NIR Technology Systems

Application Note 8: Measurement of Raw Materials in the Pharmaceutical Industry

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Introduction

Near Infrared spectra contain information about the chemical and physical character of a material. Overtone and combination absorption bands for C-H, N-H and O-H bonds provide the ability to characterise materials based on their NIR spectra in the same way as MIR finger printing. The use of Discriminant Analysis routines make the process of identifying and qualifying materials easy and reliable. A portable NIR spectrophotometer with a fibre optic probe provides the ability to identify and qualify raw materials and materials in process within a pharmaceutical manufacturing operation.

Description:

Figure 1. shows the Fibre Optic Probe (FOP) Analyser with a diffuse reflectance probe. The instrument scans the visible through to the 3rd overtone NIR region, ie, 500-1050nm. Within this region a broad range of chemical entities can be observed, including, sugars, alcohol, protein, triglyceride, aliphatic and aromatic carbon-hydrogen, water, amines and amides.

Figure 1. NIR FOP Analyser

By building a library of known spectra, the FOP Analyser can be trained to identify specific materials based on their NIR spectra. The discriminant analysis routine prompts the operator to scan the sample by inserting the probe into a container or

drum of the material. The program then searches the library and picks the spectra with the lowest Mahalanobis distance. A list of the top 3 matches is shown with the best match at the top of the list.

The program can also qualify a materials as being within specification. This procedure uses a file which contains several spectra of the same material which represents the natural variation encountered from the supplier. The sample spectra is compared to the reference file and the Mahalanobis distance computation is used to decide whether the sample spectrum is the 'Same As' the other spectra. If the sample spectra lies within the 'Cluster' of the reference spectra, then the material is 'Accepted'.

Conclusion

NIR Discriminant analysis is a powerful technique for the non destructive identification and qualification of materials. The benefits of NIR spectroscopy are in the ease of spectral collection. A portable NIR spectrophotometer with a fibre optic probe makes this technique an ideal tool for the pharmaceutical industry.

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