

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 makes the process of identifying and qualifying materials easy and reliable. The Sameness Meter is a portable NIR spectrophotometer with a fibre optic probe that provides the ability to identify and qualify raw materials and materials in process within a pharmaceutical manufacturing operation.

Description:

The Sameness Meter scans the wavelength range, 1200-2400nm, using a InGaAs diode array detector and a flat field spectrograph. A 6V 10Watt tungsten halogen lamp fitted into the end of a stainless steel probe, illuminates a sample of powder and 12 fibre optic cables collect the reflected light and return the light to the spectrometer. The fibre optic cable consists of 12 x 1.2m x 0.4mm diameter low hydroxyl, silica glass fibres enclosed in a stainless steel flexi coil sheath. The probe has a button on the handle so that the

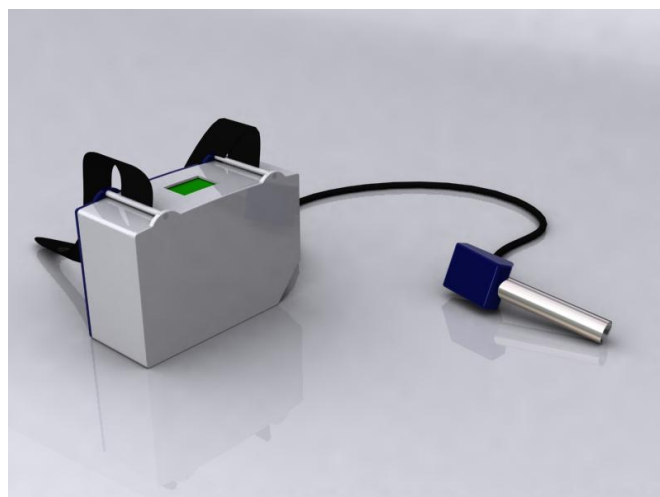


Figure 1. The Sameness Meter –

Hip-n-Holster operator can easily collect the spectrum by placing the stainless steel probe into the bag of raw material and pressing the button. The spectrum is sent by Radio Frequency Modem back to a remote PC, which runs the Discriminant Analysis program. The NIR spectrum is compared to a library of raw materials and the closest matching spectra allows the system to identify the raw material. A c is used to qualify the spectrum as being within a defined specification range. The computer determines if the spectrum is within specification or not and sends back the Name of the material, the Coefficient of Fit and an Accept or Reject decision to the Sameness Meter.

The inclusion of RF Modem allows the operator to walk from container to container and to identify and qualify the raw materials with out dragging a PC behind them. The Sameness Meter has a rechargeable battery that can operate for approximately 45 minutes before recharging.

Experimental Data:

The spectral plots below show the NIR spectra of the following materials;

Di Sodium EDTA, Glucose, Ilium Propionate, Nicotinamide, Paracetamol, Prednisolone Acetate, Paper, Polyethylene, Polystyrene, Propylparaben's.

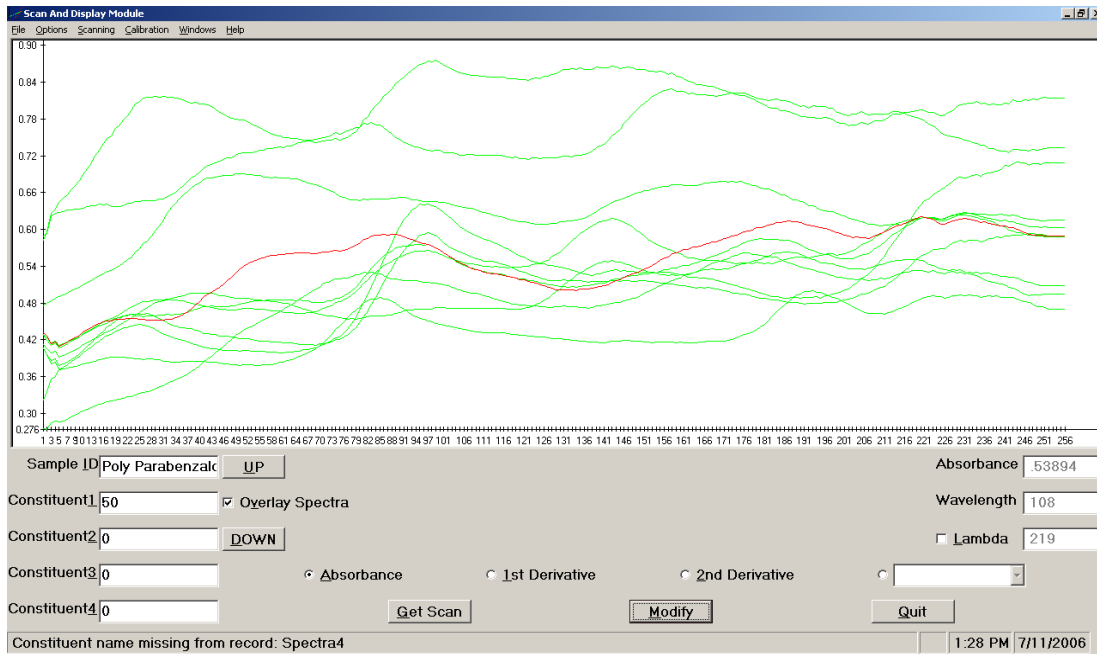


Figure 2. NIR Spectra of 9 different materials

Several spectra of each material were scanned and saved into unique files. These files made up the spectral library.

When a sample is scanned and the NIR spectrum sent from the Sameness Meter to the PC, the Discriminant Analysis program scans the library files and matches the spectrum to the closest file.

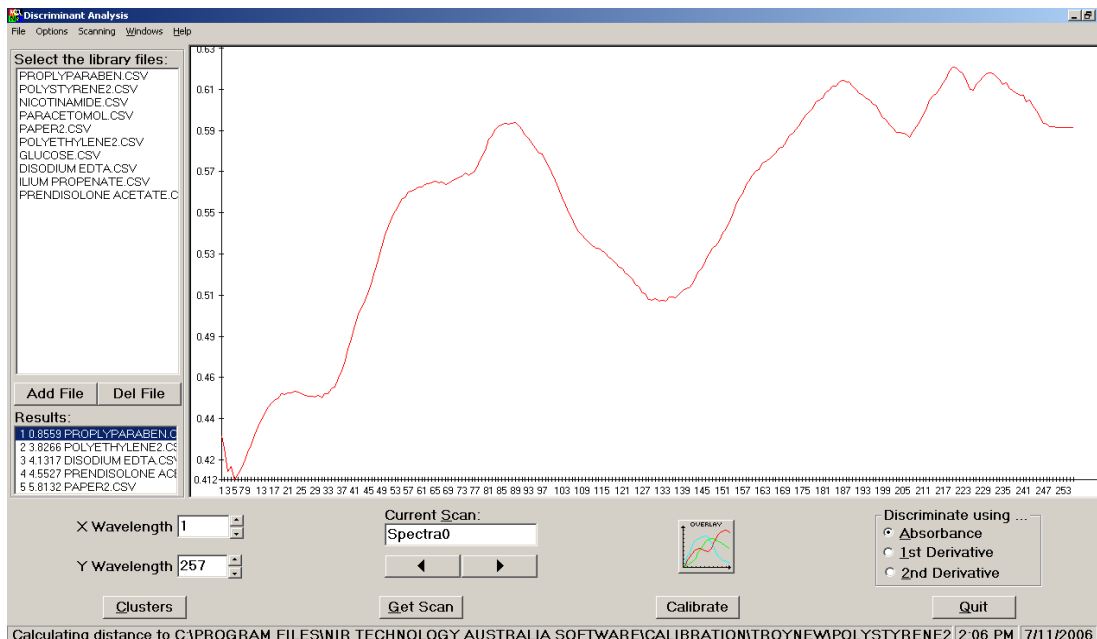


Figure 3. shows the Discriminant Analysis window on the PC. The library files are listed in the top left hand corner and the unknown spectrum is displayed on the screen. The Discriminant Analysis software lists the top 5 matches and computes the Mahalanobis Distance between the unknown spectrum and each of the library files. The one with the least Mahalanobis Distance is identified as the matching file. The program computes the Coefficient of Fit for the unknown spectrum to the matching spectral file and computes if this is within the defined specification. The PC then transmits the Name, Coefficient of Fit and an Accept or Reject message back to the Sameness Meter.

The data is displayed on the LCD screen of the Sameness Meter. By placing the probe into the next container and pressing the button, the process is repeated.

All the materials were scanned again to ensure that they were correctly identified. 100% identification was established.

Discussion:

The Sameness Meter provides a rapid means of performing raw material inspection and identification. The simplicity of operation and the convenience of portability make the Sameness Meter a cost effective tool for the Pharmaceutical industry.