Applied Instrument Technologies®

ANALECT® *RefinIR™ – Ask the Expert*

1. Why invest in the RefinIR™ analyzer in advance of initiating a process optimization project?

Upfront time must be invested to develop a spectroscopic process analyzer application. The development of the chemometric models that relate the sample spectra to the sample properties and compositions takes time. This is not due to the learning curve of the modeling software but rather because the process of collecting a suitable set of calibration samples requires time and diligence. The calibration set must represent the true variation in the process including seasonal changes and effects of unit upsets and turnarounds. The RefinIR analyzer plugs into normal lab operations to help jumpstart the model development process. Every time a process sample is brought in for the normal lab (reference) analyses, a 15 ml aliquot is transferred into an autosampler vial. With the automated RefinIR analyzer, it takes the lab very little additional effort to collect spectra on samples for which they are already getting the reference lab analyses. The models developed on the RefinIR system can be moved to the online ANALECT® Hydrocarbon SmartSystem® analyzer allowing it to do analyses immediately on startup.

2. Is the RefinIR™ analyzer useful for anything other than developing startup models for the online analyzers?

There are many cases in refining where having a snapshot of what's in a tank or pipe can be extremely useful for process troubleshooting, process planning, process control, and even for process optimization. For batch or pseudo-batch operations where you fill a tank and then process the tank, the RefinIR provides a fast, inexpensive means of characterizing what's in the tank. Real Time Optimization (RTO) applications often infer changes in feed composition based on unit performance, but a lab analysis with the RefinIR can provide a reality check on the inferred composition. If variation in the process feed is slow enough, a RefinIR lab analysis of a feed sample taken once a day or even once a week may provide a significant fraction of the credits for feed forward control. The RefinIR lab analyzer offers a less expensive way to develop these sorts of applications while still providing an avenue to transfer the application online should there be sufficient incentives.

3. What is the advantage of using our ANALECT® FTIR system over other types of spectroscopic analyzers?

The extended range ANALECT® FTIR systems made by AIT are the most versatile spectroscopic analyzers on the market. The RefinIR and Hydrocarbon SmartSystem are capable of measuring any petroleum material that is fluid at or below 125^{o}C including heavier petroleum fractions such as crude oil as well as gasoline, diesel fuel and gas oils. The RefinIR measures different materials in a single run provided the analysis can be done at the same temperature. Raman analyzers are typically limited to lower boiling, colorless samples due to fluorescence and sample heating from absorption of the laser light. Heavier petroleum fractions and crude oils are opaque in the 2nd overtone range used in NIR analyzers.

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4. Can you explain productivity achieved with the RefinIR™ analyzer over other models in the market?

Most spectroscopic lab analyzers are manually operated. The user must manually introduce the sample, wait while the spectrum is measured, wait while the sample drains from the cell, and wait for the cell to dry. With the RefinIR system, the computer does the waiting, not the user. Once the vials are positioned in the autosampler carousel, and the sample IDs are entered into the software, the RefinIR™ system will automatically collect the spectra. The system is designed for unattended operation, so the user can go on to other tasks.

5. We have never considered looking at anything but gasoline before, so how can results from your instrument benefit my company?

The RefinIR analyzer is very versatile. It can collect spectra on any material which is fluid at 125°C or less. The trick is converting that spectrum into useful information. All process control and optimization schemes have underlying process models. In turn, the process models have some underlying process analytics scheme which defines which molecular components the process separates, converts or blends. These process analytics schemes can be simple (a single GC) or convoluted (an entire crude assay), but they are generally time consuming, expensive and unsuited for online analysis. The RefinIR™ offers a path for replacing this process analytics scheme with a single, fast, inexpensive spectral measurement suited for lab or online deployment.

6. Do I have to run a whole bunch of standards to transfer models from the RefinIR™ lab system to the Hydrocarbon SmartSystem® online system?

Many spectrometer systems employ a chemometric based calibration transfer to map a “master” instrument (the one on which the model is developed) to one or more “slave” instruments (the ones on which the analyses are to be done). These calibration transfer schemes require a common set of standards be run on both the “master” and “slave” instruments. Even if it were practical to store large volumes of the standards for extended time, running the standards on process systems every time maintenance is done is at best time consuming, and at worst totally impractical.

AIT uses a proprietary instrument standardization technique to ensure that given the same sample, all ANALECT® FTIR systems, in the lab or online, will produce the same spectra to within a very tight tolerance. Every time a new background spectrum is collected, the frequency scale on the instrument is automatically re-standardized. Transferring a model on an AIT system merely involves copying the model from one computer to another. The standardization is automatically checked during instrument validation, using what ASTM E1866 defines as a Level A test. The validation ensures that the analyzer is performing properly prior to collecting and analyzing spectra of process samples.

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7. What software is included with the RefinIR™ analyzer?

The RefinIR™ analyzer uses SpectraQ™ software, a customized application that is designed to automatically operate the autosampler and spectrometer to successfully collect spectra of up to 24 samples in a single run. SpectraQ software will (1) automatically clean the IR cell, collect a new background, and standardize the instrument frequency scale, (2) automatically validate the analyzer performance by collecting and analyzing a spectrum of toluene, and comparing analysis results to historic based limits (as described in ASTM E1866 and D6122), and (3) automatically introduce and analyze up to 24 process samples. Based on the sample fluidity at the measurement temperature, the user can select among sample introduction methods to (a) avoid loss of light ends and generation of bubbles for light samples, (b) use normal sample introduction where one sample flushes out the previous samples, or (c) use heavy sample introduction where the cell is rinsed and cleaned with solvent before and after the sample measurement. SpectraQ™ software can analyze the spectra collected using models built by a variety of chemometric software packages.

AIT also offers the SpectraQuant™ chemometric model package. This software was developed for AIT in partnership with Eigenvector Research (EVRI). This allowed AIT to leverage the cutting edge software and interface tools developed by Eigenvector as part of their PLS Toolbox and Solo products. SpectraQuant software implements licensed algorithms developed and patented by Exxon Research and Engineering Company[1]. The software allows analyses to be based on discontinuous spectral regions (excluding opaque regions), allows for orthogonalization of spectra to user generated corrections (spectral baseline, water vapor and even dispersed water) to ensure models are insensitive to these type variations, and allows for inclusion of a scaling (pathlength) model which compensates for differences in pathlength between analyzer systems and also compensates for changes in sample temperature (density) thus improving transferability of models between spectrometer systems. Models developed in SpectraQuant software conform to the requirements of ASTM E1655.

[1] J.M. Brown, US5121337, Method for Correcting Spectral Data for Data Due to the Spectral Measurement Process Itself and Estimating Unknown Property and/or Composition Data of a Sample Using Such Method, June 9, 1992.