FTIR Vs. GC in Gas Analysis

Comparison of Technologies

A gas chromatograph (GC) has traditionally been the technology of choice for laboratory analysis of gas samples. GCs have been used for over 50 years in the qualification and quantification of complex mixtures of gases. The techniques and methodology required to run GCs are often a pre-requisite for any laboratory technician. Recent developments in Fourier Transform Infra-Red (FTIR) gas analysis has enabled this technology to start to replace GCs in the lab.

Both technologies are ideally suited to the identification and quantification of gas species. We discuss here the advantage and disadvantages of both techniques.

Gas Chromatography is a mass separation method. A carrier gas is permanently blown through a separation column, which is often either heated or temperature programmed. The outlet from the column goes through a detector of which there are different types. The sample to be tested is injected into the front of the column where it is separated into constituent components which appear as peaks at the detector one after the other. For different gas species or detection limits, various detectors are used. The peaks are identified by the retention time in the column after injection, given the conditions of flow and temperature. To calibrate, pure compound samples are injected in the same way and the retention times noted. The concentration is calculated from detector signal by comparing the size of the peak of the sample with the same for a concentration standard.

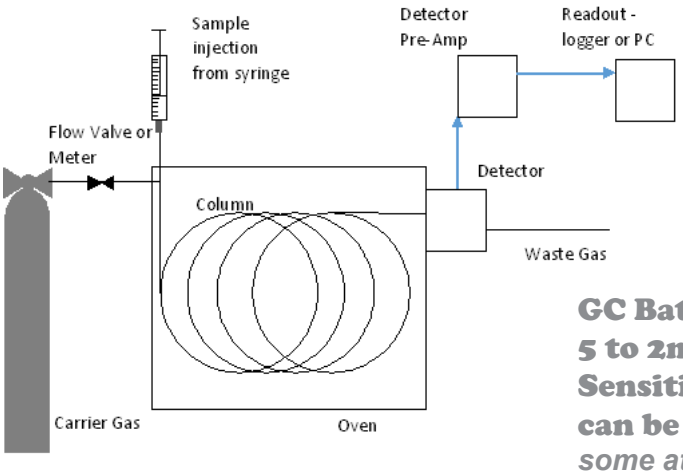

Figure 1 - Gas Chromatograph Layout.

GC Batch
5 to 2mins typical
Sensitive
can be specific !
some at Low Cost !

IR absorption spectroscopy measures the absorption of light by the molecules of the gas, based on the molecular vibrations within the gas species present. The IR absorption is a function of type of vibration within in the molecule, as well as the temperature, pressure, concentration and pathlength (distance the IR light travels in the absorbing species). The absorption is carried out in a closed gas cell, where the IR light is reflected a number of times, giving the specific pathlength. For selective gas applications, the absorption at a single frequency can be measured giving a measurement result for one gas. However with a FTIR spectrometer the full IR spectrum can be collected, enabling the detection of the absorptions peaks of all gases within the sample at once. By using chemometric software and a suitable calibration set of spectra at known concentrations, the full spectrum can be separated into the responses of each gas of interest. Quantification is made by the chemometric algorithm, with the linear absorption response of the sample being modelled against the calibration set.

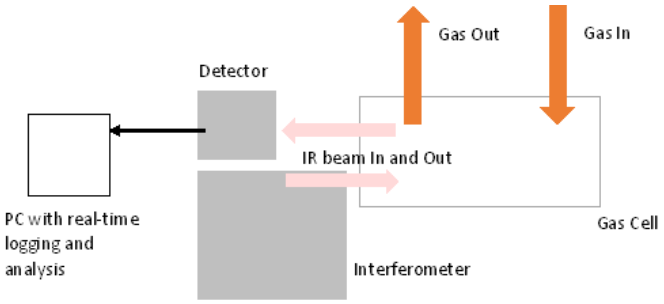

Figure 2 - FTIR Gas Analyser Layout.

Gas Mixtures *(to~50 simltaneously)*
H2O /CO2 interferences
NOT symm Mols eg He, N2, O2, Ar, CCl4(?)
- (mix) generally > complex spectra > useless?
generally limited to~C20
- HighTemp cells becoming available
- relatively expensive !

	GC	FTIR
Advantages	Good for composition analysis in measuring unknowns – by putting samples through the column with different characteristics, it's possible to obtain different separations. Column separation is good for measuring mixtures containing lots of the same types of compounds – e.g. speciation of C6+ hydrocarbons. By selection of the correct column type and detector type all gases can be measured. Detection limits down to ppb levels are readily possible by selection of a high sensitivity detector. Old and established technology has given lower initial purchase price.	An IR spectrum can be collected quickly, in as short a time as 5-10sec. Usually 1 min sampling gives the best detection limit. Simultaneous analysis of all gas components is carried out in real-time. Continuous measurement ideal for process reaction analysis. IR spectra can be re-analysed post collection for interfering gases or for other gases not programmed in the method when data was collected. Non-destructive - the sample is not affected by the measurement and passes through the gas cell to be re-used if required. Maintenance, when required, is relatively simple – replacement of IR source and detector after 5+ years, gas cell cleaning if required after 2-3 years. Lower detection limits can be achieved by choosing a high pathlength gas cell, or by choosing a low noise detector. High and low ranges of measurement can be achieved in one instrument with no change to hardware, either by sample dilution or by selection of different absorption peaks at different concentration ranges. No re-calibration needed. FTIR spectrum is repeatable. No consumables need, other than sample filters (if required) and zero gas for daily background.
Disadvantages	Non-continuous measurement – only "batch". To measure process reactions, multiple GCs are need to be sequenced together. Long measurement time which can be of the order 10-15mins, or longer if temperature programming is required and a cooling phase is required. Consumables are required – in terms of carrier gas required and H2 fuel required for FID detector. Column retention time changes with age and eventually needs replacement. Regular re-calibration for changing retention time and peak response is needed. FID detectors can block up due to small flame and jet sizes. They have short lifespans and need to be replaced. Inlet valves can be prone to leaking and need regular maintenance. Trained or expert user required. Measuring unknown samples does take a long time and a lot of expertise. GC-MS set-up is best for separation of peaks, but a lot slower and MS means a lot more expensive.	There is no response in the Mid-IR to gases such as O2, H2, N2 or inert gases so FTIR cannot measure these. Different gases give different IR absorption intensity, so some have very low detection limits and some very high. Standard detection limits for standard instruments are of the order 0.5ppm. ppb level detection requires larger and expensive components (gas cell and detector). Software has to account for interfering gases present in the background, such as H2O and CO2, as these can affect the analysis of absorption peaks. Good for speciation for C1-C6 but above C6, Total Carbon (TC) content is commonly reported for alkanes as the IR responses all overlap. Similarly for other classes of hydrocarbon, such as alcohols.

Specific Advantages of Protea atmosFIR analysers

Protea's atmosFIR range of FTIR analysers are dedicated gas analysers. As opposed to standard laboratory spectrometers that have gas cells added into the sample compartment, atmosFIR has been designed as the optimum tool for multi-species gas analysis. Software and hardware is combined to give control of the sample and analysis of the gas in real-time.

Factor	Protea atmosFIR Features	Benefits
Spectrometer	High resolution – 1cm-1 standard (0.5cm-1 as option)	High resolution needed for speciation of gases in complex mixtures.
	Automatic in-built frequency correction	Very high repeatability of spectral acquisition. No need to adjust calibrations i.e. no drift. Calibrations can be transferred from one instrument to another
	24-bit ADC with DTGS detector	Room temperature operated detector. Low noise with 24-bit sampling
Gas Cell	Very low volume to pathlength ratio	Quicker response times are achieved.
	Gas cell optics are optically matched to the full IR system	High throughput gives the best detection limit, unlike standard laboratory FTIR spectrometer with gas cell "add on". No adjustment needed by user.
	Gas cell materials optimised for reactive and corrosive gases	Gas cell can be heated if required. No losses due to absorption. Long operational life.
	In-built filter (optional)	For samples with potential dust content, the analyser can be supplied with in-built filter pre-cell.
Sampling System	In-built purge valve	Automatic zeroing. Less operator effort needed to connect/disconnect gas lines
	Sample control signal	Sample open/close signals built in for automated sampling. Less operator effort needed to connect/disconnect gas lines.
	Digital and analogue signals	Alarm output for high/low readings. Alarm output for analyser health status. 4-20mA signals for data output.
	Cell pressure and temperature sensors	Correction of readings to reporting conditions (STP) in real-time with in-built pressure sensor (FTIR spectra must be correct for pressure as spectral absorption varies with pressure).
Software	Data collected in Project and Batch format	Provides ease of data saving for laboratory test samples. Data can be reviewed and re-calculated any number of times.
	Memo feature	Data tagged with events and notes for ease of post-collection analysis and review.
	Software runs FTIR spectrometer and also sampling system	Parallel control of sample gas and measurement gives a complete measurement system in one unit.
	Interaction with PLC in customised external sampling system	Protea can supply a separation sampling system module with suitable pumps, valves, temperature controllers for bespoke applications. This is controlled by the FTIR allowing for sequential, automated measurements.
	Data output	Results can be outputted in real-time over standard protocols, such as OPC and Modbus.

Factor	Protea atmosFIR Features	Benefits
Chemometrics	Designed for gas analysis –results reported in ppb, ppm, %Vol, mgm^{-3}	Simple to report gas readings, no need for unit conversion or arbitrary readings.
	Advanced chemometric algorithms.	Software can detect and speciate individual species even in complex overlapping samples.
	Multiple algorithm support – peak analysis, CLS, PLS-1, PLS-2 algorithm features.	Can be used equally easily by the trained spectroscopists or by the newcomer to FTIR analysis.
	Component specific analysis.	Chemometrics are build specific for each gas, not a single analysis model for the entire matrix. No limit to number of gases to be analysed at once Individual methods for each gas give best analysis for each gas i.e. not limited by worst.
	Calibration method file storage and transferability.	Method is saved in calibration file that can be easily saved, loaded and sent via email. Re-calculation of results and adjustment of method is simple. Calibration file can be shared with Protea Application's team for ease of support. No need to transfer or share lots of spectra.
Cost	VCSEL laser diode for interferometer alignment	Long lifespan, >10 years, compared to conventional HeNe lasers Smaller than HeNe lasers, less power, no need for separate PSU
	Low volume cell (<300ml)	Less sample gas needed, if sample generation is costly Less zero N2 gas needed
	Single supplier of complete gas analyser	No separate vendor for spectrometer, gas cell, detector as with lab FTIR
	Very competitive price	Total cost of ownership over analyser lifetime is comparable to historically cheaper GC
	Protea's In-House support and training courses	Application support from spectroscopists with real experience of gas analysis

With dedicated gas analysers based on FTIR technology, such as Protea's atmosFIR platform, quick, repeatable and cost-effective measurements can now be made using the power of IR spectroscopy.

Figure 3 - Protea's atmosFIR FTIR gas analyser is a complete analytical system to sample, qualify and quantify gas samples quickly and effectively.

Supplier: *Restricted rights ONLY > but under review ! re viability etc*