The FTNIR Myths... Misinformation or Truth

Recently we have heard from potential customers that they have been told that FTNIR instruments are inferior to dispersive or monochromator based NIR instruments. 40 years ago when FTIR instruments first were introduced, the manufacturers of dispersive IR instruments mounted a similar campaign of misinformation. So let me provide you with some facts and you can make up your own mind.

1. FTNIR, ie, Fourier Transform Near Infrared Spectrometers, are simply another way of generating a NIR spectrum. Dispersive spectrometer which include monochromators and diode array spectrometers, generate NIR spectra. Filter based instruments also generate NIR spectra but at discrete wavelengths.
2. The issue is not how the spectra are generated but what is the signal to noise ratio, wavelength accuracy, wavelength precision and resolution of the spectra.
3. A secondary issue is what added advantages are provided by using one type of spectral generator vs other types. These advantages include;
   - calibration transferability
   - long term precision
   - resolution
   - speed of analysis
   - stray light affects
4. Mid IR spectrometers, including FTIR, use hygroscopic windows and beam splitters such as Potassium Bromide (KBr) and Sodium Chloride (NaCl). NIR spectrometers, including FTNIR, use quartz windows and beam splitters. Whereas Mid IR spectrometers require dry air purging or at least a desiccant, NIR spectrometers do not need air purging or desiccation.

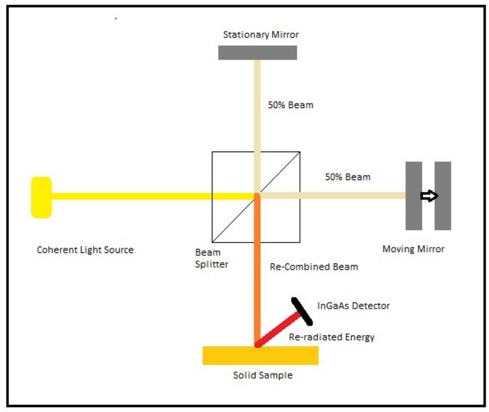
How the Series 4000 FTNIR work.

Light from a tungsten halogen lamp is collimated and passed through a beam splitter. Half the light passes through the beam splitter and onto a moving mirror adjacent to the beam splitter. The other half of the light is reflected 90 degrees to stationery mirror. The two light beams are recombined and focused onto the surface of the sample and then to the detector. As the moving mirror oscillates back and forth, the path travelled by the two beams changes and the recombined beam undergoes constructive and destructive interference. In effect the recombined beam is encoded and the InGaAs detector records the encoded signal as an Interferogram. By applying an Inverse Fourier Transform to the Interferogram, the original spectrum of the sample can be generated.

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 who 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., spectrum.

Signal to Noise Ratio: Fellgetts and Jacquinot Advantages.

This is the measure of the size of the 100% light signal as compared with the electronic and mechanical noise of the spectrometer. A UV-Vis spectrophotometer typically has a signal to noise ratio of 1000:1. A NIR spectrophotometer needs to have a signal to noise ratio of better than 50,000:1.

The noise of an instrument is limited by the following considerations;

1. Detector dark current, ie, the high frequency jitter than exists within all electronics.
2. Amplifier and digitiser range, ie, how much the analogue signal can be amplified and then digistised before the signal size is the same as the background noise.
3. Mechanical noise, ie, the vibration, thermal fluctuations and ware variations that arise from mechanical devices.

These noise components can be reduced by signal averaging. The faster the spectrometer scans, the more signal averaging that can be achieved in a given period of time. Monochromator based spectrometers typically scan at 2 scans per second FTNIR spectrometers scan at 5-30 scans per second. As such FTNIR spectrometer can provide a 2.5 to 15 times the signal averaging improvement in the signal to noise ratio.

Another way of improving the signal to noise ratio is to increase the signal size as seen by the detector. Dispersive spectrometers, by definition, use a diffraction grating to disperse the light into a continuous wavelength spectrum. The higher resolution of the diffraction grating/optics means less energy reaches the detector and a lower signal to noise ratio. A FTNIR spectrometer passes approximately 50% of the lamp energy through the optics system and onto the sample and then to the detector. As such the signal to noise ratio is typically 100 to 1000 times greater using an FTNIR spectrometer as compared to a dispersive spectrometer. This is called the Fellgetts Advantage.

Dispersive spectrometers use a slit to limit the spectral resolution of the spectrometer. Typically a slit of 0.5mm by 10mm is used on the exist of the diffraction grating. The slit excludes a very large proportion of the available energy from the lamp. A FTNIR does not use a slit but typically has a circular beam that is 10-15mm in diameter. As such more energy can be passed to the sample and then to the detector. As such FTNIR spectrometers have increased energy throughput which means higher signal to noise ratio. This is called the Jacquinot Advantage.

The net result of the Fellgetts and Jacquinots advantages is that an FTNIR spectrometer has a much higher signal to noise ratio, ie, 600,000:1.

Wavelength Accuracy: Conne’s Advantage

The wavelengths at which chemical bonds absorb energy are defined by the physical structure of the molecule and the surrounding chemical bonds. The idea behind a spectrometer is to isolate the absorbance bands at each wavelength. If the instrument cannot isolate the wavelengths then it fails as a spectrometer.

Dispersive spectrometers require an external source to calibrate the wavelength scale of the spectrometer, ie, a narrow band filter with a known wavelength. Dispersive spectrometers use diffraction gratings to disperse the spectra across the wavelength range. Diffraction gratings have a non linear dispersion from one end of the spectra to the other.

As such, dispersive spectrometers require calibration at several wavelengths. However since diffraction gratings and optics vary from instrument to instrument, the wavelength assignment can vary from instrument to instrument. As such calibrations developed on one instrument may not transfer easily to another instrument.

FTNIR spectrometers use an internal laser beam to track the mirror movement to fractions of a nm. The interference pattern generate using a FTNIR is decoded by applying an inverse Fourier Transform computation to generate the NIR spectra which has absolute wavelength accuracy and a constant resolution across the spectrum. This means that NIR spectra generated by one FTNIR is the same as generated by another FTNIR given the same spectral collection optics. This means that calibrations can be more readily transferred from one FTNIR spectrometer to another. This called the Connes Advantage.

Wavelength Precision:

It can be stated that Wavelength Accuracy in NIR spectroscopy is not as significant as it would be in Mid IR Spectroscopy. However Wavelength Precision, ie, the ability to reproduce the wavelength assignment consistently over the life of the spectrometer, is very important. Inherently due to the use of the internal laser beam, FTNIR spectrometers have extremely high wavelength precision. Most dispersive spectrometers also have very high wavelength precision because it is so important. However monochromator based spectrometers have bearings and encoders that govern the Wavelength Precision of the spectrometer. As the bearings ware the Wavelength Precision deteriorates. FTNIR spectrometers are more stable over the life of an instrument than monochromator based spectrometers.

It should be noted that Diode Array NIR spectrometers do not have bearings or encoders and as such do not deteriorate over time in respect to Wavelength Precision.

Stray Light:

Stray Light is the energy that reaches the detector without passing through the sample or the spectral generator. The sensitivity of a measurement is limited by the stray light. The following table show the absorbance limits based on 0.1%, 0.01% and 0.001% Stray Light.
A dispersive spectrometer is affected by stray light even if the NIR spectrometer is extremely well

Concentration	Transmission %	Absorbance, SL = 0	Absorbance, SL = 0.1%	Absorbance, SL = 0.01%	Absorbance, SL = 0.001%
0	100	0.000	0.000	0.000	0.000
1	10	1.000	0.996	1.000	1.000
2	1	2.000	1.959	1.996	2.000
3	0.1	3.000	2.699	2.959	2.996
4	0.01	4.000	2.959	3.699	3.959
5	0.001	5.000	2.996	3.959	4.699

made and excludes as much stray light as possible. A FTNIR spectrometer does not have stray light because the light from the lamp is encoded using the interferometer. The detector only recognises the encoded light. Exterior light from fluorescent lamps or sun light or internal reflection of windows or mirrors is completely eliminated in an FTNIR. As such, a FTNIR spectrometer has the potential of measuring far smaller levels of light than a dispersive spectrometer.

Resolution:

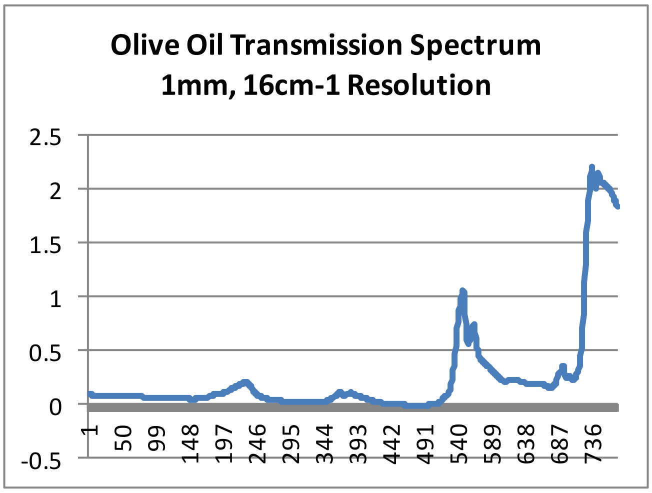
The spectral resolution of a dispersive spectrometer is fixed by the slit width and the F number of the optics. Typically a monochromator and diode array spectrometer have spectral resolution of 8-10nm half height band width at the central wavelength. The spectral resolution of a FTNIR spectrometer is variable and is based on the mirror movement. The basic resolution of a FTNIR is approximately 1nm.

The data resolution is a different term and relates to the size of increments in wavelength across the spectra. In a dispersive spectrometer, the data point resolution is determined by the encoder or the pixel width. For example, if the encoder has 1000 segments then the data resolution is the wavelength range divided by 1000. For a diode array spectrometer, the data resolution is the wavelength range divided by the number of pixels in the detector array. Different brands of dispersive spectrometers vary in their data resolution between 0.5 to 2mn. Diode array spectrometers have data resolution of approximately 3nm.

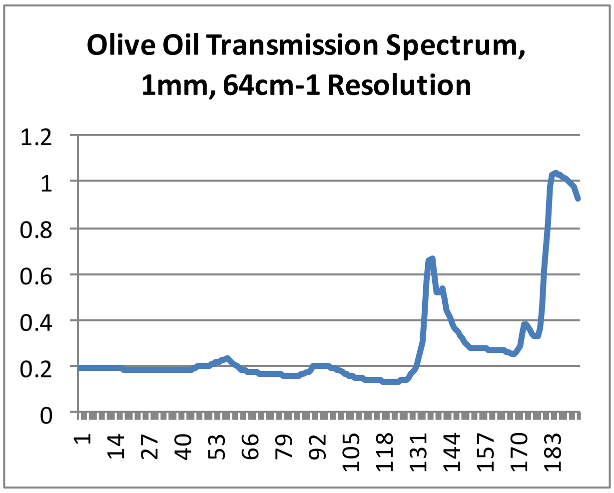
In a FTNIR, the data resolution is governed by the apodization function groups sequential data points. The most common apodization function is a simple box car smoothing, ie, averaging. As such, FTNIR spectrometers typically offer a range of resolutions, ie, 2, 4, 8, 16, 32 or 64 $cm^{-1.}$

The resolution NIR spectra is not always important. For most applications, the 10nm resolution of dispersive spectrometers is sufficient. However there are some applications where higher resolution, ie, 2 or 4nm, is a benefit. For example measuring vegetable oils for Free Fatty Acids, or measuring Amino Acids in stockfeeds, then resolution is important. Below are two spectrum of the same sample of olive oil. Note that sample A has a high resolution and the CH bands are separated.

Sample A High resolution



Sample B Low Resolution



The benefit of FTNIR lies in that the resolution can be changed through the software in seconds.

Reality vs Theory

1. The majority of dispersive spectrometers are excellent instruments that are well suited to NIR spectroscopy. For more than 35 years, monochromator based spectrometers have been the mainstay of instruments used for research and analytical NIR analyses.
2. FTNIR spectrometers first appeared approximately 25 years ago and have proven to be a very good alternative to monochromator system.
3. The latest generation of FTNIR spectrometers which use thermoelectrically cooled InGaAs detectors, self adjusting optics and 24 bit A/D converters, have leapt ahead of monochromators because they offer superior signal to noise ratio, wavelength accuracy, resolution and calibration transferability.
4. FTNIR spectrometers are like digital cameras, where as monochromator based spectrometers are like SLR cameras. Both will do the job, but technology has changed over the last 40 years and you get so much more from a digital camera, so too you will get so much more from a FTNIR spectrometer.