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Thermo Scientific Prima BT Laboratory Bench-Top Gas Analysis Mass Spectrometer

Prepared By:

The Thermo Scientific Prima is currently the world's leading process mass spectrometer system with over 1200 installed units worldwide being used for gas analysis in a wide range of industries including chemical, iron and steel and pharmaceutical. The Prima BT is the laboratory version of this instrument.

Features of the Prima BT include the following:-

- **Fast Analysis Speed:** The Prima BT can measure a process gas stream in seconds enabling improved process control through faster data acquisition.

- **Multi-component Capability:** The Prima BT's multi-component capability enables replacement of several conventional analyzers, therefore providing cost savings and reduced maintenance.

- **High Precision and Accuracy:** The excellent precision of the Prima BT means that gas analysis data can be used in feedback control with confidence, and small changes in gas stream compositions can be reliably monitored. The Prima BT's analytical performance is unmatched by any other process mass spectrometer system.

- **GasWorks and Prima Wizard Software:** Comprehensive applications software package that can be configured operated and maintained without any specialist knowledge of mass spectrometry. Prima Wizard provides a unique on line tutorial, parts manual and maintenance guide.

We trust this proposal meets with your requirements. However, if you have any further questions then please do not hesitate to contact us.

COMMERCIAL SUMMARY

Item No	Description	Order Code
1	Prima BT Laboratory Bench-Top Gas Analysis Mass Spectrometer with temperature controlled 1kV ion source, inlet probe assembly, Thoria filaments, scanning magnetic sector (scanning 0-1 Tesla) analyzer, Faraday detector, turbo drag pump and external floor mounting 8 m3/hr rotary vacuum pump. Includes embedded processor, with Gasworks Software, one serial port (RS232 or RS422) for communication with GasWorks PC (not included), two serial ports (RS 232, RS422 or RS485) for Modbus (RTU or ASCII Slave or Master, RS232, RS422 or RS485) communication, Ethernet port for Modbus-TCP, 4 digital input channels and 3 digital output channels. Includes OPC communication software. Includes documentation set (USB flash drive). Warranty - 12 months from start-up (or 18 months from delivery) includes parts, labour and travel.	BT_SYSTEM_CORE
2	30 Micron pin-hole molecular leak	PMS_LEAK_30
3	75 Micron Micro Capillary Assembly (standard - 10 ml/min)	PMS_MICRO_CAP_75
4	230V 50/60Hz Configuration	PMS_230
5	1/8" connection fittings for sample inlet and outlet	PMS_FRACT_LOW
6	Single Point Inlet, heated up to 120 deg C	BT_SINGLE_PNT
7	Modified Ion source with 1 mm exit slit for 'heavy hydrocarbon' applications; also includes Coiled W/Th filaments	PMS_STACK_1MM_W_TH_FIL
8	Kit for rotary pump gas ballast – ¼" compression inlet / ½" hose outlet, oil mist filter and oil return	BT_DRY_GAS_BALLAST
	TOTAL PRICE OF ABOVE CONFIGURATION, ITEMS 1~8, EX WORKS WINSFORD UK (INCO 2010)	
9	CPT Delivery to Salerno, Italy	
10	Commissioning visit for start-up, testing and operator training (up to 4 days maximum, including travel to and from site)	COMMISSIONING_PRIMA_BT
	TOTAL PRICE OF ABOVE CONFIGURATION INCLUDING DELIVERY & COMMISSIONING, ITEMS 1~10	
	Options	
11	Service Case comprising ion source, vacuum gauge, seals kit, fuse kit, tools, spare rotary pump oil (not included where Fomblin Rotary Pump option is used), leak, micro-capillary and FEP tubing	PMS_SERVICE_KIT+
12	Upgrade to Faraday/Secondary Electron Multiplier Single Microchannel Plate Detector system, for ppm detection (species and other component dependent)	PMS_SEM_ADDER
13	Rotary Pump Fomblin Option, for samples containing>25% O2 (explosion risk), replaces standard rotary pump	BT_FOMBL_PUMP
14	Ion chamber treatment to maximise response to OH and S containing components	PMS_SOURCE_STACK_DAG
15	Desktop PC (EMEA version) with specification optimized for GasWorks. This will be supplied with the latest version of Windows verified to be compatible with Gasworks unless otherwise specified on ordering	DESKTOP_GAWORKS_PC_EMEA
16	Prima BT Documentation Hard Copy	WIN_DOCUMENTATIONS

TERMS AND CONDITIONS - PRIMA BT

Delivery	The delivery time is currently 15 weeks for a Prima BT from acceptance of your order. This is our best estimate at the time of quoting and is subject to revision at the time of order placement.
Warranty	Standard warranty period on the Prima BT mass spectrometer is 12 months from start up or 18 months from delivery, whichever is sooner, and includes parts, labour and travel. The warranty is dependent on proper installation in line with the instrument site requirements, maintenance of the rotary pump and other system components in line with manufacturer's recommendations and other conditions listed in Thermo Onix Terms and Conditions. The warranty covers defects in goods and faulty workmanship but excludes consumable items such as filaments, SEM detector plate, flow sensor, micro-capillary, leak and filters. It also excludes failures due to ineffective sample conditioning or damage caused by the sample gas. Any commissioning, maintenance, repair, service, relocation or alteration to or of, or other tampering with, the instrument or the parts, performed by any person or entity other than Thermo Fisher Scientific without Thermo Fisher Scientific prior written approval, or any use of replacement parts not supplied by Thermo Fisher Scientific, shall immediately void and cancel all warranties with respect to the affected instrument or parts.
Commissioning date	To be agreed with Thermo Fisher Scientific with at least 6 weeks notice and to be within 6 months of date of shipment unless agreed at time of order. Note that changing commissioning dates with less than 6 weeks notice may not be possible owing to other pre-arranged commissioning visits. Thermo Fisher Scientific will give dates at the earliest opportunity in keeping with Thermo Fisher Scientific commissioning plan. Commissioning can only be carried out by a trained Thermo Fisher Scientific engineer.
Prepared site	It is essential that the customer has a prepared site, with the necessary facilities to allow efficient commissioning of the Prima system. A site readiness form will be issued prior to commissioning for completion and return to the installing Thermo Fisher Scientific office. Failure to comply with the site requirements (as enclosed) resulting in extended commissioning days or an additional visit will allow Thermo Fisher Scientific the right to charge at standard daily rate, plus expenses, for each additional day incurred.
Training	Initial operator training is provided during commissioning. Additional training (maintenance and application) can be arranged at site or our factory (at extra cost). Please contact us for details.
Calibration Gases	These are not supplied as standard, but mixtures will be recommended, as appropriate to the application. Acceptance on site is against measurement of an agreed set of calibration gas bottles supplied by the customer. Failure to have acceptance gases available at commissioning may result in additional commissioning costs, which will be charged at standard Thermo Fisher Scientific daily rate, plus expenses.
Drawings & Manuals	One set of drawings and manuals are supplied (on USB flash drive) with any system ordered, but will not be issued before an order is placed. Extra sets can be purchased. Modification to standard drawings or production of additional drawings will be charged at the appropriate rate.
Testing	Testing is performed to Thermo Fisher Scientific standard test specification. Special testing to specific customer requirements will be charged as appropriate for additional work and/or equipment/gases required.

APPLICATION SUMMARY

ANALYSIS

The Prima BT will be used for the analysis of a gas sample from catalytic dehydrogenation of Propane as follows.

Component	Mol Mass	Minimum conc %mol	Maximum conc %mol	Prima BT Lower Detection Limit %mol
Hydrogen	2	5%	30%	0.02%
Methane	16	0.10%	5%	0.005%
Water	18	19%	20%	0.05%
Ethylene	28	0.03%	0.5%	0.2%
Carbon Monoxide	28	0.0001%	1.5%	1%
Ethane	30	0.05%	2%	0.1%
Propylene	42	5%	15%	0.2%
Carbon Dioxide	44	0.0001%	0.9%	0.5%
Propane	44	50%	90%	0.05%
1-Butene	56	0.0001%	0.08%	0.005%
i-Butane	58	0.002%	0.02%	0.02%
n-Butane	58	0.002%	0.02%	0.02%

Notes

1. The analysis cycle time will be approximately 15 seconds.
2. It is assumed that no Nitrogen will be present. Any Nitrogen present will be reported as Carbon Monoxide.
3. The analysis will be performed on a normalized basis, i.e. the reported component concentrations will be adjusted so that their sum equals 100%.
4. Calibration should be checked weekly. Typical re-calibration interval is 4 weeks.
5. Analytical performance will be demonstrated during commissioning by analyzing the following calibration gas for at least 50 analysis cycles.

Component	Conc %mol	Prima BT Standard Deviation %mol
Hydrogen	15%	≤0.02%
Methane	3%	≤0.005%
Ethane	2%	≤0.01%
Propylene	10%	≤0.02%
Propane	70%	≤0.05%

CALIBRATION GASES

The following gases will be required for calibration.

%mol concentrations

	Cal Gas 1	Cal Gas 2	Cal Gas 3	Cal Gas 4	Cal Gas 5	Cal Gas 6	Cal Gas 7	Cal Gas 8	Cal Gas 9	Cal Gas 10	Cal Gas 11
Hydrogen											15%
Helium	100%		Balance	Balance				Balance	Balance	Balance	
Methane											3%
Ethylene			10%								
Carbon Monoxide				10%							
Ethane					100%						2%
Propylene						100%					10%
Carbon Dioxide							100%				
Propane		100%									70%
1-Butene								10%			
i-Butane									10%		
n-Butane										10%	

Notes

1. Calibration gases should be supplied in compressed gas cylinders with 2-stage regulators and flowmeter/needle valves to set a flow of typically 100 ml/min to the mass spectrometer inlet. For each gas each calibration will require the gas to flow at ca 100 ml/min for three minutes to complete the calibration.

2. Calibration gas 1 should use ≥ 99.999% purity.

3. Calibration gas 11 should be a certified gravimetric mixture.

4. Note on Water Calibration:

   Introduction
   Water can be measured reproducibly by the Prima BT mass spectrometer, but the calibration is not straight forward, because water vapour is not available in a standard calibration cylinder. However, the following approaches to calibration may be used:-
   a. Assume a nominal relative sensitivity of 1.25 (relative to Propane at mass 28). The results will be very reproducible but could be (always) offset by ~+/-15% relative, due to the absence of actual calibration.
   b. Adjust the value of the water relative sensitivity in the instrument so that the measured water vapour concentration on a sample stream matches a known value (either calculated/predicted or measured by another instrument).
   c. Use an accurate water vapour generator, for example, the Bronkhorst VDM (Vapour Delivery Module) which uses a built in heater/mixer and digital mass flow controller for the carrier gas and Coriolis flow meter for liquid water introduction.
   d. Using the bubbler method, as described below.

   Method of Water Calibration using the Bubbler Method
   Two streams of Propane are connected to the inlet at close to the same time, with one being a ‘wet’ stream and the other a dry stream. The ‘wet’ stream is generated using a wash bottle (e.g. FP-W from M&C Tech Group). This wash bottle contains water through which the gas forms bubbles thereby producing the ‘wet’ stream. The flow rates on the two streams are adjusted to be equal (within +/-10%) using a needle valve (e.g. Swagelok SS-4MG) on each line, so typically flow rates are 190~210 ml/min on both streams.

   A plain ¼ OD PTFE tube should be used in place of the frit tube in order to avoid completely saturating the gas with water. This avoids problems due to water condensing in the line between the wash bottle and mass spectrometer. Such an arrangement will typically produce 2~3 %mol of water vapour. The water concentration is calculated by comparing the mass 28 peak intensity of dry gas and with wet gas (assuming the same flow rates are used). The mass 28 peak intensity is expected to decrease by a percentage equal to the concentration

of water vapour present. The equation for calculating the Water relative sensitivity (relative to Propane) is the following:-

H2O relative sensitivity = [I_{18}(wet gas) - I_{18}(dry gas)] / [I_{28}(dry gas) - I_{28}(wet gas)]

This calculation needs to be performed manually offline and then the Water relative sensitivity entered into the GasWorks gas database.

5. **It is the responsibility of others** to provide calibration gas cylinders, regulators, flowmeter/needle valves, equipment for water calibration and pipe-work to the instrument.

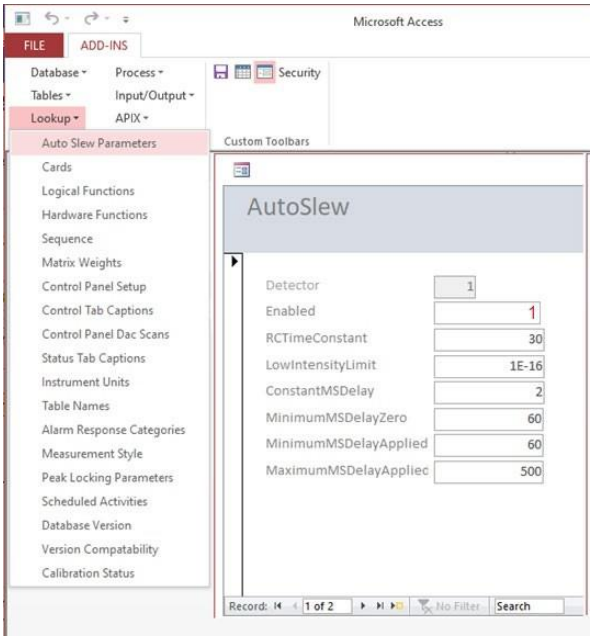
ANALYSIS SET-UP (REFERENCE INFORMATION)

The following are example values of relative sensitivities and fragmentation patterns (actual values will differ but be accurately calibrated by the instrument using the calibration gases). The Faraday detector will be used throughout.

Name	Hydrogen	Methane	Water	Carbon Monoxide	Ethylene	Ethane	Oxygen	Propylene	Carbon Dioxide	Propane	1-Butene	iso-Butane	n-Butane
Formula	H2	CH4	H2O	CO	C2H4	C2H6	O2	C3H6	CO2	C3H8	C4H8	C4H10	C4H10
Mol Wt	2	16	18	28	28	30	32	42	44	44	56	58	58
Rel Sens	0.80	1.41	1.25	1.90	1.76	1.88	1.43	1.05	2.08	1.00	0.66	2.53	2.19
2	100	0.13			0.08	0.15		0.14		0.19	0.27	0.05	0.06
16		100	0.9	0.18			4	0.10	5.03	0.11			
18		0.05	100										
26					48.79	17.72		7.40		7.71	34.76	1.01	2.73
28				100	100	100		1.29	4.42	100.00	75.40	1.35	25.30
30				0.21	0.03	30.82			0.01	3.52	1.34	0.10	0.75
32							100		0.01				
42								100		11.04	9.09	37.70	12.70
43								3.30	0.01	47.65		100	100
44								0.10	100	61.99		3.36	3.35
56											100	0.39	0.77
57											4.55	3.59	2.91
58												4.43	17.86

The base gas will be set to Propane.

In order to eliminate carry over between the measurements the Auto Slew Parameters lookup table in engconf.bat will have AutoSlew **Enabled** (set to 1) for Detector 1 (Faraday).



	Settings
Focus	700 V
Electron Energy	70 eV
Source Temperature	200 ºC
Inlet Probe Heater Setting	100%
Inlet Temperature	120 ºC

CALIBRATION SET-UP (REFERENCE INFORMATION)

The gas calibration should be configured as manual calibrations as follows, where F= Fragmentation, S = Sensitivity and B = Background. There should be one calibration method that runs all 11 calibration gases in a single calibration and 11 separate calibration methods that each use only one separate calibration gas, i.e. a method for Cal Gas 1 that only uses Cal Gas 1, a method for Cal Gas 2 that only uses Cal Gas 2, etc. The Faraday detector will be used throughout.

	Cal Gas 1	Cal Gas 2	Cal Gas 3	Cal Gas 4	Cal Gas 5	Cal Gas 6	Cal Gas 7	Cal Gas 8	Cal Gas 9	Cal Gas 10	Cal Gas 11
Settling Time	180 s	180 s	180 s	180 s	180 s	180 s	180 s	180 s	180 s	180 s	180 s
Hydrogen	B										15% SL
Helium	100%		Balance	Balance				Balance	Balance	Balance	
Methane	B										3% SL
Water	B										
Ethylene	B		10% FS								
Carbon Monoxide	B			10% FS							
Ethane	B				100% FS						2% L
Propylene	B					100% FS					10% L
Carbon Dioxide	B						100%FS				
Propane	B	100%FS									70% L
1-Butene	B							10% FS			
i-Butane	B								10% FS		
n-Butane	B									10% FS	

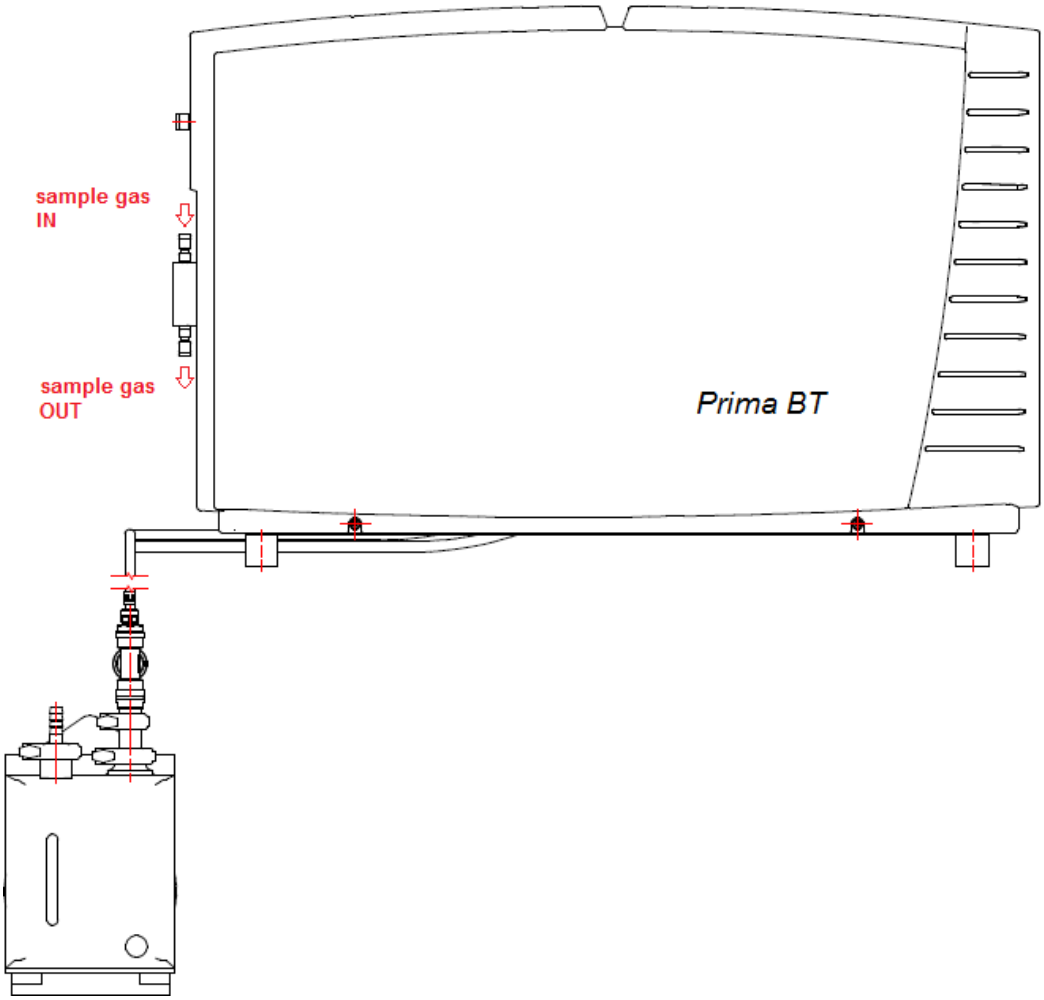
SAMPLE CONDITIONING REQUIRED

It is the responsibility of others to provide suitable sample conditioning to ensure a clean representative gas sample. To protect the Prima BT analyzer against blockage by liquids and dust we recommend the use of a hydrophobic/oleophobic membrane filter (e.g. Genie Membrane filter model 120 with type 6 membrane, A+ Corp, or Classic Filters Grade M4). Condensation in the sample lines must be avoided by ensuring the dew-point of the sample gas does not exceed the temperature of any of the sample conditioning components.

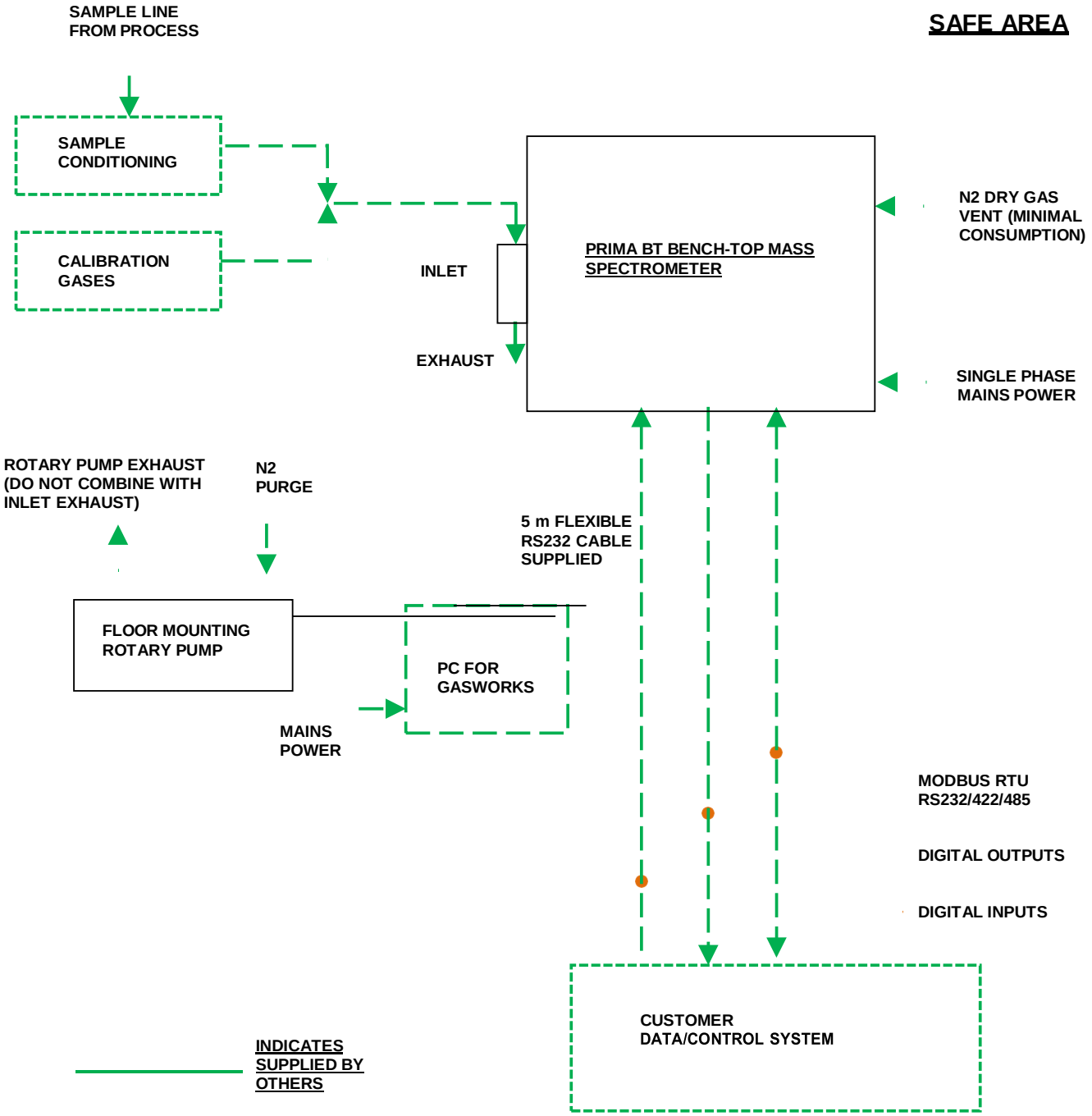
The conditioned sample gas (or calibration gas) for measurement (or calibration) needs to conform to the following specification:-

conditioned sample gas flow	20 – 1000 ml/min
conditioned sample gas dew point	≤100 °C
conditioned sample gas dust filtration	≤ 0.8 microns

The sample gas pressure should be close to atmospheric pressure, but in order to create the necessary sample gas flow, either the sample gas pressure should be slightly in excess of atmospheric pressure or a slight vacuum should be applied to the outlet. Please note the single point inlet consumes about 10 ml/min via its capillary. Therefore at the minimum sample flow rate of 20 ml/min, 10 ml/min will flow through the outlet.



INSTALLATION LAYOUT



TECHNICAL DESCRIPTION

Introduction

The Prima BT is a high performance gas analyzer based on a powerful and flexible scanning magnetic-sector mass spectrometer. The system has been designed to deliver superior analytical performance with high reliability and minimum maintenance. Apart from a floor mounting rotary pump, the instrument is contained within a fan-cooled enclosure suitable for mounting on a bench-top.

Principle of Operation

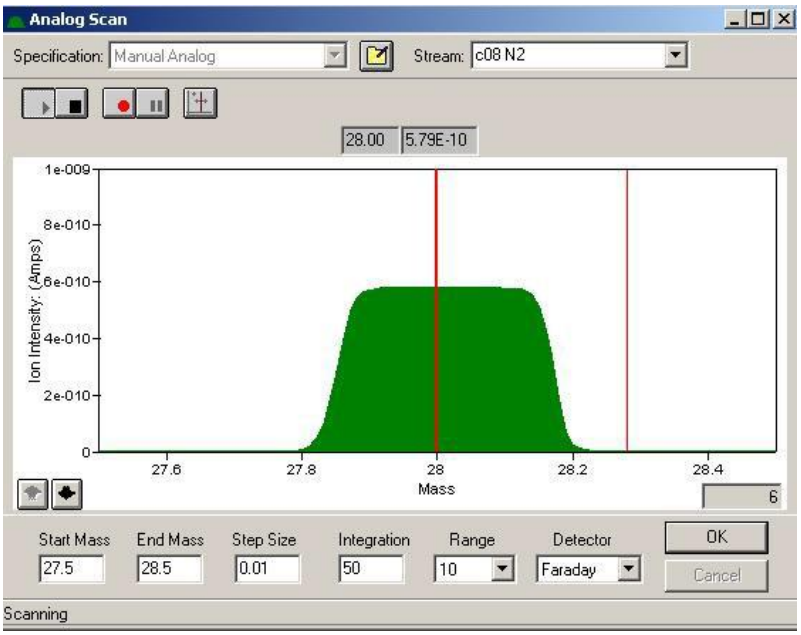
The sample gas is introduced via a stream selector and a pressure reduction system comprising a capillary and molecular leak to introduce sample gas into the ion source under vacuum. Via the capillary a small flow of sample gas is drawn past the molecular leak by a vacuum pump. A small proportion of the sample gas enters the ion source. Using an electron emitting filament, the ionization chamber converts the sample molecules into ions which are positively charged molecules or parts of molecules. These ions are then separated according to their mass by a variable magnetic field. The different mass ions are then quantified by the detector in accordance with the abundance of the signals at these masses.

Main components

Analyzer:

At the heart of the Prima BT is a magnetic sector analyzer which offers unrivalled precision and accuracy. Thermo Fisher Scientific manufactures *both* quadrupole and magnetic sector mass spectrometers. Over nearly three decades of industrial experience has shown that magnetic sector based analyzers offer the best performance for industrial on line gas analysis.

Key advantages of magnetic sector analyzers include improved precision, accuracy, long intervals between calibrations and resistance to contamination. Typically, analytical precision is between 2 and 10 times better than a quadrupole analyzer, depending on the gases analyzed and complexity of the mixture. Unlike a quadrupole analyzer which gives only rounded peaks, the magnetic sector gives flat-topped peaks which ensure the measurements **are highly reproducible.**



A unique feature of the Prima BT magnet is that it is laminated. This means that the Prima BT magnetic analyzer can scan at speeds equivalent to that of quadrupole analyzers, therefore offering the unique combination of rapid analysis and high stability. The variable magnetic field is provided by a electromagnet with a laminated core, allowing the rapid and extremely stable analysis of a number of user-defined gases. The scanning magnetic sector is controlled with 24-bit precision using a magnetic flux measuring device for extremely stable mass alignment.

The ion source is an enclosed type for high sensitivity, minimum background interference and maximum contamination resistance. This is a high-energy (1000 eV) analyzer that offers extremely rugged performance in the presence of gases and vapors that have the potential for contaminating the internal vacuum components. As the ions are extracted from the ion source at high energy, excellent stability is achieved for low molecular weight compounds such as hydrogen and helium.

The ion optics is under full computer control, removing the need for manual tuning of the analyzer. Options are available for both single and dual detector ion sources. Temperature control to 0.1 degree C is a standard feature of the ion source, providing maximum stability and fast response to polar compounds.

Ion detection and amplification is encoded and transmitted to the local Processor using fiber-optic cable for maximum noise immunity. With the continually updated zero reading, minor components can be measured more reliably in complex mixtures. Concentrations in the 10ppm - 100% can be quantified using the standard Faraday detector. Concentrations as low as 10ppb can be measured using the optional multiplier but in practice the lower limit of detection will depend upon the degree of spectral overlap in the sample gas mixture and instrument background.

Inlet System Options:

Available options include stepper motor controlled Rapid, Multi-stream Sampling (RMS), single point solenoid inlet and single point inlet.

The unique RMS sample selection system sets new standards for multi-stream sampling, offering an unmatched combination of sampling speed and reliability, which allow selection of the gas sample from 1 of 16 streams. Stream settling times are application dependent and completely user configurable. The RMS includes digital sample flow recording for every selected stream. This can be used to trigger an alarm in case of fall off in sample flow, for example due to a blocked filter in the sample conditioning system.

This unit includes inlet control electronics, which provides electronic control of the stepper motor, calibration panel and RMS temperature (up to 80 deg. C). The position of the stream selector is optically encoded for reliable, computer controlled stream selection. The temperature and position control signals are communicated via the VG*i* network, which will accommodate multiple inlet systems on a single analyzer.

Calibration Panel Option:
For automatic calibration a calibration panel assembly with 6 solenoid valves is used to select calibration gases. This option is available when the RMS or single point solenoid inlets are ordered.

Electronics

Mass Spectrometer Power Supplies:

Power supply and distribution has been engineered to ensure minimum power consumption and maximum reliability with extensive system monitoring at all points around the network. The principles of fault-tolerant design have been implemented throughout.

Local Computer:

The local processor provides embedded processing power for true, stand-alone control of all mass spectrometer functions. A local network provides control of all ancillary equipment. A serial port is provided for connection to a PC and an additional two configurable serial ports are provided for remote communication. As standard Modbus protocol communications are supplied (RTU or ASCII, both data logging and external control).

The Vacuum System:

Includes the external floor mounting rotary pump that provides backing vacuum for evacuating the analyzer and also provides pumping for the inlet bypass capillary, the pump controller which controls the operation of the high-performance combination turbomolecular pump and an active cold-cathode vacuum gauge for interlock protection of the ion source filaments. As an option the external floor mounting rotary pump is replaced by an internal diaphragm pump which fits within the instrument enclosure.

Please note the standard rotary pump is only suitable for samples having O2 concentration <25%. Above this concentration, an explosion hazard exists and special configuration options need to be included – consult Thermo Fisher Scientific for details

PRIMA BT PROCESS MASS SPECTROMETER SPECIFICATIONS

Ion Source	Enclosed Electron Impact with Dual Filaments, temperature controlled (settable over range 120-200 degrees C, to ± 0.1 degrees C)
Analyzer Type	Scanning Laminated Electromagnet, 6 cm radius, 80 degrees deflection
Mass Range	Adjustable, default is 1-150 amu at 1000 eV ion acceleration voltage, (at 750 eV ion acceleration voltage, mass range is 1-200 amu)
Resolution	Switchable between two collector resolving slits, resolving powers of 60 (1mm) and 20 (4 mm) are standard. Optionally 140/85 (0.36 mm/0.69 mm) or 100/45 (0.56 mm/1.45 mm) or 140/45 (0.36 mm/1.45 mm) may be fitted
Mass scale stability	Measured at mass 28 < 0.013 amu over 24 hours
Peak Shape	At 60 resolution, the ratio of the width of the flat-top (99% height width) to the base peak width (5% height width) 0.4 (or 0.2 with 1 mm ion exit slit)
Abundance sensitivity	<250 ppm for 27/28
Detector	Faraday and optional Faraday/SEM dual detector
Inlet Type	Capillary with Molecular leak and bypass (standard configuration)
Vacuum System	Turbomolecular Pump and Rotary Pump
Sample Flow	Digitally measured and recorded for each stream for any instrument with RMS option
Precision*	<0.1% relative (typical, application dependent)
Linearity*	<1% rel over decade change in concentration (typical, application dependent)
Dynamic range*	Faraday: 10 ppm – 100% (theoretical, application dependent) Optional single MCP SEM: 1 ppm – 1000 ppm (theoretical, application dependent) Optional twin MCP SEM: 10 ppb – 1000 ppm (theoretical, application dependent)
Stability*	<1% relative over 1 week (typical, application dependent)

*These specifications refer to the standard instrument using an external rotary pump.

COMMUNICATION OPTIONS

Serial Communications

The Prima BT supports many communication protocols on its serial ports (both RS-232C and RS-422 or RS-485). These may be used for both data logging and instrument control and may be intermixed as required. Connections may be made using either 7 or 8 data bits with one stop bit and parity may be set to None, Odd or Even. The baud rate may be chosen from the following list: 300, 1200, 2400, 4800, 9600, 19200 and 38400.

The supported protocols are:

VGCP
Simple ASCII
Siemens 3964
Modbus
OPC

The protocols are implemented in various flavours and the facilities they each support depend on the chosen style. Only one style for each protocol may be implemented in a single instrument. I.e. while it is reasonable to have both a PVGCP Slave and a Modbus ASCII Master, it is not possible to have both a Modbus ASCII Master and a Modbus RTU Master within a single instrument.

VGCP is available in these styles:

VGCP Master (Data Logger)
In this style, the only function available is transmission of Analysis results after each sample is completed. The message includes time-stamped instrument status and derived values as well as the Analysis concentrations.

PVGCP Master (Data Logger)
This adds checksumming and retries to the basic VGCP Master but no further features.

VGCP Slave
As a slave, VGCP requires the connected host to poll for Analysis results. The slave may also be commanded to control instrument functions such as: Enable Stream, Disable Stream, Start Scheduling, Start Calibration and Stop Activity.

PVGCP Slave
This adds checksumming and retries to the VGCP slave to provide a secure protected link to external gateways such as the X-Link.

A test program, written to operate on a PC under Windows, is included on the GasWorks distribution CD so that all four styles can be fully exercised on site. Xon/Xoff flow control (Software flow control) is supported in all styles.

Simple ASCII
Simple ASCII is available only as data logging, un-polled connection, which transmits Analysis, results after each sample is completed. Its format is suitable for connection to simple programs or even direct to a printer. There is no checksumming or retrying and Xon/Xoff flow control is supported.

Siemens 3964
Siemens 3964 is available in these styles:

3964
In this style, the format conveys Analysis results after each sample is completed. The message can include instrument status and derived values as well as the Analysis concentrations.

3964R
This style adds a checksum to the transmissions and expects the responses from the host to be similarly enhanced.

No flow control is supported for these styles.

Modbus is available in these styles:

Modbus ASCII Master
In this style, Analysis results are transmitted as scaled integers. The register map is user-definable and may be to more than one slave (RTU). Transmitted registers may contain values for time stamps, instrument status, Analysis concentrations and derived values.

Modbus RTU Master
This style transmits the above register data in the more common 8-bit RTU format.

Modbus ASCII Slave
As a full slave, the instrument may be commanded to control instrument functions such as: Enable Stream, Disable Stream, Start Scheduling, Start Calibration and Stop Activity. The host may also read all measured concentrations and derived values as well as the time stamps, stream alarm states and instrument hardware condition from a user-defined register map. The slave can be configured as any unit in the range 1 to 255.

Modbus RTU Slave
This style supports the above functions in the more common 8-bit RTU format.

Xon/Xoff flow control is supported for the ASCII Master and Slave styles only.

OPC

We offer two options for OPC (OLE for Process Control or Open Process Control): -

GasWorks OPC Data Logger (via GasWorks)
This allows simple read-only OPC access to instrument statuses and stream analysis data (alarm indications, concentration values and derived values) via the GasWorks application. These OPC items are only available when the PC running the GasWorks workstation software is connected to the instrument.

GasWorks OPC Server (via a dedicated MODBUS connection)
As well as access to instrument statuses, stream analysis data (alarm indications, concentration values and derived values), this provides the ability to control the instrument - to start/stop analyses, enable/disable streams etc. It provides a direct connection to the instrument at all times and hence doesn't rely upon the PC running the GasWorks workstation software being connected to the instrument.

This functionality is provided by a separate application that can run on any PC having a dedicated serial link to the instrument (this link is in addition to any serial connection used to connect the GasWorks workstation to the instrument).

Digital I/O

Four digital inputs and three digital outputs are provided for the following functions.

Digital external control
The function of the inputs is to allow the user to perform a number of tasks without operating via the PC. These can be used to either 'Start or Stop Schedule' or 'Run Calibration Now'.

Instrument activity outputs
The function of these outputs is to indicate the status of the analyzer: -

- External Control Active
- Running Scheduled Analysis
- Calibrating
- In Stand-by

Stream inhibit digital inputs
The function of this series of digital inputs is to allow the user to enable or disable any of the sample streams, which have been previously enabled for multi-point Analysis in the software. This function allows the user to effectively change the multi-point sequence without interrupting the Analysis; indeed it permits changes in the multi-point

sequence to be made without making any operation on the PC or with the PC disconnected (i.e. in the stand-alone state).

Component alarm outputs
The I/O system may be configured to provide component alarm outputs on any or all sample streams; these may be associated with up to 10 different response categories (e.g. H2 20 mole % may be a response 1 category, N2 < 30% may be a response 2 category, Wobbe < 2 may be a response 8 category). Each response category utilized requires a separate output module. Also, if the alarm is to be stream specific, each specified stream uses a separate output module.

Hardware alarm outputs
The I/O system may be configured to provide hardware alarm outputs for up to 10 different response categories, each representing one or more hardware alarm states. For example: -

Hardware Alarm (user configurable)	Response Category (user configurable)
Vacuum failure	Response 1
Emission (filament) failure	Response 2
Ion Energy low	Response 3
Cabinet temperature high	Response 4
Source Pressure 3.9×10^{-5} mbar	Response 4
Source temperature not at set-point	Response 5

Note on Digital Inputs
Digital input modules can be configured to switch on with either high or low signals. The high signal voltage is in the range of 10 - 32 volts.

Notes on Digital Outputs
Digital outputs provide voltage free contacts that can be configured either open or closed contact for any particular function. Digital outputs can be configured as either static or pulsed (selectable as either 0.5 or 1.0 seconds).

ANALYSIS BY PRIMA BT: ACCURACY AND LOWER DETECTION LIMIT CONSIDERATIONS

Gas analysis by mass spectrometry is performed by continuously introducing the sample gas into an ion source, where an electron beam interacts with the sample gas, causing a proportion of the sample molecules, as they pass through, to become ionized as various molecular, fragment and atomic ions. The resultant ion beam is accelerated and extracted by an electric field and then subjected to mass separation. The resultant separated component ion beams of different mass-to-charge ratio (m/z) are recorded by the ion detector as a series of peaks. Characteristic peak signal strengths are (within limits) linearly proportional to concentrations. However, the results are subjected to a normalization process, in order to correct for the following effects:-

- Pressure and temperature effects in sample
- Gas flow effects: different gas viscosities cause the same partial pressure in the sample gas to give rise to different partial pressures in the ion source
- Sensitivity variation with time

Normalization is carried out as follows:-

Non-normalized Concentration (that is concentration prior to normalisation) is calculated
= (Measured Intensity – Background Intensity)/Sensitivity

Normalised Concentration = Non-normalized Concentration x 100/ [Sum of Non-normalized Concentrations]

This assumes is that all significant components in the gas sample are being accounted for in the analysis method. Therefore some components may be measured which are not of interest to the user, but are required in order to normalize the results. Frequently water is not included in the analysis, so that the normalized results have to be considered to be on a dry basis.

It is often the case, that the peaks being measured are ‘overlapped’ or composite with contributions from more than one component. A de-convoluting data reduction technique is involved in deducing the component contributions to the peaks. On the Prima BT this is performed automatically by an embedded processor in the mass spectrometer. An important assumption is made (and is generally obeyed) that the overlapping peaks, when combined, obey the principle of linear peak superposition. The principle of linear peak superposition is that the composite peak height at a particular mass is simply equal to the sum of the peak heights which correspond linearly to the individual concentrations of the contributing components in the complex mixture. This may be represented as follows:-

$$i_1 = s_1 f_{11} c_1 + s_2 f_{21} c_2 + s_3 f_{31} c_3 + \ldots s_n f_{1n} c_n$$

where i is a composite peak height, and for 1 to n components contributing to this peak, s is the base peak sensitivity, f is its cracking pattern and c is its concentration. Values of s and f are determined for each component during calibration. During analysis the peak heights (i) are measured for 1 to n (or >n) masses so that there are at least n simultaneous equations to determine the n unknown values of c. Matrix inversion is used to solve these sets of simultaneous equations. These calculations are executed by the instrument computer to generate the concentration results. Some components may be measured which are not of interest to the user, but are required in order to deconvolute these interferences.

There can be small variations in the values of s and c caused by at least four effects. One effect is space charge which influences the behavior of the ions as they are transmitted from the ion source through the mass spectrometer to the detector. However, there are variations in space charge resulting from the fact that different gases produce ions at different rates; this is a fundamental physical property of the different gases and is unavoidable. The influence of space charge is reduced in a magnetic sector instrument, such as the Prima BT, because the ion acceleration voltage is very high (typically 1000 volts compared with only a few volts on a quadrupole instrument) thereby minimizing the effects of deviating voltages caused by space charge. A second effect is the influence of the gas being measured on the thermionic properties of the filament. This is due to interaction of the gas with the filament, thereby changing its temperature of emission and therefore altering the behaviour of the electron beam and ion beam. A third effect is that of the ageing of the filament which influences its work function and physical position which again changes the behaviour of the electron beam and ion beam. A fourth effect is that of ambient temperature changes causing dimensional changes to the analyzer and causing variations in analyzer lens voltages. The extent of the influence of some of these effects can be minimized by running a calibration gas mixture at regular intervals to decide when re-calibration is necessary. This is most easily accomplished by scheduling an automatic calibration which a pre-check with appropriately set tolerances on the

calibration gas mixture, for example on a daily basis. If the check analysis of the calibration gas mixture in the pre-check falls outside any of the tolerances, a complete calibration is performed

The result of the above effects is such that during normal operation of the instrument the relative values of s and f may change by up to 1% relative and 1.5% relative respectively.

As a 'rule of thumb' the uncertainty due to interference of measurement of particular component A using a particular peak intensity will be equal to 0.015 x (intensity due to overlapping components) / sensitivity of A

This can be expressed as:-

0.015 x (∑concentration x sensitivity of overlapping component) / sensitivity of A

The above assumes the Faraday detector is being used (which is normally the case for measurements over the range of 100 ppm – 100%). For measurements on the SEM detector the variations in the relative values of s and f may be much greater: these may change by up to 5% relative.

This effect of overlapping peaks will particularly influence the accuracy of measurement and even the ability to detect a component in the presence of interfering components. The lower the sensitivity of the component being measured relative to the overlapping component, the worse the effect.

Consideration should also be paid to possible errors due to errors in the concentrations of the calibration gases themselves.

Another limitation to the detection of a component is the background. Generally a component can be detected down to a concentration for which the peak intensity is $1/10^{th}$ of the background peak intensity. There are a number of background peaks of significance in a mass spectrometer. Typical levels for those peaks which are equivalent to greater than 1 ppm in the Prima BT are shown below:-

m/z	Background ppm
2	50
14	50
15	1
16	50
17	250
18	1000
19	1
20	5
28	500
29	5
20	20
32	200
40	10
44	5

Lastly, a further limitation on detection is the noise of the detector. The noise of the detector depends on the integration time, being inversely proportional to the square root of the integration time. It also depends on which detector is used. The Faraday detector uses a 1×10^{10} ohm amplifier feedback resistor and the maximum voltage that can be measured is 10 volts, corresponding to 1×10^{-9} amps. The Faraday detector noise is typically 1×10^{-15} amps (expressed as the standard deviation of the baseline) for a 1 second integration time. The SEM detector uses a 1×10^{9} ohm amplifier feedback resistor and is operated with a gain typically between 1000 (single MCP) and 10,000 (twin MCPs). The detector electron output noise due to the amplifier is typically ~2×10^{-14} amps (expressed as the standard deviation of the baseline) for a 1 second integration time. Depending on the gain of the SEM this is equivalent to between 2×10^{-17} amps ion current at 1000 gain or 2×10^{-18} amps ion current at 10,000 gain. However there is another significant contribution to noise on the SEM besides the amplifier. This is statistical noise. Statistical noise arises from the fact that the ion current is a beam of discrete charged particles and therefore each particle has

a certain probability it will reach the detector within a certain measurement window (during the integrated measurement). The standard deviation of the ion current due to statistical noise is given by:-

St Dev = $n^{1/2}$/n x ion current

where n is number of ions measured during the integration time

for a 1 second integration time n = ion current / 1.6×10^{-19}
since 1.6×10^{-19} is the charge in coulombs on each singly charged ion and amps = coulombs per second.

Therefore St Dev = (ion current x 1.6×10^{-19})$^{1/2}$ amps.

GAS*WORKS* SOFTWARE FOR WINDOWS 10 & 11

Introduction

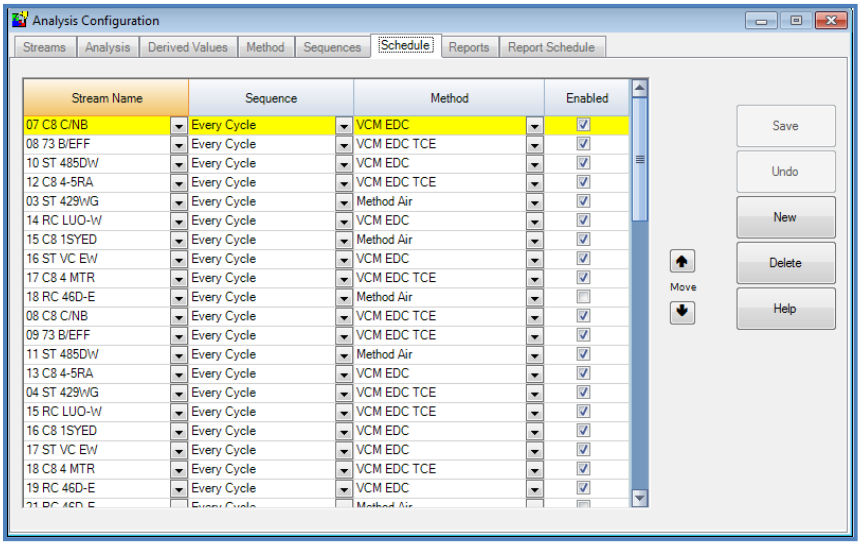
GasWorks has been designed to ensure that the Thermo Scientific gas analysis mass spectrometers can be easily configured, operated and maintained without specialist knowledge of mass spectrometry. The system is based on our extensive experience of the needs of process users and, as such, includes industry standard communication protocols, multilevel security, event logging, automatic calibration and tuning, diagnostics and on-line help. The software suite also benefits from an extensive array of data presentation forms that can be configured to meet the needs of a variety of control-room or laboratory situations. This document provides only a brief overview of what can only be described as the most comprehensive software package provided by any analyzer manufacturer in the world.

System Architecture

GasWorks is a two-processor system. The primary machine is the control engine built into the instrument. It provides a fully multitasking 32-bit real time control system which manages all aspects of instrument control. It contains a database of all instrument configuration and operational details and retains this through power fail thus allowing restart without user intervention. Since this database contains all data needed for instrument operation, the analyzer can be configured and then left to run through its scheduled processes with no further intervention, simply sending its results to the DCS and calibrating itself when necessary. The instrument controller needs no installation since its program is burned-in and its data is loaded from the host GasWorks machine.

The host GasWorks machine is a PC operating under Windows 10 and 11. It provides a convenient graphical user interface for configuring analysis methods, derived value calculations, calibration routines, communication protocols, I/O, alarm levels, etc. The host GasWorks machine also provides real-time analysis numeric and trend displays, together with various mass spectral scan modes, data logging in csv spreadsheet format and OPC for presentation of the data over a network. Also provided are comprehensive data review programs for numeric and trend displays and statistical calculations of stored data.

The primary machine can operate in stand-alone mode: i.e. analyze, auto-calibrate and provide data without connection of the host GasWorks machine.

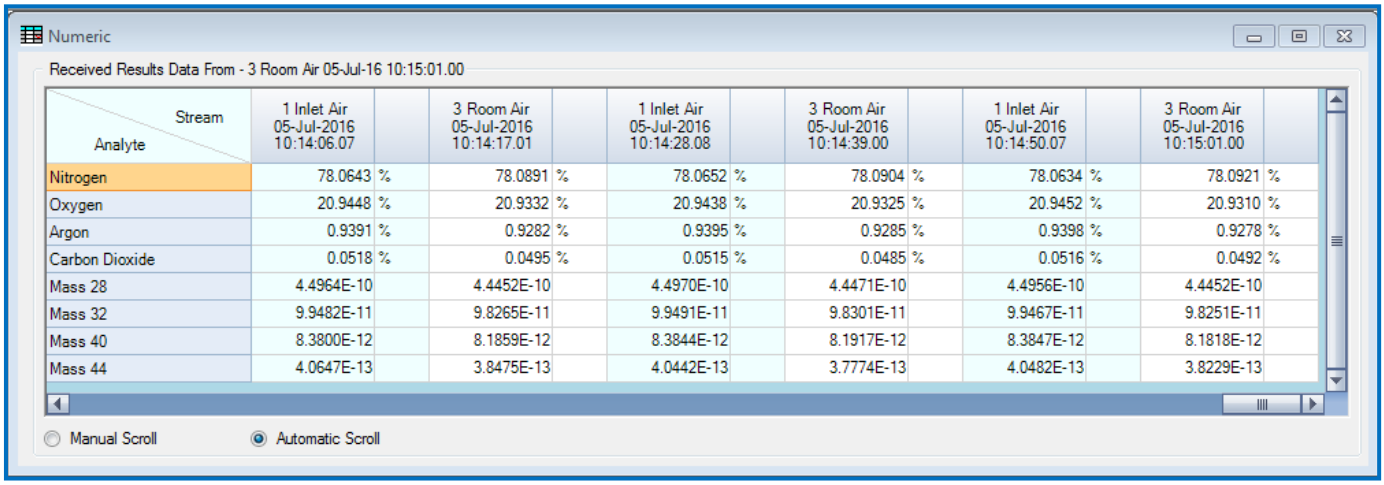


Analysis Configuration

The analysis configuration for an application is normally pre-programmed by Thermo Fisher Scientific application engineers. However components can simply be added or removed from the analysis by the user if this is required. GasWorks is designed to treat sample streams differently if the application demands, with the user having full control over the analysis performed, alarm levels and actions, auxiliary inputs and outputs, data logging and report generation.

Data Presentation

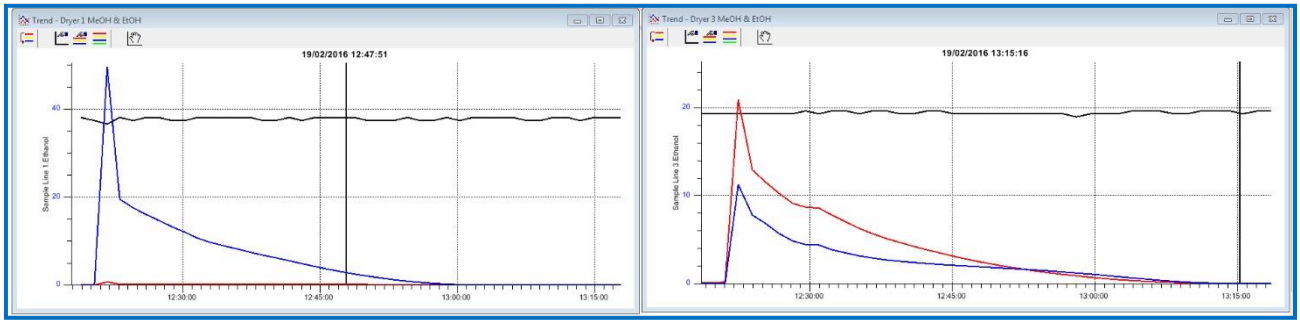
The “Numeric” screen provides a spreadsheet view of the data as it is generated by the mass spectrometer. The user can manually scroll through the data to view recently generated data on any of the enabled sample streams or this form can be configured to auto-scroll so that the most recent data is always presented.



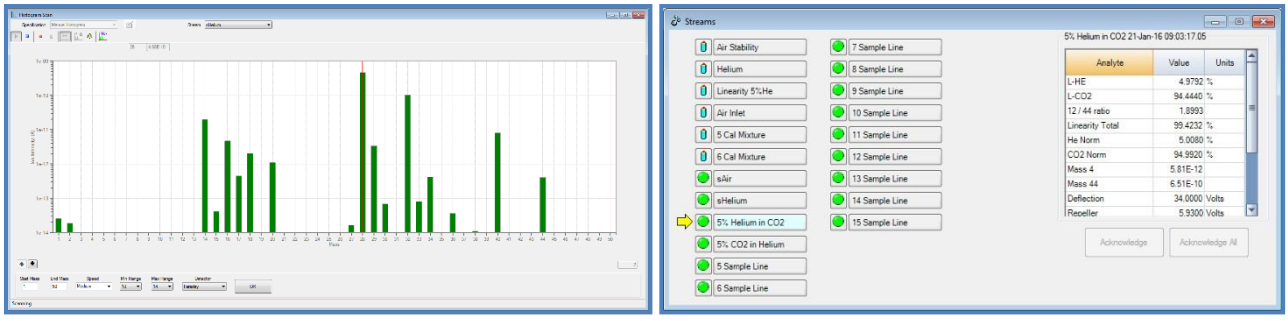
Analyte \ Stream	1 Inlet Air 05-Jul-2016 10:14:06.07		3 Room Air 05-Jul-2016 10:14:17.01		1 Inlet Air 05-Jul-2016 10:14:28.08		3 Room Air 05-Jul-2016 10:14:39.00		1 Inlet Air 05-Jul-2016 10:14:50.07		3 Room Air 05-Jul-2016 10:15:01.00	
Nitrogen	78.0643	%	78.0891	%	78.0652	%	78.0904	%	78.0634	%	78.0921	%
Oxygen	20.9448	%	20.9332	%	20.9438	%	20.9325	%	20.9452	%	20.9310	%
Argon	0.9391	%	0.9282	%	0.9395	%	0.9285	%	0.9398	%	0.9278	%
Carbon Dioxide	0.0518	%	0.0495	%	0.0515	%	0.0485	%	0.0516	%	0.0492	%
Mass 28	4.4964E-10		4.4452E-10		4.4970E-10		4.4471E-10		4.4956E-10		4.4452E-10	
Mass 32	9.9482E-11		9.8265E-11		9.9491E-11		9.8301E-11		9.9467E-11		9.8251E-11	
Mass 40	8.3800E-12		8.1859E-12		8.3844E-12		8.1917E-12		8.3847E-12		8.1818E-12	
Mass 44	4.0647E-13		3.8475E-13		4.0442E-13		3.7774E-13		4.0482E-13		3.8229E-13	

No limits on the number of components are imposed by the software, which can present raw mass spec data, on- line calculations (derived values), system parameters and external analog signals in addition to the calculated gas concentrations as shown above.

Multiple trend screens can also be provided for graphical presentation of data. This is of particular importance where the mass spectrometer is used to monitor a number of independent processes. Where this is the case, each process would have its own trend form, which is made available for display by selection from a drop-down list.



Each new trend form is configured using a set-up wizard which provides easy component and stream selection, axis configuration (log mode, linear mode, manual & automatic dynamic range, time, etc.) and trace color. Where a complex set of axes is required to present both logarithmic and linear plots on a single form then multiple y-axes are supported. Each form can be positioned and sized to make the best use of the available display area.

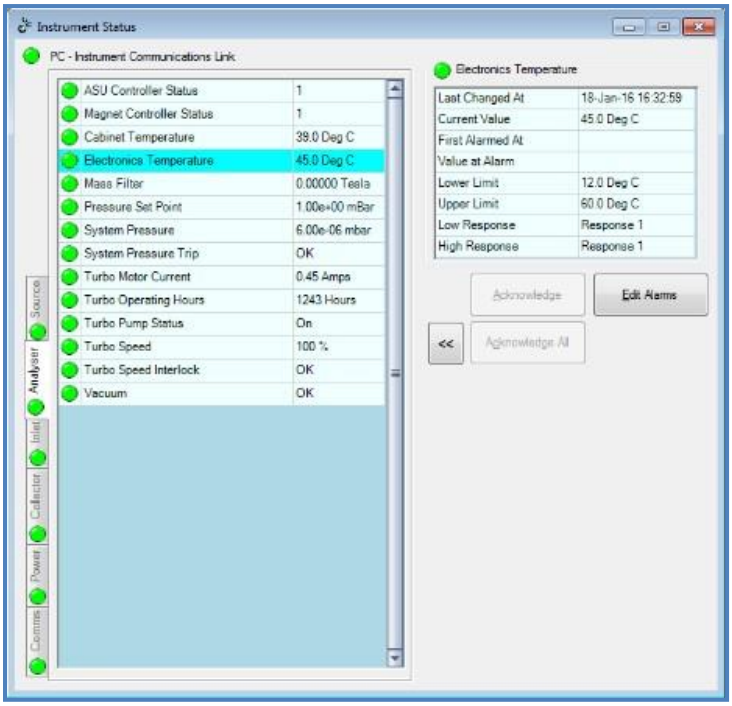


Many other data display forms are included in the standard GasWorks package including the “Scan” and “Streams View” forms shown above. The Streams View is particularly useful when the analyzer is used for environmental monitoring. Each sample stream is provided with a green/red LED style indicator and a button that is used to display

the gas concentrations in the stream window. If a gas concentration goes above its alarm set-point, then the operator simply clicks on the button with the red alarm indicator and he or she will see the offending component hi-lighted in red. This display also indicates the currently selected stream – a feature that allows the operator to judge when the next measurement will be made on any given sample port.

System Status Monitor

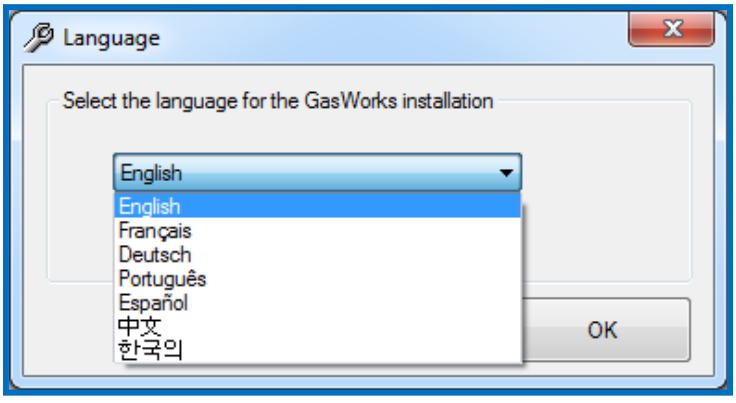
GasWorks continuously monitors over 60 instrument read-backs. The Status window displays information in a series of tables covering all aspects of the system – ion source, analyzer, inlet, collector, power and communications - listing the parameters being monitored, the current state or value of the parameter and a colored LED indicating the alarm status of the parameter. More detailed information is obtained by clicking on a parameter button, includingtime of alarm, value at alarm and user defined alarm limits.



System Security

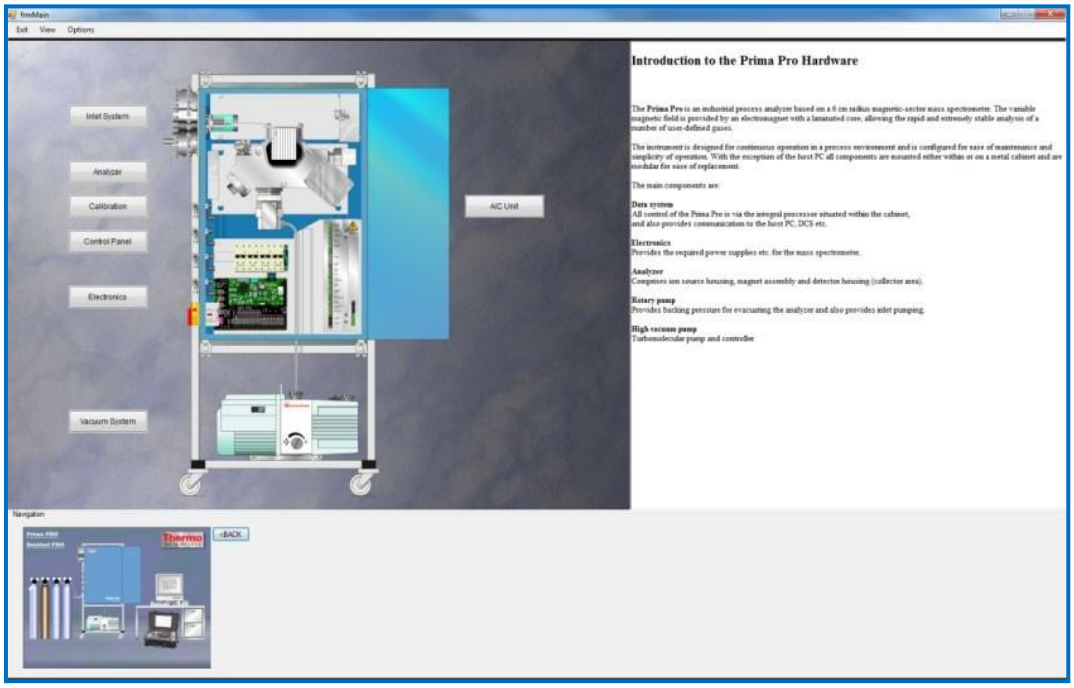
GasWorks incorporates full multi-layered and user-definable security mechanisms and accommodates FDA 21 CFR Part 11 requirements for electronic data storage. The operator must log in to gain operational authority before making any changes and password checking is performed before the operator is granted access to any of the system functions.

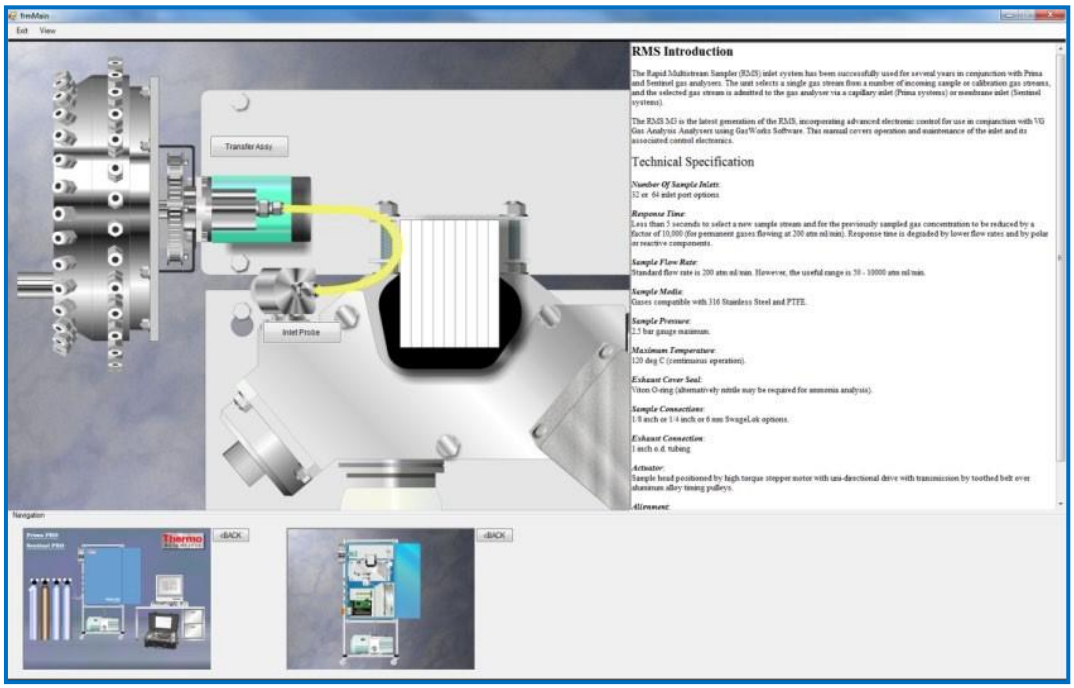
Multi-Language Support



GasWorks allows the user to choose between English, French, German, Portuguese, Spanish, Chinese and Korean for all HMI screens.

WizardPro: Expert System Software
This software package is an extensive knowledge base for the Prima PRO, Sentinel PRO and Prima BT systems, provided so the user has all the information needed to operate and maintain the analyzer right where it is needed - at the mass spectrometer. The software is easily navigated using command buttons and pull-down menus, with each subassembly having a number of views that can be selected to display the information needed. These views include tutorials, parts manuals, assembly dimensions, animations, videos, electronic schematics, electrical connections and component options.

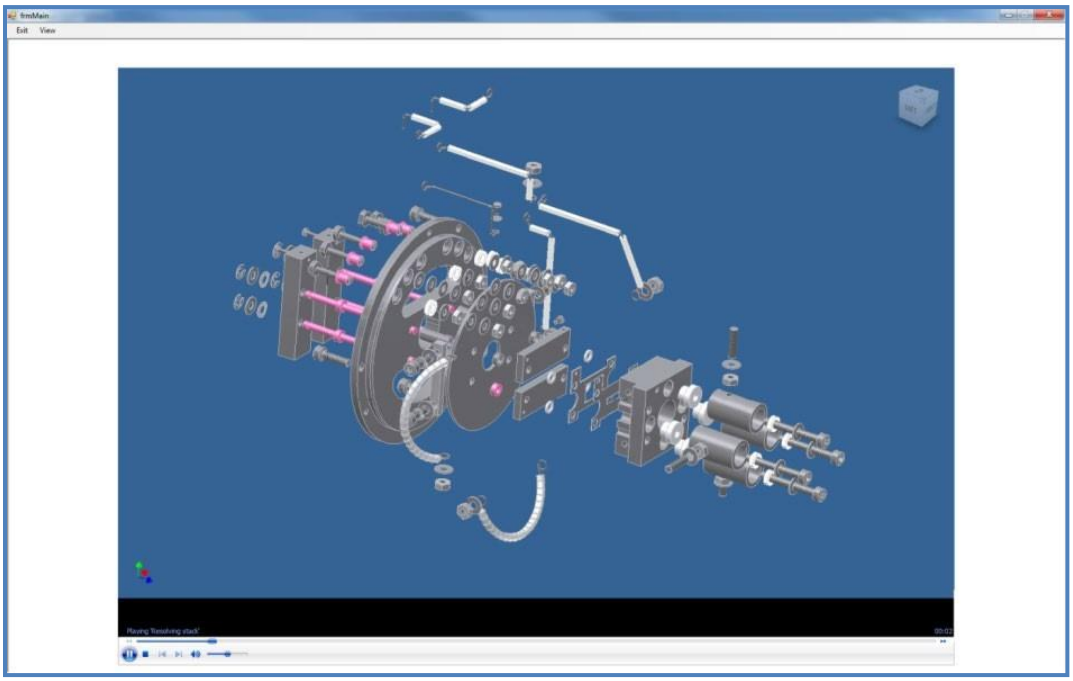




Maintenance
Preventative maintenance procedures are presented with clear and concise illustrated text to help guide the maintenance technician through the recommended routines.

Tutorials

Since users are more likely to get maximum benefit from the mass spectrometer data if they understand the underlying concepts of the technology, we have included a series of tutorials that explain the fundamental operating principles of the system. The illustrations, text, animations and videos are used extensively during operator training at the time of installation and are often reused if in-house training is required at a later date.



SITE REQUIREMENTS

Environmental operating conditions
ambient conditions should fall with the following guidelines:
The temperature of the room in which the Prima BT is located should ideally be between 18 and 22°C; permissible range is 12 °C to 30°C.
Humidity can be up to 90% maximum, non-condensing.
The vibration frequency and amplitude should be within the following limits:

Frequency	Maximum Amplitude
≤ 20 Hz	5 mm
≤ 60 Hz	1 mm
≤ 200 Hz	0.05 mm
> 200 Hz	0.01 mm

Location
The requirement is a bench space of at least 80 x 53 cm for the Prima BT, with the possibility of floor mounting the rotary pump.

The dimensions of the Prima BT are: width = 86 cm, height = 53 cm, depth = 56 cm.
Prima BT weight is 100 kg.

There is also a floor mounting rotary pump, dimensions: width = 16 cm, height = 23 cm, depth = 47 cm; weight = 30 kg.

Electrical supply
Mains voltage socket, only one is required to run the system. A single 230 VAC (± 10VAC) 50/60 Hz mains outlet is required. Power consumption under normal operating conditions is 1500W.

Sample and Calibration Gas Connections
These are connected via a 1/8" compression fitting. Sample gas should be suitably conditioned – please refer to application summary section.

Exhaust Gas Connections
There are two outlets, which should be exhausted to the outside or into a vent, i.e. not into the work area. These are:

(i) Rotary pump exhaust - 1/2 inch hose connection.
(ii) Inlet exhaust – 1/8" compression fitting.

Please note that interconnection of these two exhausts MUST be avoided. This is because the rotary pump exhaust contains an oil mist which could cause very serious contamination problems if allowed to enter the inlet (and hence the capillary the mass spectrometer). If interconnection is unavoidable, it should take place several metres downstream, and a positive flow on the inlet exhaust guaranteed, to reduce the chances of back flow.

The possibility of any condensation in either exhaust back draining to the instrument should be avoided by either ensuring a continuous downward gradient on the line, or fitting of suitable traps. It is the customer responsibility to supply all the necessary pipework to connect the two exhaust outlets to a suitable location.

Dry Gas Vent
When the vacuum system shuts down it automatically vents so that the internal pressure rises to ambient. Atmospheric air contains quantities of water vapour that can prolong the system evacuation time. This facility is provided to allow the vacuum system to be vented with a clean dry gas (most commonly nitrogen), which significantly reduces the time required for the subsequent pump down.

Connection is ¼" compression. Pressure should be in the range 0.5 – 2 bar(g), minimal flow requirement. Nitrogen supply can be from a cylinder or a plant nitrogen line.

Nitrogen Purge for Rotary Pump Ballast
This purge primarily prevents formation of liquids from any potentially condensable vapours being pumped. Connection is ¼" compression. Pressure should be supplied at between 0.2 and 0.5 bar(g). Nitrogen supply can be from a cylinder or a plant nitrogen line. Consumption rate will be within the range 0.1~1 l/min.

Computer and Communications
The PC system typically comprises computer, monitor and printer. A detailed specification for the PC is detailed below. The PC is connected to the instrument enclosure by means of a serial link.

Serial link connections to the instrument are made via 9 pin D-sockets.

A number of different formats for the serial links are possible.

a) RS232. Simple 3 wire link, transmission distance 5 metres. May be extended by the use of good quality screened cable.
b) RS422. 4 wire link, extended transmission distances.
c) RS485. 2 wire link, extended transmission distances (not available for host PC communication).

GasWorks PC Specification
If a PC is not purchased with the instrument, then a PC with Windows 10 or 11 operating system needs to be supplied.

The following requirements must be met.

Display	Minimum 14" (1024 x 768) Colour
Mouse	Any Windows supported mouse
Keyboard	Any Windows supported keyboard
USB ports	At least one available USB port: For installing GasWorks software from flash drive supplied with instrument For GasWorks communication with the instrument (using the USB-RS232 or USB-RS422 converter supplied with the instrument)

The GasWorks PC may be networked.

The usability of GasWorks improves with increasing PC performance. However, this has insignificant effect on the analytical speed of the instrument as all measurement and calculation is performed within the instrument.

Important
It is essential that the Microsoft .NET Framework v3.5 is installed prior to installing the GasWorks software. This will require the Windows distribution media or the ability to connect the PC to the internet for the software download and installation.

Notes on Delivery

Note on Instrument Packing and Transportation
The instrument is packed using a wooden crate in which it is sealed in foil with desiccant. Although it is secured within the wooden crate, the instrument assembly itself is susceptible to possible misalignment or even damage by excessive vibrations or shocks. Accordingly the crate is fitted with 'shock-watch' and 'tilt-watch' indicators. The only exception to the above is in the case of a direct UK delivery to site where it has been specifically requested by the customer that the instrument be delivered un-crated (for example for the convenience of immediate installation).

We recommend that any transportation by road should be by vehicle fitted with **air ride suspension** to minimise vibration and shock transmission and a tail lift capable of handling at least 500 kg.

Note on Instrument Storage

Whether for an extended period or simply prior to installation the instrument should be stored in the following manner:

- In a secure location
- Upright
- Dry (protected from standing and falling water etc.)
- Between 5 degC and 40 degC (40 degF and 105 degF)
- 90% Maximum humidity – Non condensing
- All packages together