Emphasis Shifts to Testing All Critical Phases of a Process

Providing faster results than traditional methods, FT-IR and FT-NIR technologies are growing in popularity in the chemical processing industry

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Fourier-Transform Infrared (FT-IR) and Fourier-Transform Near-Infrared (FT-NIR) are two technologies that are being increasingly used in the chemical processing industry. While these two technologies are similar, there are important differences between them that make each better suited for particular applications. FT-IR and FT-NIR can be utilized at many stages of chemical processing, including raw material, intermediate product and final product testing. This article will explain the differences between these two technologies and describe how they can be used to improve the quality of chemical processing operations. Chemical manufacturers typically use a range of analytical chemistry tools to separate and identify the components of their final products and often to evaluate raw and intermediate materials as well. But traditional analytical methods such as HPLC can require hours to prepare samples for analysis and complete a run. These techniques are often not well suited for process analysis because it’s usually too expensive and time intensive to hold up the manufacturing process while testing is underway. In addition, they require specialized sample preparation methods that are difficult to perform in a manufacturing environment. Another problem with many conventional analytical methods is they generally are not capable of measuring the physical properties that are sometimes critical in raw materials and process testing. The trouble with relying exclusively on traditional methods is that problems are often identified only at the last stage of manufacturing, sometimes making it necessary to destroy a batch after large amounts of money have been invested. For this reason, chemical processing manufacturers are putting an increasing emphasis on testing at critical phases throughout the manufacturing process. Testing performed upstream does not eliminate the need for testing of the finished product, but it does usually reduce manufacturing costs by avoiding waste and providing diagnostic information that can be used to correct problems and optimize upstream processes. The popularity of FT-IR and FT-NIR technologies is increasingly in the chemical processing industry because they can provide much faster results than traditional methods, often delivering a pass or fail reading in a matter of seconds. FT-IR and FT-NIR take advantage of the fact that each molecule’s functional groups absorb radiation to generate a characteristic absorption or transmission spectrum that is rich in information and unique to that molecule. Spectra can be analyzed or searched against libraries of reference materials to identify unknown materials positively. Just like human fingerprints, infrared spectroscopy provides a spectral fingerprint that uniquely identifies a chemical compound. Modern FT-IR and FT-NIR instruments combine a wide spectral operating range, higher spectral resolution and superior wavelength precision, potentially providing a wealth of important information not available to old technology systems.

The PerkinElmer Spectrum 100 is an FT-IR spectrometer that can be used for a wide range of samples.

There are several types of IR and NIR spectrometers, each suited to different applications. For high-throughput in-process measurements, simple filter instruments are often used successfully. Dispersive NIR spectrometers have also been used for QA/QC measurements. However, for materials quality and product development measurements in the lab or at-line, FT-IR and FT-NIR spectroscopy have been established as leading technologies, primarily because of their speed, reliability and robustness in a manufacturing setting. While FT-IR and FT-NIR are similar, there are important differences between them, which makes each better suited for particular applications. Mid-IR range spectra are typically very strong, which means very sensitive detections, but they also require a degree of sample preparation that is usually best performed in a laboratory setting. Mid-IR spectra are also relatively simple to interpret, enabling an unknown material’s composition to be derived easily. FT-IR instruments are most commonly used to perform detailed analyses of raw materials, intermediate products and final products and for troubleshooting. An example of an FT-IR application involves a major consumer goods producer. The company ensures compliance with strict internal quality standards by generating a unique fingerprint of incoming shipments using FT-IR. Any change in the incoming material from what has been approved previously is immediately detected and the material is not accepted unless it can be proven that it will not have a negative impact on the finished product. The use of automated instruments and software makes this unique level of inspection cost-effective by allowing users without scientific training to generate infrared spectra from a sample and validate them against reference spectra in about five minutes. The ability to provide positive identification of incoming raw materials quickly helps the company maintain the highest possible quality standards while saving time that can be applied to other quality control procedures. In addition, FT-IR has been useful in troubleshooting tough specialty chemical applications. In one case, an electronics cleaning solution worked perfectly with the previous process, but after a process change, an unacceptable discoloration remained on the surface of the carrier. A specialty chemical manufacturer that competed with the original supplier analyzed the residue and discovered it was a particular surfactant used by its competitor. This provided valuable guidance in helping to identify a formulation that solved the problem quickly. FT-NIR absorbencies on the other hand, are not as strong, which in most cases eliminates the need for sample preparation, increasing analysis speed and enabling non-destructive testing. FT-NIR instruments are thus much more suitable for use in a manufacturing environment. FT-NIR can be utilized at many stages of chemical processing including raw material, intermediate product and final product testing. The result can be substantial improvements in quality as well as reductions in costs as problems are identified and fixed before additional resources are invested. For example, a fiber-optic NIR probe can be inserted into a bin of raw materials or a blend and, within seconds, the chemical and often the physical properties of the material can be analyzed with a “go” or “no go” result presented to the operator &#151 sometimes on an LCD display on the probe itself. FT-NIR provides an excellent tool for diagnosing processing operations. The speed and lack of special skills required to use this method make it possible to employ it to make frequent samples of intermediate products such as after a blending operation. All in all, FT-IR and FT-NIR spectroscopy provides important advantages to the chemical processing industry. The speed and ability of these technologies to provide analysis results with little or no sample preparation make them useful at any stage of the manufacturing cycle. As a result, in many applications, they can enable cost reductions and quality improvements. *Sharon Williams is the infrared business manager at PerkinElmer Life & Analytical Sciences, Chalfont Road, Seer Green, Beaconsfield, England, which specializes in the health sciences and photonics markets. Questions about this article can be addressed to Williams at 011 44 1494 679020. Additional information is available at www.perkinelmer.com/spectrum100.*