CIC Photonics

FREQUENTLY ASKED QUESTIONS

A. IRGAS HARDWARE

1. Alternative FTIRs

Q: Which FTIR spectrometers can be incorporated into the IRGAS package?

A: Currently the IRGAS hardware and the SPGAS software are configured for use with the Bomem WorkIR spectrometer, with custom optical couplings to the long path gas cell. The hardware package can be customized for other FTIRs to which either the 4Runner or Ranger gas cells can be coupled. The accompanying SPGAS software also has to be customized to that spectrometer.

2. Gas Cell Selection

Q: Which long path gas cell is most compatible with the IRGAS?

A: The IRGAS was designed to provide ppb-level sensitivity for impurities in the electronic specialty gases. For that regime, a 4-meter to 10-meter pathlength has proven to be the cell of choice among the gas producers. CICP offers either its Ranger-EN 9.6-meter cell or its 4Runner 4- or 6-meter with the IRGAS. Both cells are capable of detecting moisture at the 5 to 25 ppb impurity level in such gases as HCl, HBr, Cl2, WF6, NH3, H2, SiH4, GeH4, etc.

3. Alternative Gas Manifolds

Q: Can the IRGAS-400 version stainless steel gas manifold be modified either to incorporate additional components or to delete some items for a simpler system?

A: The existing manifold is designed to meet SEMI Standards and to provide total computerized control of the supply and purge gases. For less stringent or simpler applications, the system can be reduced in scale or converted to manual operation.

Several other gas sampling configurations, from simple manual valve controls to more complex multipoint electronic valves, are available to meet customer requirements.

4. Purge Gas and Purifier

Q: What is the purpose of the purge gas stream and why is a gas purifier needed?

A: Purge gas (e.g. high purity dry nitrogen) is used both to purge the long path gas cell between process gas samples and to purge the FTIR spectrometer and the optical conduits. The former use hastens the sweep-out of adsorbed impurities in the gas cell, particularly if a cycled flushing procedure is used. The latter maintains the FTIR and optics in a state of very low moisture content. The moisture purifier delivers dry nitrogen that is even drier than the nitrogen source; hence the “background” reference spectra are more free of interfering moisture peaks.

5. Motorized Transfer Mirrors

Q: What enhancement is offered by having the transfer mirrors within the purge box on a motorized track for moving them in and out of position with respect to the FTIR beam?

A: The motorized transfer mirrors can be either manually operated or driven by a computer program. In either case, the positioning of the mirrors is more reproducible. But the major advantage of the computerized control comes with the use of the SpectraStream™ software module; SpectraStream provides an "early warning" indication of sudden changes in the gas composition.

6. Temperature and Pressure Monitors

Q: How and where are the temperature and pressure monitors for the process gas flow through the long path gas cell?

A: The gas cell is heated with a sheet or band heater that is cylindrically-wrapped around the body of the gas cell. A Type K thermocouple is embedded in the heater; the heater and cell body are covered with thick insulation to provide temperature uniformity and stability. The thermocouple measures the temperature of the outer surface of the stainless steel cell body and not of the internal gas sample. The gas pressure is controlled and monitored via a pressure sensor in the gas manifold.

Temperature and pressure sensors are also available for direct sensing within the long path gas cell. These sensors are read by a PLC unit which permits the IRGAS software to adjust calculated gas concentrations via the Ideal Gas Law.

7. Temperature Controller

Q: What are the specifications for the temperature controller?

A: The temperature controller is a PID-type microprocessor, equipped with EIA/TIA-485 computer communications protocol. It measures and controls the load temperature to +/- 2 deg C, using a Type K thermocouple or to +/- 1.3 deg C with a RTD device. A single channel unit (500 watts) is used with the 4Runner gas cell and a dual channel (1000 watts) unit is used with the Ranger-EN. The SPGAS software provides communication with the temperature controller and displays the gas cell temperature continuously on the monitor.

8. Alternative Enclosures

Q: What is the enclosure that is displayed with the IRGAS system? Are other enclosures also available?

A: The enclosure shown for the IRGAS-400 configuration meets SEMI standards. It is a custom powder-coated steel cabinet configured to house all the major components of that hardware package: gas cell, FTIR, optics, gas manifold, temperature controller, CPU, PLC, and electronics; only a vacuum pump and monitor are not included within the enclosure. The optional PC monitor may be mounted on an external pivotal shelf. An auxiliary vacuum pump is available on a "sidecar."

Other enclosures are available for the IRGAS-XSA, IRGAS-LPA, and IRGAS-SPA products. These may be stainless steel, powder-coated steel, plastic composites, Plexiglass, or none at all. Rack-mounted configurations are also available.

9. Vacuum pumps or Venturi gas generators

Q: Are these options available and for what applications are they recommended?

A: Either or both an auxiliary diaphragm-type vacuum pump and a Venturi unit can be provided with the IRGAS packages. The Venturi is a standard feature of the IRGAS-400 gas manifold. It is operated off of a separate connection from the high pressure purge gas supply. The Venturi is capable of pumping the gas cell down to the Torr level between gas samples. For higher concentrations of impurities or components (> ppm), this may be sufficient.

For quick impurity determinations at the ppb level, the gas cell needs to be evacuated rapidly to the millitorr level in order to remove contaminations from the preceding gas sample. Hence, an auxiliary vacuum pump is required. A Scroll pump or a small turbomolecular pump will provide this capability.

10. Vibration and other environmental conditions

Q: What are the temperature, pressure, humidity, vibration, and noise constraints on the operation of the IRGAS in an industrial plant environment?

A: The following conditions apply:

- Temperature:
  - Storage temperature range: -10ºC to 50ºC
  - Operating temperature range: 0ºC to 30ºC
- Pressure: Atmospheric
- Humidity: 0% to 40% non-condensing
- Noise and Vibration:

High levels of audible noise and vibration can adversely affect the operation of the WorkIR, by adding spectral noise of artifacts or by causing an excessive number of bad scans. If noise and vibration conditions prevent the WorkIR from meeting its performance specifications, a vibration absorption interface and/or noise barrier may be required. Low frequency vibrations, less than 20 Hz, will normally be compensated for by the electronics feedback control loop. Vibrations above 20 Hz can cause scan rejection and should be attenuated to a level where the analyzer does not reject scans. Severe, audible noise may reduce spectroscopic performance or cause bad scans that will rejected by the WorkIR. The following table gives ranges of frequencies that can cause spectral artifacts or interference.

Model	**Minimum frequency**	**Maximum frequency**
WorkIR 100	130 Hz	3 Khz

When severe audible noise conditions are encountered, a noise control strategy must be developed and implemented. The best approach is to eliminate the noise at the source. If this is not possible, noise barriers must be used. The WorkIR has a considerable noise damping by virtue of its sealed enclosure. A second enclosure with acoustic damping panels is effective in reducing excessive noise effects.

11. Remote plant locations

Q: What options exist for where the IRGAS can be placed in a semiconductor wafer fab plant, gas purification facility, or other industrial chemical plant?

A: The IRGAS is designed to be placed as close as physically-possible to the point at which a gas line connection can be made to a process tool, purification chain, or a gas tank. The IRGAS-400 comes with a coaxial gas fitting for direct welding to a process gas line. The purge gas fitting is a VCR. For gas monitoring at a wafer tool, it is preferable to locate the IRGAS right at the tool in order to minimize the time between gas samples. For checking the purity of gas cylinders containing purified specialty gases, the IRGAS may be located in a remote analytical lab.

For situations where fast time response is required, the FTIR, gas cell, and optics must be close to the source point; but the CPU, monitor, and vacuum pump can be located elsewhere, so long as electronic and plumbing conduits are provided. In this case, the FTIR, gas cell, and optics may be contained in a smaller enclosure, or integrated into the cabinetry of the process

B. Software

1. SPGAS and SpectraStream

Q: What are SPGAS and SpectraStream and how do they differ from other commercial software packages? (Briefly)

A: SPGAS is a state-of-the-art gas analysis system built into a complete hardware management system. SPGAS was designed to provide turnkey industrial real-time gas analysis.

The SpectraStream technology was developed by CIC Photonics. SpectraStream works as an add-on module for SPGAS, and provides a higher sensitivity detection of impurities, reduces the time response typically associated with FTIR (from minutes to seconds), and greatly reduces the effects of spectrometer drift over the collected spectrum. Other commercial software packages were designed to work as laboratory bench applications. SPGAS is specifically designed to address the requirements of an industrial application.

2. Other Commercial Software

Q: Can software like GRAMS, OMNIC, and other commercial chemometric software packages be used with the IRGAS hardware?

A: No, these commercial software packages do not offer a hardware management option; but a special software interface between SPGAS and these commercial software packages can be built, allowing them to receive spectral data from the IRGAS hardware.

3. Applicability to other FTIRs

Q: Can SPGAS be applied to FTIR spectrometers other than Bomem units?

A: Not at this point, but there is work in progress to make our SPGAS spectrometer interface module compliant with ThermoGalactic's My Instrument specifications (see www.myinstrument.com). This will open the doors for SPGAS to a great variety of FTIR instruments.

4. SPGAS separately available

Q: Is the SPGAS software available apart from the IRGAS hardware system? If so, what if any customization is required?

A: Yes, it is available separately from the IRGAS Hardware. The level of customization is directly related to the customer's needs and hardware requirements.

5. Acquisition drivers and communication protocols

Q: Are acquisition drivers available for application of the SPGAS software to other FTIR spectrometers?

A: There are other instrument manufacturers who are open to the idea of the creation of a standard interface to communicate with all FTIR instruments. This group supports and are members of the "My Instrument" effort (see www.myinstrument.com). CIC Photonics supports this effort and has work in progress to follow its specifications.

6. Multiple Species Measurements

Q: How many gas species can be measured essentially simultaneously with the IRGAS/SPGAS system?

A: Theoretically, all the gas species that absorb infrared light can be measured simultaneously, since our chemometric analysis is based on a multivariate method. But there are limiting factors like very high concentrations of a gas species which may absorb all the infrared light at certain frequencies; thus acting as a filter at those frequencies and preventing other gas species that have overlapping frequencies from been detected.

7. Species sensitivity

Q: What determines the ultimate sensitivity of the IRGAS/SPGAS system for various gaseous species?

A: There are seven main parameters that determine the ultimate sensitivity of the IRGAS/SPGAS system: FTIR detector, gas cell pathlength, gas pressure, gas temperature, calibration spectra, spectrometer drift, and purity of the background or reference spectrum forthe gas species being analyzed. All of them play a very important role in the chemometric analysis.
CICP does offer IRGAS Systems that can detect certain species at ppb levels.

8. Chemometrics

Q: What version of chemometrics is incorporated within SPGAS and why?

A: Our chemometric package is based upon a variation of the classical CLS analysis. We provide a weighted multi-band CLS analysis. This method outperforms other methods like PLS and PCR and provides a higher immunity to false positives in the detection and estimation of gas species.

9. Temperature and pressure corrections

Q: Are temperature and pressure correcting algorithms incorporated within SPGAS to match gas calibration data with the actual gas sample parameters? How is this performed?

A: Yes, SPGAS has pressure and temperature correction algorithms. This algorithm uses the temperature and pressure parameters inside the gas cell, which need to be monitored to provide the correct gas calibration data to the quantification algorithm and to obtain an optimal quantification analysis. The pressure and temperature inside the gas cell are obtained by using temperature and pressure transducers connected to the gas cell body. There is also work in progress on a software self-correcting algorithm that will obtain the pressure and temperature parameters from the spectral data instead of using pressure and temperature transducers connected to the gas cell.

10. MALT and HITRAN

Q: Please explain what these are and how they are used within SPGAS.

A: MALT is a software program that calculates the spectra of gas-phase molecules based on line parameters such as the HITRAN database. MALT calculates the monochromatic spectrum at each specific temperature, pressure, pathlength, and concentration and then convolves them with a specific instrument function, which includes resolution, field of view and apodization. The calculated spectra simulate real measured spectra which can be used in place of actual measured spectra for the purposes of calibration, qualitative and quantitative analyses.

HITRAN is an acronym for high-resolution transmission molecular absorption database. HITRAN is a compilation of spectroscopic parameters which a variety of computer codes use to predict and simulate the transmission and emission of light in the atmosphere. The database is a long-running project started by the Air Force Cambridge Research Laboratories (AFCRL) in the late 1960's in response to the need for detailed knowledge of the infrared properties of the atmosphere. The HITRAN compilation is now being developed at the Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics under the continued direction of Dr. Laurence S. Rothman.

11. SpectraStream

Q: What are the features of SpectraStream that are distinct from SPGAS?

A: SpectraStream is not a stand-alone product; it is an add-on module for SPGAS that enhances its data collection capabilities. SPGAS without SpectraStream, as well as commercial software packages, uses a standard collection technique or “Passive Spectra Collection” to generate an absorption spectrum. On the other hand, SPGAS with SpectraStream uses a “Active Spectra Collection” technique that generates an absorption spectrum in less time, less affected by the effects of spectrometer drift, and able to produce spectra with a higher signal to noise ratio than the absorption produced by SPGAS without SpectraStream.

12. Baseline drift

Q: Is baseline drift a significant problem with IRGAS? How is it managed?

A: Baseline drift is a general problem for all the FTIR spectrometer benches. The baseline drift can affect the quantification analysis if the chemometric software package does not address this problem. This problem becomes more evident when working around the detection limit of the instrument. The SPGAS chemometric module uses baseline correction parameters to compensate for the effects of baseline drifting during the quantification analysis. SpectraStream is a unique active spectra collection approach to produce a nearly flat and static baseline which is easier to model.

13. Record archiving

Q: To what extent can SPGAS data records be stored for future recovery? How are they identified and tracked?

A: All the quantification analysis results can be stored and time stamped for purposes of trace-ability and report generation. It is up to the customer to define their requirement of how much data they would like the system to store. The system uses at least 6Kb/hr per molecule to store the time stamp, molecule concentration, and standard error information at a rate of one concentration analysis every 10 seconds. Of course other information can be included like the gas tank serial number, process lot, etc.

14. Warning signals

Q: What types of warning and alarm signals are built into SPGAS? Can they be coupled to a master process control computer?

A: SPGAS not only actively monitors the concentration levels of the desired gas components, but also actively monitors all the hardware components to ensure its proper operation. The type of alarm signal can vary from reporting concentration levels to hardware status. SPGAS can be adapted to connect to a master process control computer. This adaptation is manufactured according to customer needs.

C. Applications

1. Response times

Q: What factors determine the ultimate response time of the IRGAS in industrial applications?

A: The time response of the IRGAS is governed by the scan rate of the FTIR spectrometer, the volume of the gas cell, the lengths of the sample gas supply lines from the sampling point to the IRGAS console, and the flowrate of the sample gas. The FTIR spectrometer and the SPGAS software can generate reliable data within seconds; however, the flowrate and piping distance will lead to a delay time element between real-time and time of measurement. In addition, a period of time for the exchange of gas within the volume of the gas cell applies.

2. Candidate gases and impurities

Q: Which carrier gases and impurities can be analyzed with the IRGAS? Which gases are excluded? Are the corrosive and toxic acid gases candidates?

A: All gases and impurities can be analyzed, but the FTIR spectrometer provides quantitative data only for the infrared, vibrationally-active species. Impurities within the monatomic and homopolar diatomic gases can be measured but not the absolute abundances of those carrier gases. The IRGAS was specifically designed to measure the electronic specialty gases, including the corrosive and toxic gases commonly used in the semiconductor industry.

3. Chemical resistance

Q: What materials are used to permit analysis of the corrosive acid gases? Cell body, mirrors, windows, coatings, seals, etc.?

A: The materials of construction consist of 304, 316, and/or 316L stainless steel, Kalrez 4079 O-rings, either gold- or nickel-coated Inconel C-seals, MgF_2-coated gold mirrors, transmission windows of ZnSe, BaF_2, CaF_2, AgCl, and others. Certain corrosive gases require specific combinations of these materials for the highest performance.

4. Exposure to gold issue

Q: If a process gas application can not tolerate exposure to bare gold, what alternatives exist for mirror coatings and seals?

A: MgF_2 is a frequently used protective coating for gold-coated mirrors; it provides both physical and chemical protection. Where C-seals are used, the nickel-coated Inconel C-seals are applicable.

5. Monitor reactant and product gases

Q: Can the IRGAS be applied to both reactant and product gases of a process operation?

A: With proper conditioning of the process gases and the gas cell and its piping conduits, many different gas compositions can be analyzed. The long path gas cell can be heated up to 200 or 300 deg C to prevent condensation and maintain the samples in their vapor phases. For gas samples that are highly diluted with carrier gases such as argon or hydrogen, the possibility of condensation is reduced even further.

6. Existing placement of IRGAS Systems

Q: How many IRGAS Systems are in lab and field use with customers?

A: As of September 30, 2007, more than 60 systems are in various customer applications around the world.