

Real-Time Reaction Monitoring with the **VERAX™** and **VizRaman™** Software

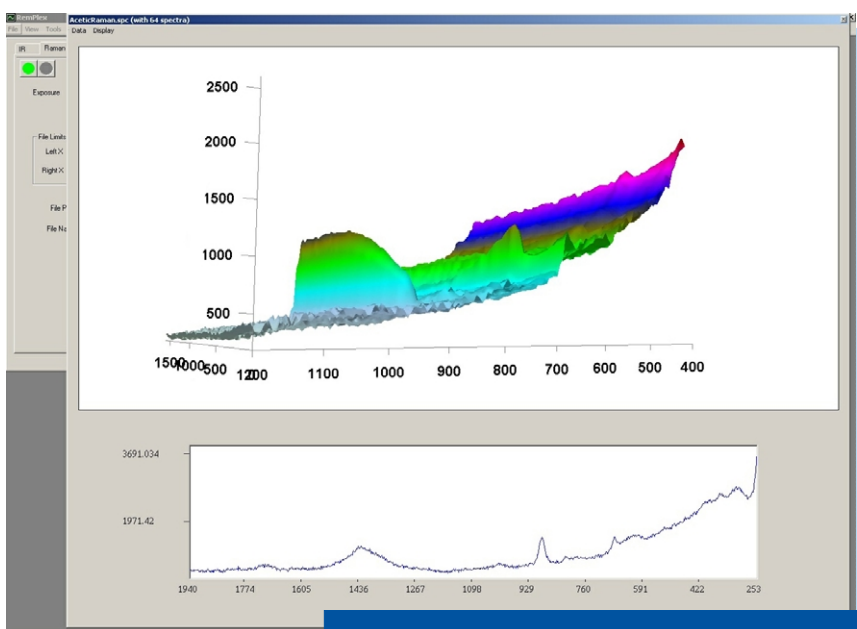
Why Raman?

Raman spectroscopy continues to emerge as an important tool for monitoring reactions in real time. Raman scattering provides complementary information to traditional FT-IR (mid-IR) and NIR spectroscopy, and has advantages over both:

- Raman measures fundamental vibrational modes that are easily attributed to molecular structure.
- Measurements can often be made through glass reaction vessels.
- Immersible fiber optic probes can be manufactured with inexpensive silica fibers and quartz or sapphire optics.
- Water is a weak Raman scatterer, so aqueous solutions do not pose any additional difficulties.
- Most Raman bands are not sensitive to minor temperature fluctuations.

The VERAX System

The VERAX™ Raman system combines a high quality spectrometer, wide array of fiber optic probes, and VizRaman™ software to enable monitoring of experiments in real time. At the heart of the system is the high-throughput spectrometer providing excellent data in the “fingerprint” region of the spectrum. High resolution (4 cm^{-1}) ensures that small spectral changes can be clearly discriminated. The VERAX is available with a variety of RamanProbe™ fiber optic probes



Real-time spectral display with VizRaman and the VERAX spectrometer.

for through-vessel or immersion measurements. Various diameters of probes are available to fit into lab-scale reaction glassware or an ALR (Automated Laboratory Reactor). Because silica fiber optics are highly transmissive, laboratory results are readily transferrable to on-line process monitoring.

Real-Time Display

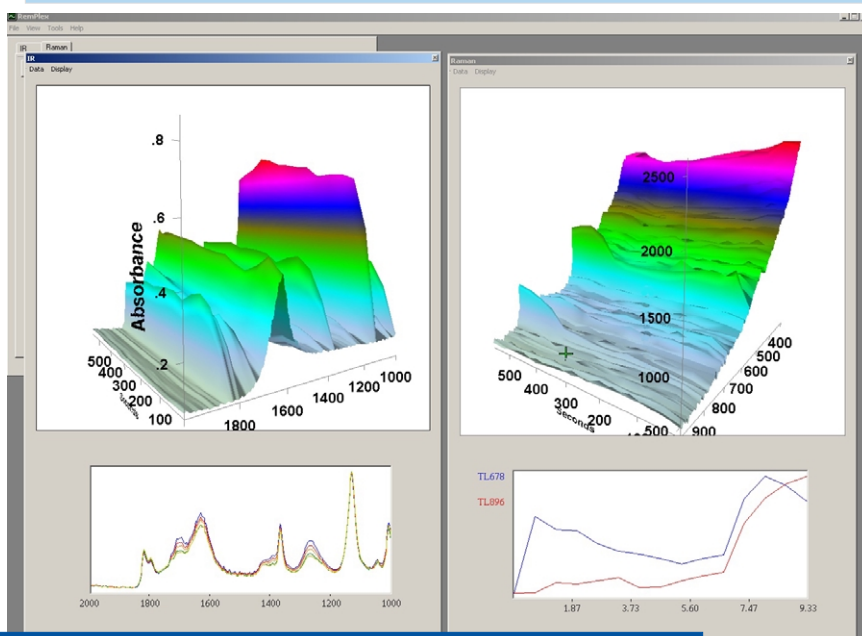
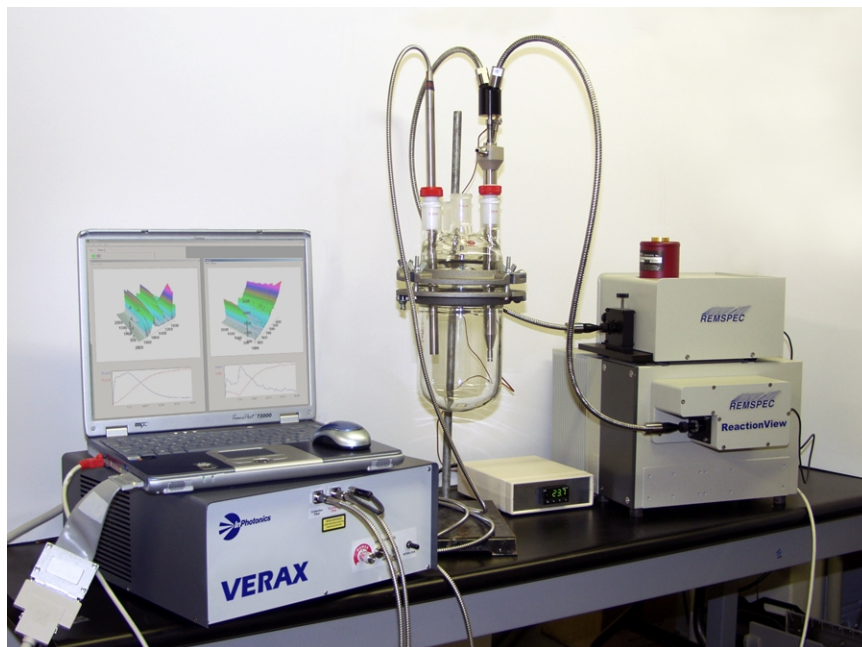
VizRaman software provides a simple but powerful interface for setting up and running reaction monitoring experiments. The Exposure Time (or measurement time) can be set

on the main control panel enabling either single spectra or a set of successive spectra to be collected. Large data sets are not a problem, and the overall reaction time does not need to be defined prior to data collection. The “Stop” button can be pressed at any time to halt the data acquisition and save all data. An interactive 3D display allows the full visualization of the spectral data while the reaction is still in progress. An optional second window can be added to show the most recent spectra, or a trend line of the height of a selected peak versus time. All individual spectra, and any calculated trendlines, are stored for later detailed analysis.

Combined FT-IR and Raman

FT-IR and Raman are complementary vibrational spectroscopic methods. The selection rules for the two techniques are quite different: FT-IR is very sensitive to changes in polar functions such as carbonyl and nitrile groups, whereas Raman is particularly useful for observing molecular linkages involving multiple bonds and heavier atoms. FT-IR is an absorbance technique and is inherently more sensitive to dilute constituents. Raman is a scattering technique with a larger sample volume, and can detect changes in phase and morphology in addition to molecular properties. In a crystallization study, for example, an FT-IR system equipped with an ATR (attenuated total reflectance) probe will provide information about the liquid phase, while the Raman spectra will include morphological information about the crystals that are forming. Mixing information about multi-phase systems and emulsions is also accessible using Raman spectroscopy.

The VERAX Raman system coupled with a ReactionView™ fiber-optic FT-IR spectrometer provide a wealth of chemical information in real time. The RamIR™ multichannel reaction monitoring software can be used to control both systems simultaneously, resulting in complete vibrational spectroscopic characterization of a given system. The FT-IR data extends through the R-H stretching regions beyond 3000 cm⁻¹, while the Raman data spans below 300 cm⁻¹, enabling monitoring of low-frequency bending modes and halogen-containing vibrations. Together, the VERAX and ReactionView form a complete solution for monitoring reaction chemistry, phase changes, and crystallization.



The VERAX and ReactionView combined FT-IR and Raman reaction monitoring system with RamIR software.

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