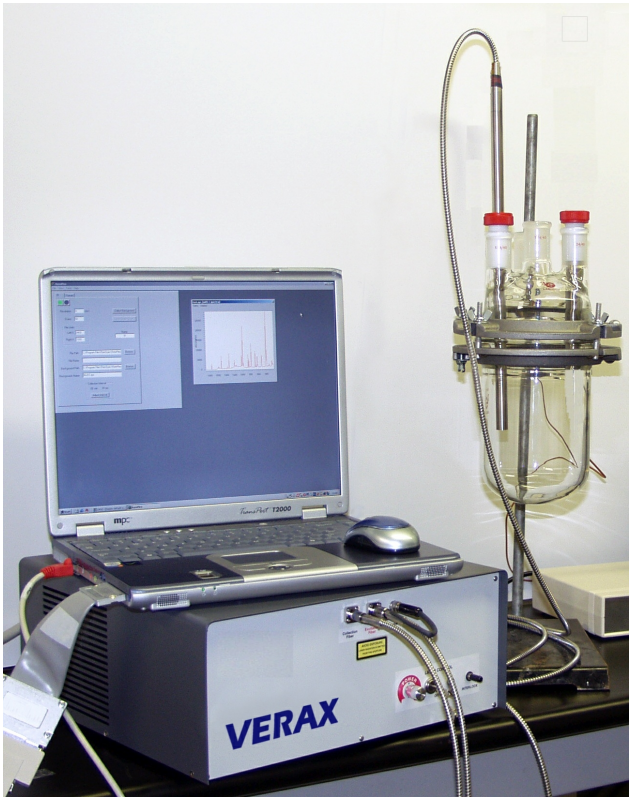
REMSPEC

Real-Time Raman *in-situ* Reaction Monitoring with VERAX™



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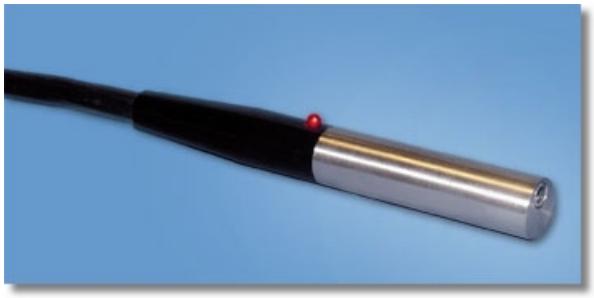
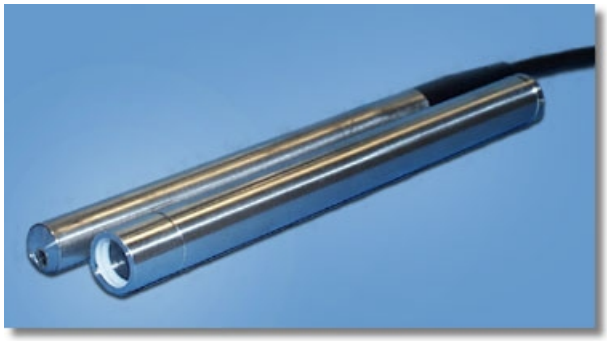
In-Situ Spectroscopy

The VERAX™ reaction monitoring system turns Raman spectroscopy into a truly in-situ technique, allowing you to carry out Raman analysis in real time as a reaction evolves. The VERAX™ spectrometer has a range of 250–1940 cm^{-1}, uses a 785 nm diode laser and a TE-cooled CCD array detector, and comes with a fiber-optic probe from the RamanProbe™ range. The patented RamanProbe™ design completely filters Rayleigh scattering with an attenuation of 10^8; the probe also eliminates background signals arising in the fiber optic cables for optimum data quality. You can use the VERAX™ inside a conventional lab-scale reaction vessel or your choice of ALR (Automated Laboratory Reactor) to generate real-time data on the reactions and chemical changes that are taking place - all without perturbing the process to remove samples. Reactor modifications are kept to a minimum - often avoided completely - since RamanProbes™ are compact enough to fit into many existing reactor ports and can collect data through the walls of glass reactors.

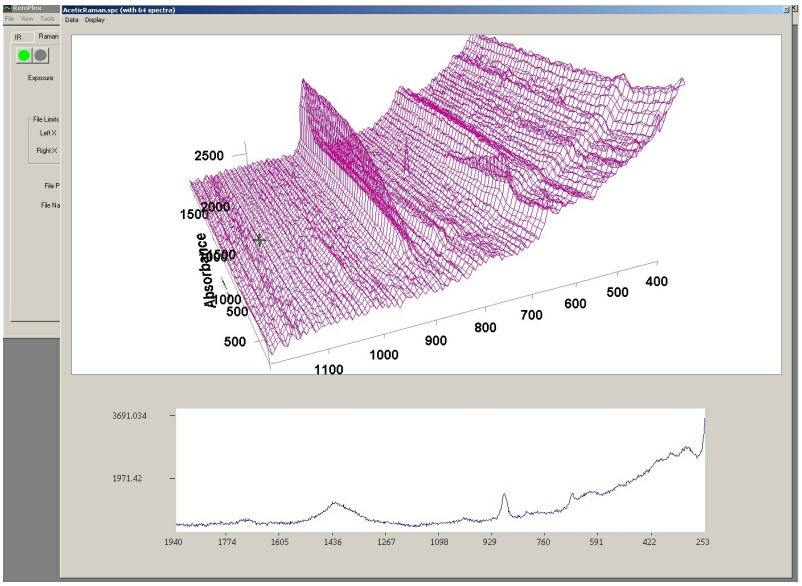


A RamanProbe™ for through-glass measurements



A RamanProbe™ 2 with removable immersion sleeve

Real-Time Display with VizRaman™ Software

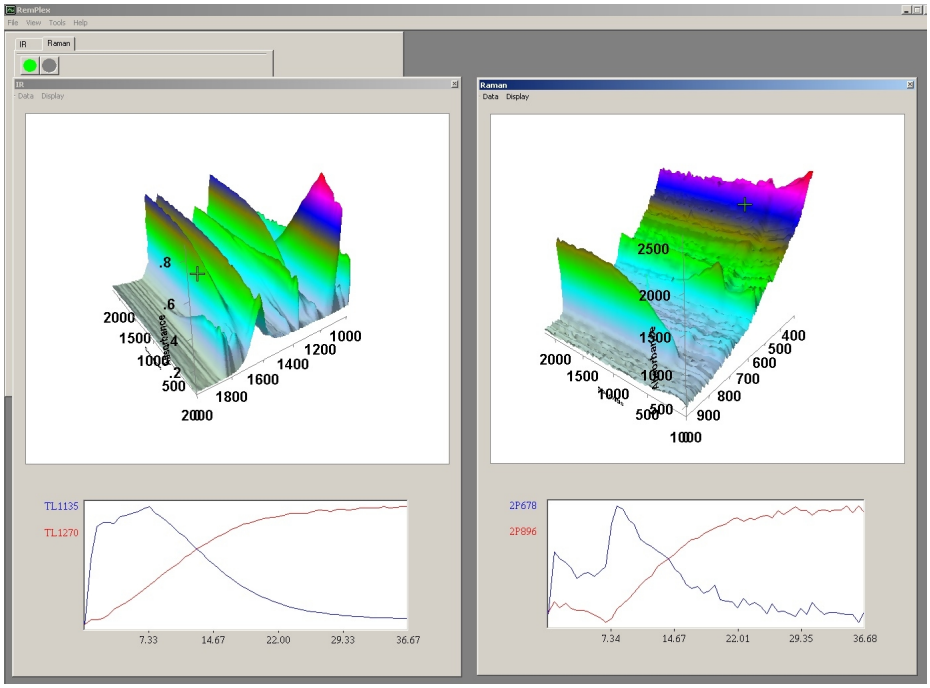


VizRaman™ software provides a simple but powerful interface for setting up and running reaction monitoring experiments. Parameters such as Exposure Time are set on the main control panel, then either a single spectrum or a set of successive spectra are collected. Large data sets are not a problem and you do not have to commit to a reaction time when you start the run. Just press the red button when you are finished and the data is saved in Galactic SPC format. The display includes

a true 3D display of spectra as they are collected – you can manipulate the 3D image without disrupting data collection to take advantage of its full visual power. An optional second window can be added to show the most recent single spectrum, or a trend line of the height of a selected peak versus time. All of the individual spectra, and the calculated trendlines, are stored for later detailed analysis.

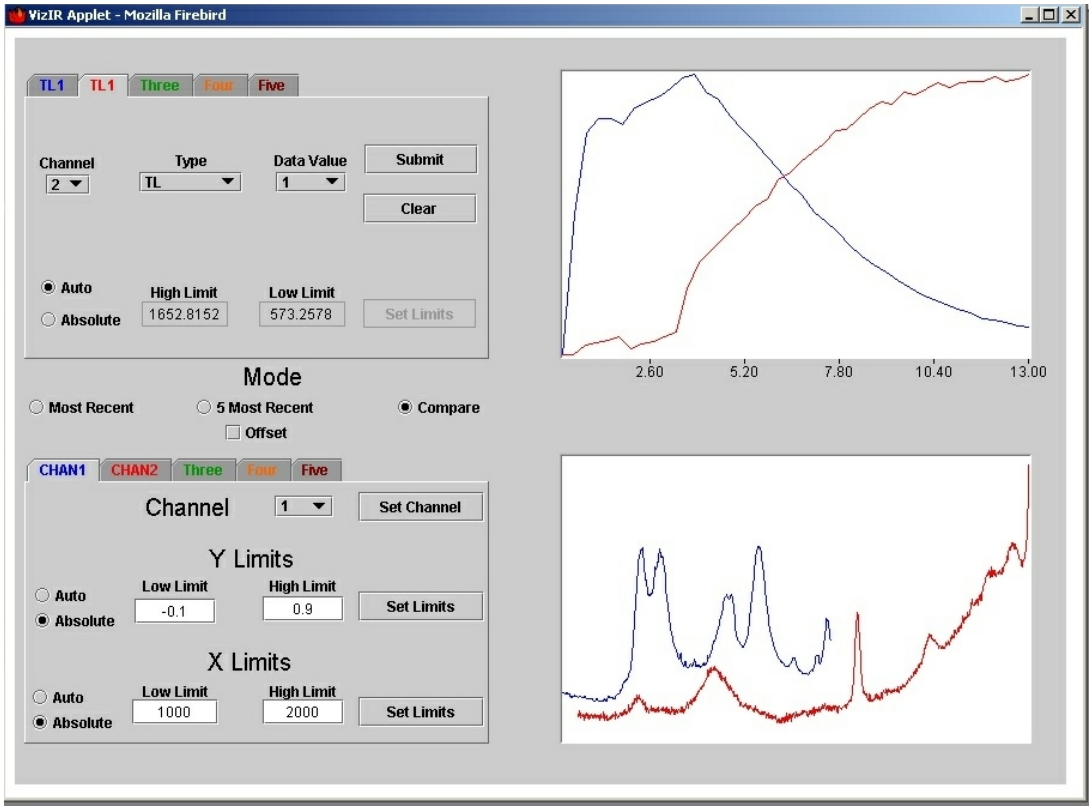
VERAX™ and ReactionView™ Together: Raman and FTIR Combined

In the mid-IR region, Raman and FTIR can be regarded as complementary spectroscopy methods. For one thing, the selection rules for each method are different, so that FTIR is particularly sensitive to changes in polar functions such as carbonyl and nitrile groups while Raman can be superior for observing carbon-carbon bonds in aromatic systems, for instance. The different modes of obtaining the two spectra are also a factor. Since FTIR is a true absorbance technique, molecular-level information dominates the spectrum. Raman is a scattering technique using near-IR radiation to carry the signal, and the spectra are sensitive to changes in phase and morphology, as well as molecular properties. In a crystallization study, for example, this means that a ReactionView™ FTIR probe with an ATR head will give spectra of the liquid phase, while the Raman spectra from the VERAX™ system will include morphological information about the crystals that are forming. Mixing information about multi-phase systems and emulsions is also accessible using Raman spectroscopy.



This screenshot from RamIR™, Remspec's multichannel reaction monitoring software, was taken during the hydrolysis of acetic anhydride. The 3D spectral plots of the FTIR and Raman channels show changes as the anhydride is added and slowly hydrolyzes. Trendlines based on each data set show the anhydride (blue lines) increasing rapidly then diminishing, while acetic acid (red lines) builds up. The poor mixing of acetic anhydride and water at the beginning of the reaction is reflected particularly strongly in the Raman spectra, with considerable discontinuities in the observed spectral trends during the first few minutes of the reaction. This effect is much less pronounced in the FTIR data.

Another advantage of combining the FTIR capability of ReactionView™ with VERAX™ Raman is the extended wavelength range that becomes available – all the way from 5000 cm^{-1} in the FTIR to 250 cm^{-1} in the Raman without sacrificing the flexibility and versatility of slim fiber-optic probes.



A screen shot from the RamIR™ remote-viewing applet illustrates this. The FTIR spectrum from 2000 – 900 cm^{-1} (blue) and the Raman spectrum from 1948 – 252 cm^{-1} (red) are compared in the lower window, while the evolution of the FTIR peak at 1135 cm^{-1} and the Raman peak at 895 cm^{-1} are followed in the upper window.

VERAX™ alone provides a cost-effective, versatile, and flexible Raman reaction monitoring system. Combined with the FTIR power of ReactionView, it provides a complete solution for monitoring reaction chemistry, phase changes, and crystallization – all at the same cost as many stand-alone Raman systems.

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