NIR Chemometrics Software

NTAS(NIR Technology Analysis Software) is a complete suite of spectral analysis and calibration routines for use with the MultiScan Series of NIR Analyser

Scan and Display

Scan and Displays provides a means of scanning samples and displaying the spectra on the screen. The NIR spectra can be transformed into 1st and 2nd derivative as well as Standard Normal Variant and Multiplicative Scatter Correction algorithms. Spectra can be overlayed, marquee and zoom in functions. A unique feature of Scan and Display is to display the probable chemical bonds at each wavelength in the spectra. As the cursor is moved along the spectrum, a chemical bond is displayed.

Calibration

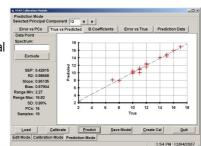
NTAS provides a comprehensive calibration routine using Partial Least Squares (PLS) Regression. Samples can be scanned and saved using the Scan and Display routine. The reference values can be added to the spectral files using the Edit feature. Then the calibration spectral file can be imported into the Calibration Creation routine. A few simple keystrokes and a PLS model can be created and saved. Up to four models can be developed and saved in the one product file.

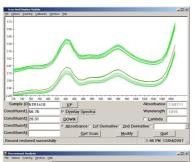
Analysis

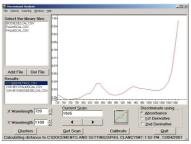
Series 4000 is operated directly from NTAS using a PC. The Analysis program in NTAS allows the operator to connect to the analyser and thereby control the instrument's operation. Simply select the Product from the memory and perform an analysis by following the screen prompts. The results of up to four components are displayed on the screen in either a Trend Plot or a Table of Results. Results can be stored in memory for later reporting or further analysis.

Discriminant Analysis

NTAS also provides a Library Search routine called "Discriminant Analysis". A set of spectra files for a wide range of materials, e.g., raw materials used in a food or a pharmaceutical manufacturer, are stored in memory as a library file. Incoming or unknown materials can be scanned quickly and identified based on their spectrum. This technique does not require any calibration and provides a rapid means of ensuring that the material is the "Same As" described on the label and the "Same As" last batch. The Discriminant Analysis routine uses Mahalanobis Distance between spectra to match a test sample to the closest library file.



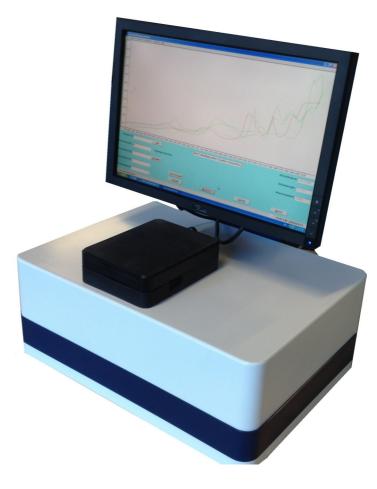




Specification	Series 4000 FTNIR
Wavelength Range	4000- 8300cm ⁻¹ , 800-2500nm
Opics/Detector	Michelson Interferometer/InGaAs
Lamp	Tungsten Halogen 12VDC, 20W
Scan Rate	Up to 5 per sec
Resolution	1,2,4,8,16,32 and 64cm ⁻¹
Display	Touch Screen PC
Power	19VDC using 110 –240VAC
Dimensions (cm) Weight (Kg)	60 W x 40 D x 18 H 22Kg



MultiScan Series 4000 FTNIR Spectrophotometer



The Next Generation of Near Infrared Analysers

Manufactured by: NIR Technology Systems

B1 366 Edgar Street, Condell Park, NSW, 2200, Australia Tel: 612 9771 5444, fax: 612 9771 5255 Email: sales@nextinstruments.net Web: www.nextinstruments.net





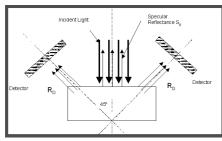
Near Infrared Spectroscopy

In the Near Infrared spectral region, 700 to 2500nm. chemical entities such Carbon-Hydrogen, Oxygen-Hydrogen and Nitrogen-Hydrogen absorb light passed through or reflected off a sample. The amount of light that is absorbed by these chemical bonds is proportional to the concentration of the compounds containing the C-H, O-H and N-H bonds. Compounds such as amines, amides, hydrocarbons, carbohydrates, phenolics, alcohols and water can be measured in slurries, emulsions, granules, liquids and powders. As such, NIR spectroscopy is an excellent analytical technique for measuring a broad range of organic materials across many industries.

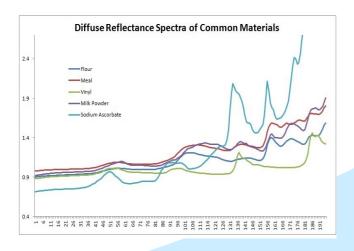
Near Infrared Reflectance (NIR)

Diffuse Reflectance Spectroscopy is performed by illuminating a solid sample, e.g., powder, textile, film, etc. at 0 degrees and collecting the re-radiated energy at 45 degrees to the illumination beam. The schematic below shows a typical Diffuse Reflectance NIR spectrometer.

The optimum spectral region for collecting diffuse reflectance spectrum is between 1200



and 2500nm. The combination stretch and bend vibrations of C-H, N-H and O-H bonds lies between 1900 and 2500nm, while the first and second overtone vibrations occur between 1200 and 1800nm. The 1st and 2nd overtone regions provide good absorption spectra for transmission through liquids or reflectance off high water content solids.



MultiScan Series 4000 FTNIR Spectrometer

The Series 4000 FTNIR Spectrometer is a powerful Fourier Transform Near Infrared spectrometer designed to measure reflectance and transmission spectra through liquids,

powders, granules and slurries. The Series 4000 measures the O-H (water and alcohol), N-H (proteins, amides and amines) and C-H (fats, oils, surfactants, carbohydrates and hydrocarbons) bonds in a broad range of materials.

The Series 4000 is based on a Michelson interferometer using a InGaAs detector. The systems offers far superior performance over dispersive NIR spectrometers.

The Series 4000 has a range of samples cells available to measure liquids, slurries, granules, pellets, powders, films and woven materials. NTAS(NIR Technology Analysis Software) is included in this system and provides a comprehensive Chemometrics software package that includes;

- Scan and Display
- Discriminant Analysis
- Analysis
- Calibration Creation
- Spectral Matching

Applications for the Series 4000 FTNIR include:

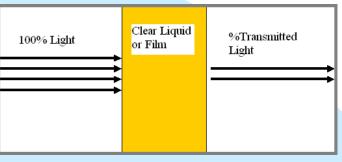
- · Stockfeeds and Meals
- · Food and Food Ingredients
- Petrochemicals
- Chemicals
- Pharmaceuticals
- Plastics and Polymers

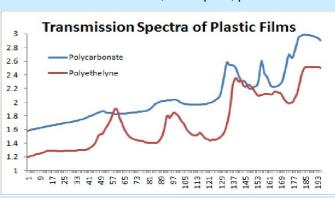


through the sample is focused onto the InGaAs detector where the electronics and software collect the interferogram. The inverse Fourier transform is applied to the interferogram to generate the NIR spectrum. For materials that are clear, i.e. Liquids, plastic films or

Near Infrared Transmission and Transflectance. (NIT)

The schematic below shows the optical configuration for transmission spectroscopy. Light from the interferometer passes through a sample cell containing liquids, slurries or films. The light is absorbed by the C-H, O-H and N-H bonds in the sample in direct proportion the concentration of each bond. The light that passes





sheets, the light passes through the sample without deviation. This technique is classical transmission spectroscopy. Typically the pathlength of such samples is between 0.5 and 2mm thick.

For materials that have a high solids to water content, i.e., slurries, pastes or emulsions, the light actually passes through the material by internal reflectance off the solid particles and through the liquid phase. This is referred to as Transflectance, i.e., a combination of reflectance and transmission. For samples with high water content, transflectance offers the advantage in that the NIT spectrum represents the whole of the sample not just the surface. In this spectral region, NIR light can pass through a sample up to 30mm thick. Typically cheese, meat and high moisture content foods are measured using a 10mm pathlength.

How the Series 4000 FTNIR work.

The Series 4000 FTNIR spectrometer is based on a Michelson interferometer as shown in the schematic. Coherent light passes into a 50:50 beam splitter, where half the light is deflected to the Stationary Mirror and half to the Moving Mirror. As the Moving Mirror moves back and forth, the reflected beams from both mirrors are re-combined and emerge from the bottom of the beam splitter. The re-combined beam illuminates the surface of the sample and re-radiated energy is collected by the InGaAs* detector. As the Moving Mirror oscillates the pathlength of the two beams differs so that when they are re-combined, they undergo constructive and destructive interference. The detector scans the re-combined beam over the time it takes for the mirrors to move in and out of phase. The signal collected by the detector is the interference pattern but it is called an Interferogram.

The interferogram is an encoded signal where every point in the interferogram is a summation of the light absorbed at each frequency. To decode this signal, an inverse Fourier** transform is applied and the underlying spectrum is reconstructed.

An internal laser beam is used in an interferometer to measure the movement of the Moving Mirror. When the two mirrors are exactly the same distance apart, i.e., they are in phase, then the laser beam is detected. As the beams move out of phase the laser beam intensity is modulated directly in proportion to the distance travelled by the mirror. The modulated laser beam provides an absolute reference for the wavelength of the re-combined beam.

The following advantages are inherent in an interferometer (FTNIR) spectrometer;

- · Fellgett's advantage: All wavelengths of light pass through the sample simultaneously and produces higher S/N ratio.
- Jacquinot advantage: Large beam sizes allows higher light throughput.
- · Conne's advantage: Absolute wavelength accuracy based on an internal laser beam.
- Stray Light advantage: Encoded light signal is independent of stray light.
- Speed: Interferometers generate spectra at very high rates.
- InGaAs—Indium Gallium Arsenide Semi-Conductor Detector.
- ** Fourier—A French mathematician that showed that all waveforms could be described by a series of sine and cosine functions. Conversely an interference pattern can be deconstructed using an inverse transform to reconstruct the underlying waveform, i.e.,