 1.

Figure 1: Infrared radiation is found between visible light and microwaves. It is divided into three wavelength groups: near-, mid- and far-IR.

Infrared is itself divided into three distinct regions, based on the frequency of the IR radiation relative to the visible spectrum. Thus, near-IR is closest to visible light, typically 760nm to 3µm; mid-IR is from 3 to 14µm; while far-IR is the broadest of the three, ranging from 14µm to 1mm.

Infrared sensors can be active (emitter and detector) or passive (detector only). Passive IR sensors in the mid-IR and far-IR regions are generally thermal IR detectors, while near-IR sensors are typically quantum detectors, also known as photodetectors. Photodetectors can have faster response times and greater sensitivity than thermal detectors, but typically have to be cooled in order to cut thermal noise. This paper focuses on passive pyroelectric IR sensors, which do not need external cooling.

Passive IR sensors are particularly useful for analysis as they do not influence the samples or the environment within which they are operating. They are generally based on certain pyroelectric materials, typically crystals. Pyroelectric materials generate an electrical voltage when heated or cooled. The pyroelectric effect is described as a response to changes in the thermal radiation of an object, which in turn produces a change in voltage across a crystal. In simple terms, IR sensors turn incoming IR radiation into an electrical signal.
A passive IR sensor may comprise one, two, four or many individual detector cells, available in various package styles, including TO cans and arrays, for conventional through-hole board or SMD mounting. The sensor’s outputs can be very small, so an amplifier or pre-amplifier is typically integrated into the package with an internal voltage regulator. Outputs may be analogue or digital or both, with the latter incorporating an analogue-to-digital converter.

Most IR sensors require integration with a microcontroller, either incorporated into the package or interfaced externally, via I2C, USB or other protocols that allow for system integration.

Additionally, an optical filter or lens can be placed in front of the sensor, enabling it to converge or focus specific frequencies or wavelengths. For some applications, a lens assembly may be incorporated to focus distant IR radiation on to the pyroelectric detector. In order to limit spectral response, an optical band-pass filter can be used to block certain radiation wavelengths, to avoid false alarms, for example, or to detect specific substances. When multiple elements are integrated into a sensor array, the application may call for different wavelengths of IR light detected on each pixel. In this case, a device such as a linear variable filter (LVF) can be integrated. See Figure 2.

IR sensors in operation

All objects emit some form of thermal radiation, usually in the infrared spectrum, and different materials absorb different wavelengths of infrared energy. Thus, IR sensors can be used to analyse substances, including solids, liquids and gases, and identify specific elements within those substances. Additionally, they can be used to measure flames, as well as to detect presence and motion.

The benefit of using IR sensors for spectroscopy is the ability to capture a wealth of information from the sample, including considerable detail to determine sample composition and concentration, sample identification, and the presence of contaminants or additives, as well as atomic structure and molecular interactions.

IR energy from the sample excites vibrational motions in the covalent bonds in molecules. These vibrational modes have been proven to be unique to a specific chemical structure, thereby providing a ‘fingerprint’ of the sample material for identification purposes.

IR sensors for spectroscopy can be constructed on thin-film pyroelectric materials, which may be thin-film PZT (piezoelectric) or lithium tantalate (LiTaO3) based. Alternatively, thermopile devices can be used. Thermopiles consist of a stack of thermocouples forming an electrical series of alternating materials. When a temperature difference is applied between the joints, an electrical voltage (signal) is produced.

While thermopiles are a mature technology delivering a reasonably good signal-to-noise ratio (SNR) and small pixels in an SMD format if required, responsivity is low. Pyroelectric thin-film PZT, meanwhile, has a superior SNR and high responsivity, and is faster and more accurate. In addition, devices can be smaller with denser arrays. Manufacturing is scalable and transferable, and the technology offers strong potential for improved performance.

Conversely, pyroelectric LiTaO3-based IR detectors have comparable performance to thin film, with a good SNR and high responsivity. However, resolution may be lower, they generally feature large elements and they are not available as SMDs. Devices are manufactured in dedicated fabs, and consequently are often more expensive.
Mid-IR sensor formats

For most spectroscopy applications, and particularly those requiring materials identification, such as food safety, fuel and oil analysis, and detection of counterfeit materials, mid-IR sensors are preferred. The interaction of mid-IR radiation with a given sample has been shown to provide the most useful spectral fingerprint, being very specific to the chemical structure of the sample. The spectra, derived from the fundamental bands measured, are higher intensity and less convoluted than the overtone/harmonic bands derived from near-IR radiation. Near-IR spectroscopy, however, can be useful for non-homogeneous samples and trace analysis, although mid-IR devices are now becoming available to meet some trace detection requirements.

Pyreos offers mid-IR sensors in a number of different formats, including unpackaged die, discrete sensors, 2D arrays and linear arrays. See Figure 3. At the heart of the company’s core skills lies its unique thin-film PZT, mid-IR sensor technology, together with the required materials, deposition/process, optics, sensor-level firmware and applications knowledge. From this base, Pyreos has developed many compatible and complementary product ranges, and has the capability to develop new pixel geometries and tailored designs to meet specific customer requirements.

Catalogue parts include single, dual and quad IR detectors, which may be analogue or digital and are typically packaged in TO-39 cans or in an SMD format. While both analogue and digital versions can be used for gas and flame detection, and material analysis, the digital devices are also suited to motion detection. The digital range, called ezPyro, is available in single-element and 2 x 2 pixel versions. Supplied with an integrated, configurable ASIC containing an I2C interface, these ultra-low-power devices are the smallest available, in an SMD package measuring just 5.65 x 3.7 x 1.55mm. More information on both digital and analogue single, dual and quad mid-IR sensors for gas and flame detection applications can be found in the white paper on our website at https://pyreos.com/resource-centre

Pyreos linear IR sensor arrays, meanwhile, are best described as a spectroscopy engine in a package. Devices are available with 128, 255 or 510 pixels. They can be used in three different ways to suit a variety of spectroscopy applications. See Figure 4.

Figure 3: Package styles for Pyreos digital and analogue products include TO-39 cans, SMDs and 16-pin dual in-line packages.

Figure 4: Three approaches to using Pyreos linear arrays for spectroscopy applications.
Transmission spectroscopy uses a linear variable filter integrated into the array package, enabling different wavelengths of IR light to be detected on each pixel. The technology enables systems offering high-performance, very low-power operation in a portable package for a range of general-purpose spectroscopy applications.

Attenuated total reflection (ATR) spectroscopy uses the IR array with LVF, in conjunction with an ATR crystal and IR light beam, again enabling sophisticated spectroscopy techniques to be taken out of the laboratory and used in a compact, fast, repeatable and easy-to-use system. It is particularly suited to analysing samples of fuel oil.

Grating spectroscopy, meanwhile, uses the linear IR detector array with a standard silicon or germanium filter typically used in conventional laboratory equipment, and requiring high performance.

Choosing sensors for spectrometry

There are two distinct aspects to using IR sensor-based detector for spectrometry applications in food safety and oil analysis applications. The first is where there are suspected unknown substances in a sample that need to be identified. A linear IR sensor array is the best option in this case, enabling the collection of data across the spectrum, and then analysing and quantifying it as necessary. The second is in applications where the composition of a substance is known, but the requirement is to quantify the various elements. In this case, a solution using discrete sensors, is an option. Analogue or digital devices can feature up to 4 channel detectors.

While the end application will generally determine which spectroscopy approach to take, there are some key specifications and features that engineers should look for when choosing and selecting sensor components for a new design, particularly for use in portable equipment.

- **Small size**: PZT thin-film processes produce the tiniest IR sensor components, enabling smaller and denser high-resolution arrays and modules.
- **Physically robust**: With no moving parts, the technology is innately rugged, withstanding shock and vibration and high operating temperatures.
- **No cooling required**: PZT can be easily patterned to provide individual sensor pixels on a thermally isolating membrane layer.
- **Minimal calibration**: Rugged thin-film PTZ technology delivers stable and accurate operation, with no degradation over time or due to higher temperatures.
- **High responsivity**: Current-mode read-out provides high responsivity over voltage mode types. Output signals do not depend on sensor capacitance, giving faster response times. See Figure 5.
- **Excellent SNR and high sensitivity**: Thin-film pyroelectric IR sensors deliver the highest specifications.
- **Low power**: Passive devices offer the lowest-power operation with lower duty cycle. Read-out circuits can be as low as 0.9µA, with wake-up via IR radiation.
- **Modular**: There are packaging options from chip to array, plus a range of filters, digital interfaces and complementary products for easy systems integration.
- **Economical**: Manufactured in standard semiconductor foundries, taking advantage of competitive process options. Small, dense arrays enable lower-cost modules for portable systems.
- **Scalable production**: Technology is easily scalable for low or high volumes.
- **Developing (yet proven) technology**: New R&D investment is likely to lead to improved performance and broader application scope. Design flexibility for easy customisation.

Pyreos’ innovative current mode read-out technology delivers high, stable and fast responsivity

- Traditionally pyroelectric sensors are read-out in voltage mode
- Pyreos’ current mode technology provides extremely high responsivity over a broad frequency range up to 100Hz
- Since output signals do not depend on sensor capacitance, response times are extremely fast

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Typical voltage mode sensor</th>
<th>Pyreos current mode sensor</th>
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<tbody>
<tr>
<td>Responsivity</td>
<td>≤ 5 kV/W</td>
<td>100–500 kV/W</td>
</tr>
<tr>
<td>Thermal frequency response</td>
<td>Peak at 9.1–1.0 Hz</td>
<td>Stable up to 100 Hz</td>
</tr>
<tr>
<td>Time constant</td>
<td>&gt; 100 ms</td>
<td>~19 ms</td>
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Figure 5: Current-mode sensing delivers higher, faster and more stable responsivity than traditional voltage mode.
Application examples

Food safety is a major concern, as the world’s population grows, and globalisation sees food products becoming an increasingly valuable commodity. Spectrometers using Pyreos’ mid-IR sensor arrays have been successfully deployed in India since 2015, analysing milk. Portable instruments are used in the field or in-line in during processing, to check on the composition of milk products, and to detect adulterants such as added water, sugar, maltodextrin, urea and trace chemicals (i.e. from fertiliser products or tainted cattle feed). Each adulterant can be specifically identified from its unique ‘fingerprint’ dependent on the IR radiation detected by the sensors. More sensitive than near-IR, mid-IR sensors are the most reliable means of providing a fast and accurate response from a given sample.

The option of using linear variable filters on the Pyreos 128 element arrays allows for a much broader spectrum to be covered. LVFs are available to cover the 2.5 to 5µm range and the 5.5 to 11µm range.

Mid-IR spectroscopy is used for analysing the composition of edible oils and detecting adulterants or inferior-quality products that might be used to bulk out a shipment. Counterfeit wine and whisky are becoming increasingly common. Portable analysers are useful for confirming critical parameters like alcohol and sugar content at any point along the supply chain.

Reducing reliance on fossil fuels is giving rise to alternative energy sources, such as bio-fuels. Increasingly, detailed fuel characterisation and testing is required to ensure optimum performance and to assess environmental impact. Mid-IR spectrometers can be developed to analyse the content of these new bio-fuels. Instruments can check octane levels in conventional fuels, and check for the presence of fuel additives like ethanol. Again, it is the use of mid-IR sensors that enables modular instruments to detect the adulterants or contaminants specific to an application. And high-density thin-film mid-IR arrays are the key to building an affordable, easy-to-use and effective spectrometer.

As an example, the Parker Kittiwake ATR analyser can be used on board ship, to check the condition of engine oil while it is hot and the ship is cruising. (weblink: https://www.hellenicshippingnews.com/parker-kittiwake-launches-breakthrough-analysers-which-tests-four-parameters-at-once-to-prevent-engine-damage/ ) The ability to test simultaneously for water content, base number, total acid number, soot loading, viscosity and fatty acid methyl ester (FAME) allows engineers to assess the state of the oil. Frequent testing ensures that unnecessary engine damage due to contaminants is avoided, but also that oil is not changed before it needs to be. See Figure 6.

![Figure 6: Differences between new and used oil are easily visible in the IR spectrum.](image)

Other upcoming application areas for mid-IR spectroscopy include chemical and pharmaceutical production (confirming the composition of incoming materials, or in QA and testing of finished products) and environmental monitoring, such as measuring air quality and detecting contamination in high-risk areas.

A recent Pyreos development is its 128+1 linear IR sensor array. The addition of an extra, super-sensitive, large pixel is a boon to many spectroscopy applications. For example, with an appropriate optical filter, the extra pixel can be used to focus on specific infrared wavelengths with the LVF spectral range, with a much higher sensitivity (SNR can be 10 to 50 times higher). This allows lower concentrations of a key substance to be detected, while the line array measures the broader spectrum. Alternatively, it can be tuned to look at wavelengths outside the spectrum of the LVF.
Conclusion

To summarise the key advantages of mid-IR sensor technology for food safety and fuel and oil analysis applications:

- Mid-IR sensors are optimal for determining sample composition due to their ability to generate a clear ‘fingerprint’ of components detected.
- The construction of thin-film PZT mid-IR sensors makes them ideal for building multi-sensor arrays that are small and robust, both physically and thermally, for portable equipment.
- The technology delivers higher responsivity, superior SNR and lower-power operation over alternative approaches.
- The modular design approach and scalable manufacturing potential afforded by mid-IR linear arrays, plus the range of optical filter options, ensure that the technology will suit a wide range of portable spectroscopy applications at low cost.
- Easy interfacing to microcontrollers using industry-standard protocols enables OEMs to build equipment that is easy to use and tailored for the specific end-user application.