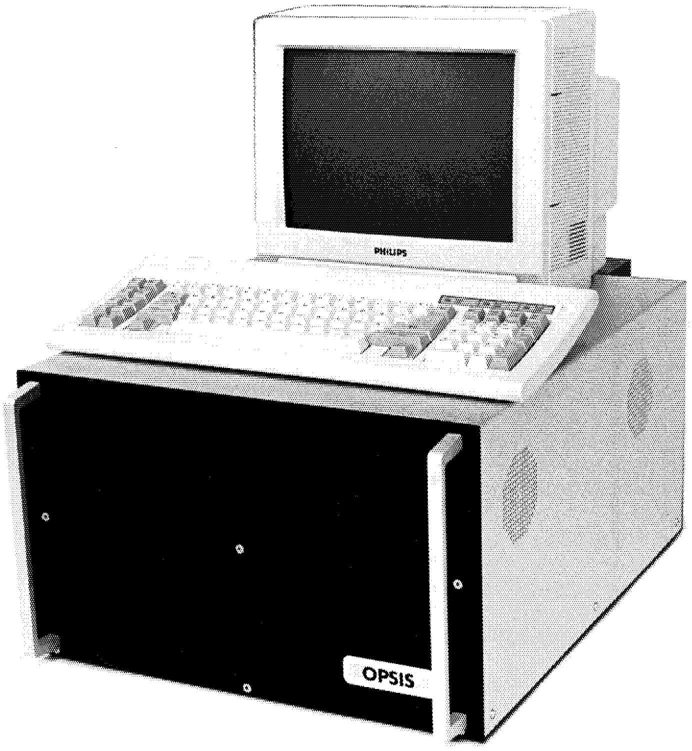
OPSIS®



AR500, AR600
AR550, AR650
Software version 7.21

Analyser Reference Manual

Release 2

Copyright

Trademarks

Limited warranty on software

The warranty conditions of this software are described in the purchase agreement between the buyer and the seller. However, a condition for any warranty is that the software is installed, operated and maintained in accordance with the specifications and instructions issued by Opsis AB including this manual. This warranty is limited to replacement of defective diskette or documentation supplied by Opsis AB and in no event shall Opsis AB or its suppliers be liable for any loss of profit or any other commercial damage, including but not limited to direct or indirect, special, incidental, contingent or consequential damages resulting from any defects in the software or its documentation including damages from loss of data, downtime, loss of goodwill, damage to or replacement of equipment or property.

Contact information

Adress	Opsis AB Box 244 SE-244 02 Furulund, Sweden
Telephone	+46 46 72 25 00
Fax	+46 46 72 25 01
Web-site	http://www.opsis.se
E-mail	info@opsis.se

Contents

Introduction 1

1.1 The monitoring path

The positioning of the emitter and the receiver define the monitoring path. The light source in the emitter is a high-pressure xenon lamp. This type of light source radiates an almost smooth spectrum ranging from approximately 200 nm up to 500 nm, and from about 1200 to 3000 nm. Within these ranges a number of gaseous substances show specific absorption spectra. The lamp spectrum is however not prefectly smooth, but the remaining "hills" in the spectral output are being taken care of in the evaluation.

The emitted light beam is directed towards the receiver, and on its way the intensity is affected by scattering and absorption in molecules and particles.

From the receiver the captured light is led via an opto-fibre to the analyser. The function of the fibre is only to avoid exposing the opto-analyser to dust, high humidity, temperature variations, etc.

1.1.1 The opto-analyser AR500 and AR600

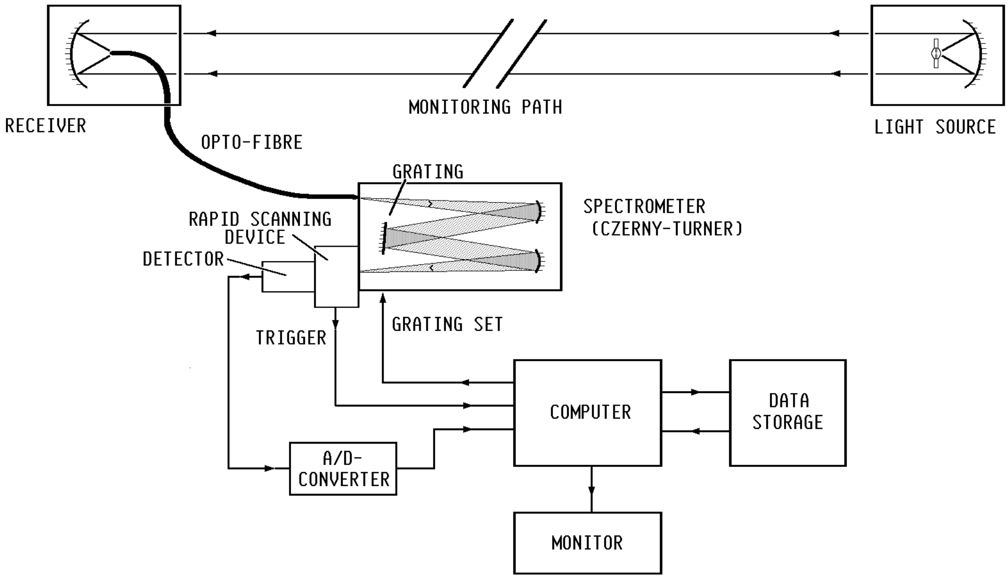


Figure 1.1. An Opsis AR500 or AR600 system consists of a light source, a receiver, an opto-fibre, and an opto-analyser. The analyser consists of a spectrometer, a detection system, electronics for the operation of the grating, the detection system, etc. and a computer for the evaluation and signal processing.

When the light reaches the analyser, it enters a spectrometer. Inside the spectrometer, a grating refracts the light into its wavelength components. The refracted light is then projected onto a rapid scanning slit in front of a photo-multiplier detector or an infrared sensitive diode, where a selected part of the spectrum is detected. The scanning slit device makes it possible to record all wavelengths separately, although only one detector is used.

As the grating is moveable, any chosen part of the spectrum can be detected. The wavelength window can thus be optimised for a certain component, with respect to parameters such as sensitivity and interfering pollutants. Approximately 100 scans per second are recorded.

The current from the detector is converted into digital signals by a 12 bit analogue-to-digital converter, and the signal is stored and accumulated in a multi-channel register. The detected spectrum is typically 40 nm wide in the UV range and approximately twice as wide in the IR range. Each scan is digitised into 1000 points.

Each pollutant is monitored during a time period entered by the operator. When the data accumulation is finished, the evaluation process is started. At the same time the next data accumulation period starts.

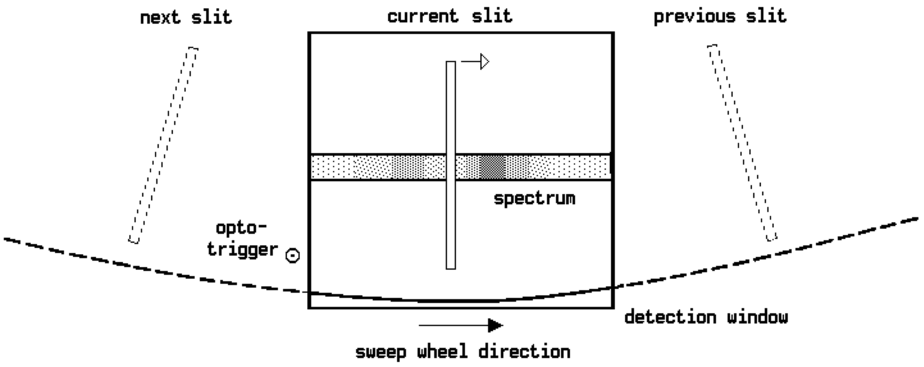


Figure 1.2. Schematic drawing of the exit window and the scanning slit in the spectrometer. The detector's "eye" covers the whole window. Due to turbulence in the air the recording time for one spectrum has to be in the order of 10 ms. A fixed slit is thus not applicable. A slotted disk, rotating with about 300 rpm, provides the detection system with the required time resolution. The opto-trigger signal is used by the computer to prepare the multi-channel memory for a new scan, and to reset the analogue-to-digital converter.

1.1.2 The opto-analyser AR550 and AR650

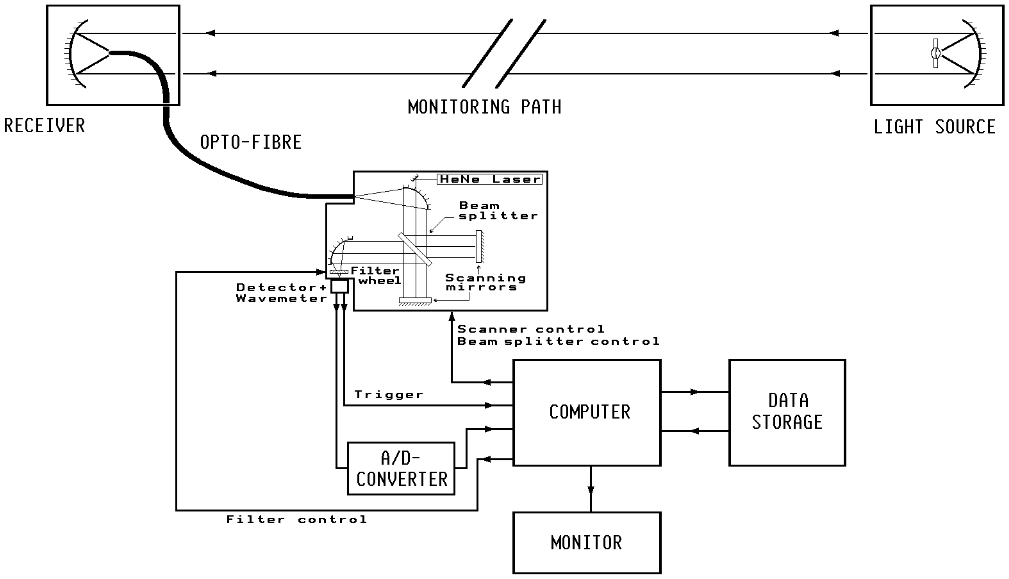


Figure 1.3. An Opsis AR550 or AR650 system consists of a light source, a receiver, an opto-fibre, and an opto-analyser. The analyser consists of a interferometer, a detection system, electronics for the operation of the grating, the detection system, etc. and a computer for the evaluation and signal processing

When the light reaches the analyser, it enters an interferometer. Inside the interferometer, a beam splitter refracts the light into two light paths. The light in each path is reflected back to the beam splitter by a mirror, whereby an optical interference is produced. (Michelson-interferometer). This interferred light is focused on an IR-detector, and by moving the reflection mirrors, a signal, which contains the parts of the spectrum where the detector is sensitive, is produced. The longer movement of the mirrors, the higher wavelength resolution is acheived. The signals from the IR-detector is A/D converted syncronous with the mirror movement. This is done by a signal from a HeNe-Laser which passes through the interferometer the same way as the opto-fiber light. To optimize the detection limit, a filter can be put in front of the detector. Each pollutant is monitored during a time period entered by the operator. When the data accumulation is finished, the evaluation process is started. At the same time the next data accumulation period starts.

The absorption spectrum is divided by the lamp spectrum and the result is a raw spectrum for further treatment.

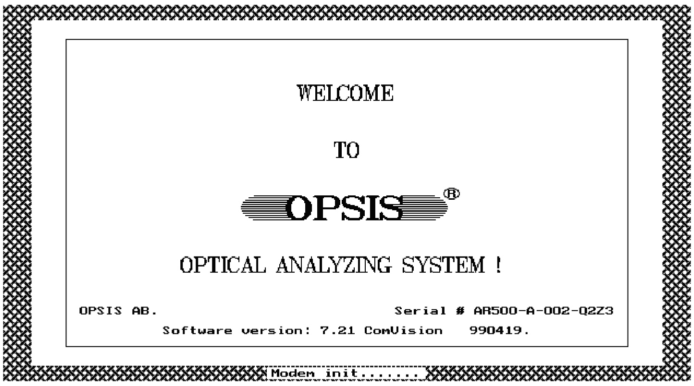
1.2 The Opsis Software

This section gives an introduction to the software controlling the Opsis UV- and IR-DOAS analysers in the AR500, 550, 600 and 650 product series.

The Opsis software is responsible for the entire function of the analyser in all parts; among other things, the operation of the data acquisition system and the optical components, the evaluations and the calculations as well as the communication to and from the analyser. The program is specific for each analyser, and can not be run on any other analyser than the one it is compiled for.

1.2.1 Starting the analyser

When power is switched on, the analyser starts a boot sequence. This includes basic initialisation of the operating system, start of the datalogger software, if used, and necessary initialisation of the mechanical and electrical parts of the analyser. During the latter part of the start sequence, the analyser displays a screen as shown in figure 1.4.



WELCOME

TO

OPSIS®

OPTICAL ANALYZING SYSTEM !

```
OPSIS AB.                          Serial # AR500-A-002-Q2Z3
        Software version: 7.21 ComVision   990419.
```

```
Modem init.......
```

Figure 1.4. The initialisation screen.

The initialisation screen gives information about:

- The registered user name, "OPSIS AB" in the above figure.

- The serial number and hardware configuration, see section 1.2.4, The analyser serial number.
- The software version, 7.21 in this example.
- The release date of this software, here April 19, 1999.

When all initialisation is ready, a one to five minute warm-up period starts to allow for stabilising of the hardware. The length depends on the analyser model. When the five minutes have passed, the analyser will start its measurement sequence, as described in section 6, Measurements. The countdown can be interrupted by pressing any key on the keyboard. This leads directly to the root menu, described in section 1.2.2, The Root menu. From here, all configuration, presentation and calibration procedures can be accessed.

The root menu can be password protected. This is described in section 1.2.3, Password protection.

1.2.2 The Root menu

The Analyser Root menu is the main menu for the software functions. To access a submenu, use the indicated function keys directly, or use the arrow keys to move the highlighted text and then press [Enter] to confirm the selection. These methods can be used throughout all software menus.

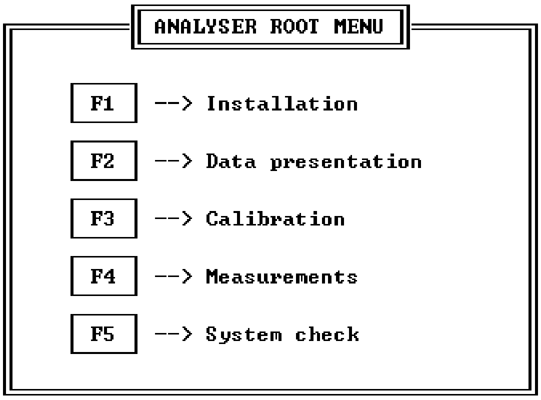


Figure 1.5. The analyser root menu.

- [F1] Installation. Used to initiate all important parameters for the instrument, such as measurement period, length of measurement path, the substances to be monitored, and to initialise a datalogger, serial communication, etc.
- [F2] Data presentation. Used for analysis and presentation of measurement results. It is also possible to make backup of data files in this menu.
- [F3] Calibration. This is the menu in which reference, zero and span calibrations of the analyser are initialised and performed.
- [F4] Measurements. This activates the measurement mode. The analyser will automatically enter this mode five minutes after start-up, unless a key is pressed manually during the countdown. The software is also provided with a timer function,

which takes one step towards the automatic measurement mode approximately every fifth minute, when the keyboard is not used. This means that the instrument will always end up measuring, no matter what sub-menu was active last.

- [F5] System check. Initiates a check of the performance of the instrument.

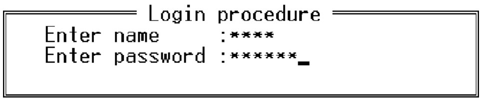
The five functions in the root menu are described in separate sections.

1.2.3 Password protection

The access to the menus in the software may be protected by passwords. Upon accessing the root menu, a user name and a password will then have to be entered. Once the password is entered, access is given to all parts of the analyser software available to the user with the given password. Different passwords may give access to different parts of the software. The functions which may be accessed individually are:

- Installation of system parameters
- Calibration procedures, available in two levels
- Data presentation
- File management
- System check.

The password set-up is described in section 7.2.3, Password setup.



```
Login procedure
Enter name     :****
Enter password :******_
```

Figure 1.6. The menus may be protected by user names and passwords. The entered text will appear as stars on the screen.

1.2.4 The analyser serial number

In the initialising menu, which is presented when the analyser is warming up, the serial number is shown. As an example, in figure 1.4, the number is "AR500-A-002-Q2Z3". This number gives some important information on the hardware configuration in the analyser. Given the format:

ARnnn-N-iii-ABCD

the different sections have the following meanings:

Analyser serial number information	
nnn	Information on analyser model. Possible numbers are 500 to 503, 510-513, 520-523, 550, the corresponding numbers for the 600 series, and 300 or 400.
N	Also information on analyser designation. A-E or I.
iii	Analyser serial number, 001 to 999

Analyser serial number information		
A	O, P or Q:	O: Old 186 processor card P: New 186 card, old PROM Q: New 186 card, new PROM
B	1, 2 or 3:	1: analogue-to-digital card, old version 2: analogue-to-digital card, model A/D2 3: analogue-to-digital card, model A/D3
C	S, X, Z or F:	S: grating drive unit, museum model X: grating unit, DC motor operated Z: grating unit with stepper motor F: fixed grating
D	X, A, 3, 4 or 5:	X: computer motherboard, model XT A: AT computer 3: computer working with 386 processor 4: computer with 486 processor 5: computer with Pentium processor

For analysers in the AR550 and AR650 series, only the information under item D is relevant. A through C are thus not presented.

Hardware AR500, AR600 2

This chapter describes dimensions and electrical specifications of the AR500/600 instrument. It also includes drawings of the exterior and interior of the instrument, including location of the main mechanical and electrical components, and fuses.

Technical specification: AR500 and AR600 series	
Flash disk	512 MB or more
Floppy disk drive	3 ½" 1.44 MB
Power supply, consumption	230 V_{AC} (+6 %, -10 %), 110 W, or 115 V_{AC} (± 10 %), 110 W
Dimensions (L × W × H)	600 × 440 × 266 mm^3
Weight	Approx. 30 kg
Degree of protection	IP 20
Temperature range	Storage 0 to 45 °C Operating 5 to 30 °C
Humidity range	0 to 80 % relative humidity, non-condensing

***Note**: It is vital that the humidity range is kept also during storage, when the instrument is not in use. Failure to do so may result on permanent damage of the optics of the instrument.*

2.1 Instrument housing

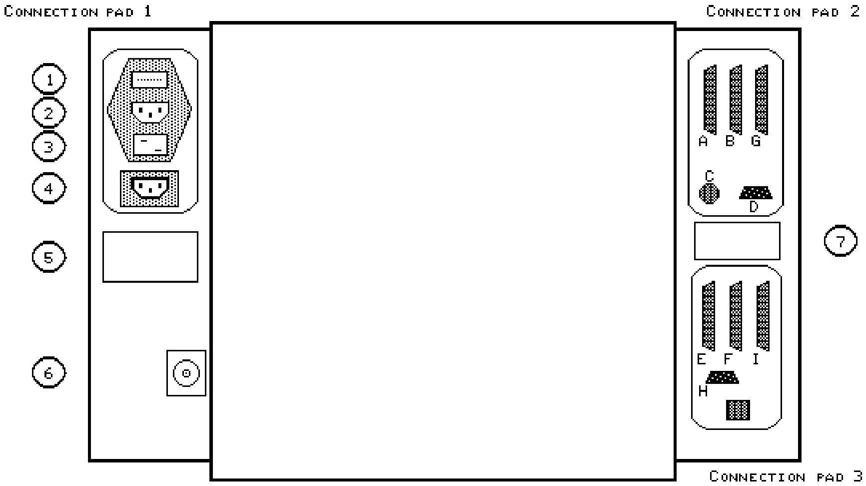


Figure 2.1. Analyser housing, rear view.

AR500/AR600 analyser housing			
1	Mains power on/off	2	Mains input
3	Fuse holder, 115/230 V programmable, see figure 2.2 for correct position	4	Power outlet for monitor
5	Warning sign	6	Fibre optic connector
7	Type/serial number label		
A	Serial port, COM1	B	Serial port, COM2
C	Keyboard connector	D	Output connector for monitor
E	Serial port, COM3	F	Serial port, COM4
G	Not used (option: serial port)	H	MX004/MX012/MX024/CA004 output connector
I	Not used (option: serial port)		

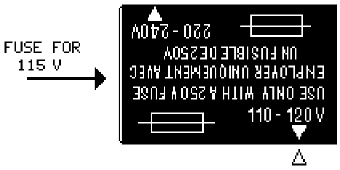


Figure 2.2. Fuse holder, here set at 115 V mains supply.

__Note__: The use of the peripheral ports may vary depending on analyser configuration. Please refer to the individual analyser test sheet and the label attached next to the connectors.

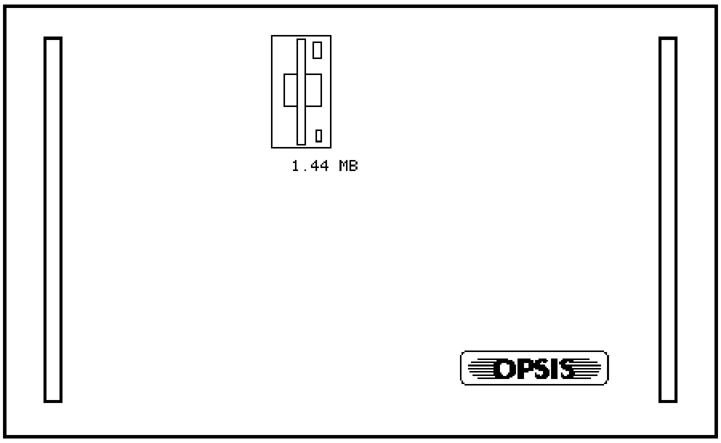


Figure 2.3. The front side of the AR500 and AR600 analyser.

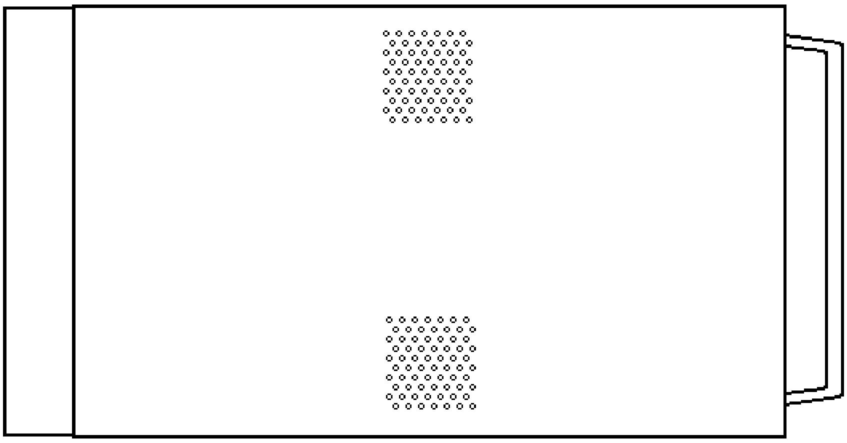


Figure 2.4. The left side of the AR500 and AR600 analyser.

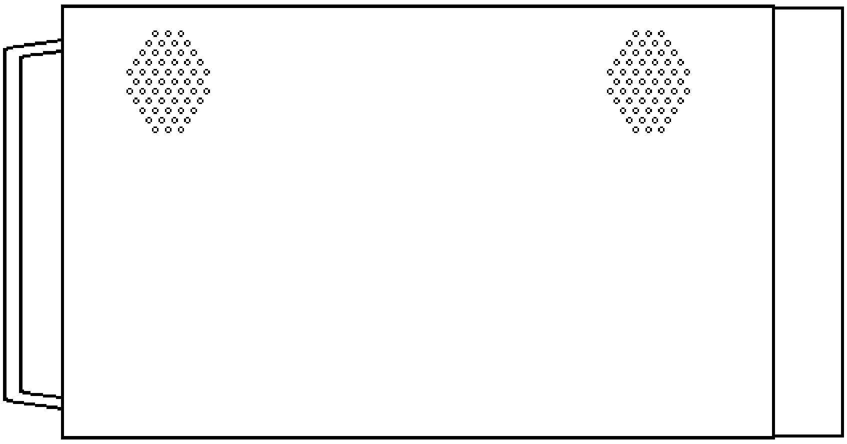


Figure 2.5. The right side of the AR500 and AR600 analyser.

2.2 Component layout, lower deck

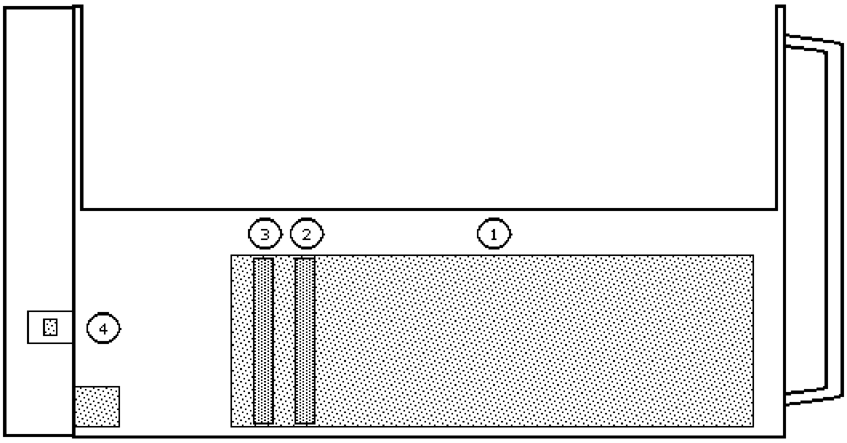


Figure 2.6. Component layout, lower deck (side view).

Component layout AR500/AR600, lower deck	
1	Rack for euro-cards
2	Photo-multiplier voltage and IR diode control card - PMT-IR (1-3 pcs.)
3	Analogue to digital conversion card - A/D-3 (1-3 pcs.)
4	Sweep trig cards

2.3 Component layout, upper deck

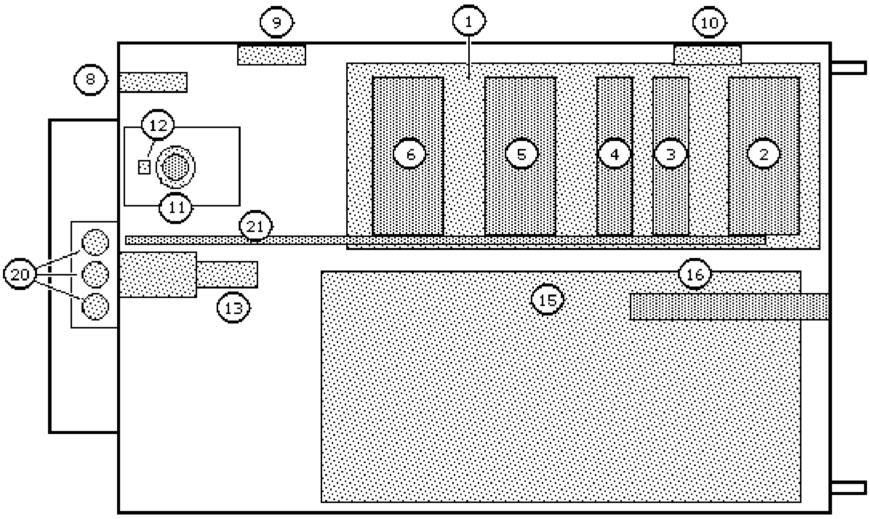


Figure 2.7. Component layout, upper deck (top view).

Component layout AR500/AR600, upper deck			
1	Rack for euro-cards	2	Power module 0 - PM0
3	Power module 1- PM1	4	Power module 2 - PM2
5	Sweep motor drive - PFC	6	Grating motor drive - D631
8	Mains filter	9	Fan
10	Fan	11	Grating motor
12	Grating trig card	13	Sweep motor
15	Computer unit*	16	Floppy disk drive
20	Photo-multiplier/high voltage power base and/or IR diodes (1-3 pcs.)	21	Interconnection card - BP1

* The computer unit includes three horizontally mounted cards:

- PC main board
- COM3, COM4 card
- Co186 card

and the flash disk (vertically mounted on the unit).

2.4 Fuses

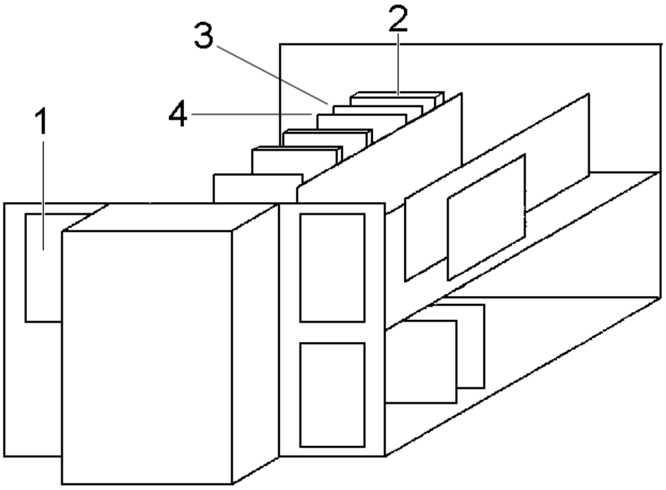


Figure 2.8. Fuse locations.

No.	**Position**	**European version** **(230 V_{AC}, +6 %, - 10 %)**	**US version** **(115 V_{AC}, ±10 %)**
1	Fuse socket	2 × 2.5 A slow/250 V	1 × 5 A slow/250 V
2	Power module 0 - PM0	1 × 8 A slow/250 V (size 6.3 × 35 mm)	1 × 8 A slow/250 V (size 6.3 × 35 mm)
3	Power module 1 - PM1	1 × 5 A slow/250 V (size 5 × 20 mm)	1 × 5 A slow/250 V (size 5 × 20 mm)
4	Power module 2 - PM2		
	F1, F2:	1 × 2 A slow/250 V (size 5 × 20 mm)	1 × 2 A slow/250 V (size 5 × 20 mm)
	F3:	1 × 5 A slow/250 V (size 5 × 20 mm)	1 × 5 A slow/250 V (size 5 × 20 mm)

Warning*: For continued protection against risk of fire, replace only with fuse of the specified type and current ratings.*

Note*: The protective housing of the instrument may only be opened by authorised service personnel.*

Hardware AR550, AR650 3

This chapter describes dimensions and electrical specifications of the AR550/650 instrument. It also includes drawings of the exterior and interior of the instrument, including location of the main mechanical and electrical components, and fuses.

Technical specification: AR550 and AR650 series	
Flash disk	512 MB or more
Floppy disk drive	3 ½" 1.44 MB
Power supply, consumption	230 V_{AC} (+6 %, -10 %), 110 W, or 115 V_{AC} (±10 %), 110 W
Dimensions (L × W × H)	$600 \times 440 \times 266$ mm^3
Weight	Approx. 30 kg
Degree of protection	IP 20
Temperature range	Storage 0 to 45 °C Operating 5 to 30 °C
Humidity range	0 to 80 % relative humidity, non-condensing

***Note**: It is vital that the humidity range is kept also during storage, when the instrument is not in use. Failure to do so may result on permanent damage of the optics of the instrument.*

3.1 Instrument housing

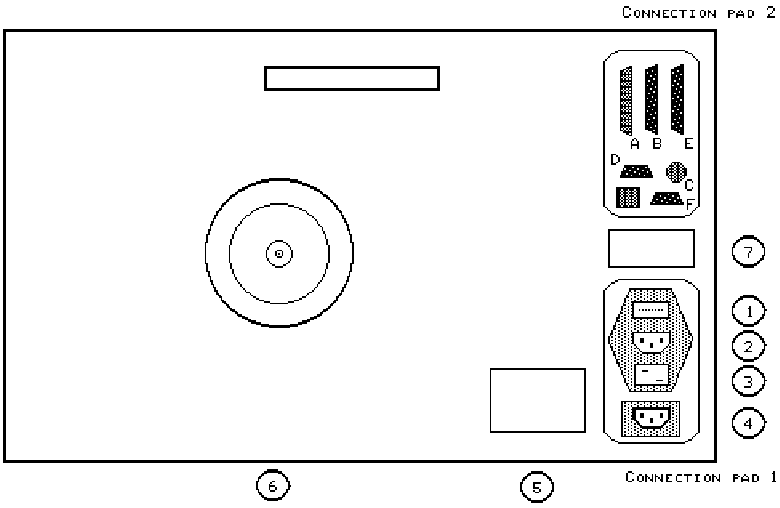


Figure 3.1. Analyser housing, rear view.

AR550/AR650 analyser housing			
1	Mains power on/off	2	Mains input
3	Fuse holder, 115/230 V programmable, see figure 3.2 for correct position	4	Power outlet for monitor
5	Warning sign	6	Fibre optic connector
7	Type/serial number label	A	Serial port COM2
B	Serial port COM3	C	Keyboard connector
D	Output connector for monitor	E	Serial port COM4
F	MX004/MX012 output connector		

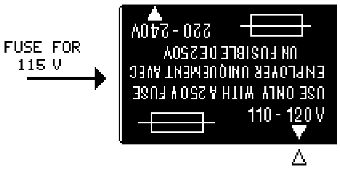


Figure 3.2. Fuse holder, here set at 115 V mains supply.

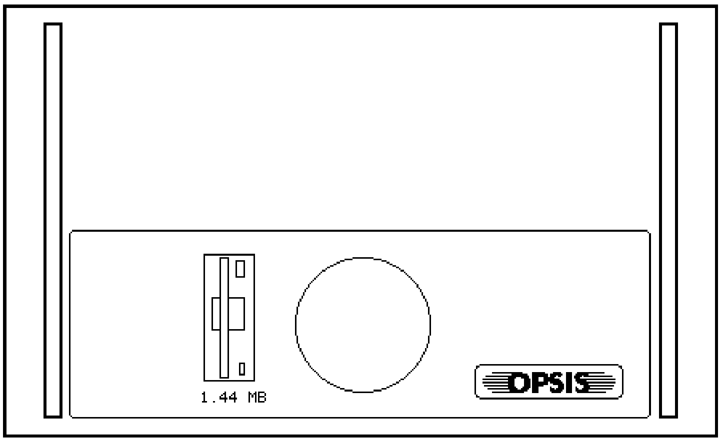


Figure 3.3. The front side of the AR550 and AR650 analyser.

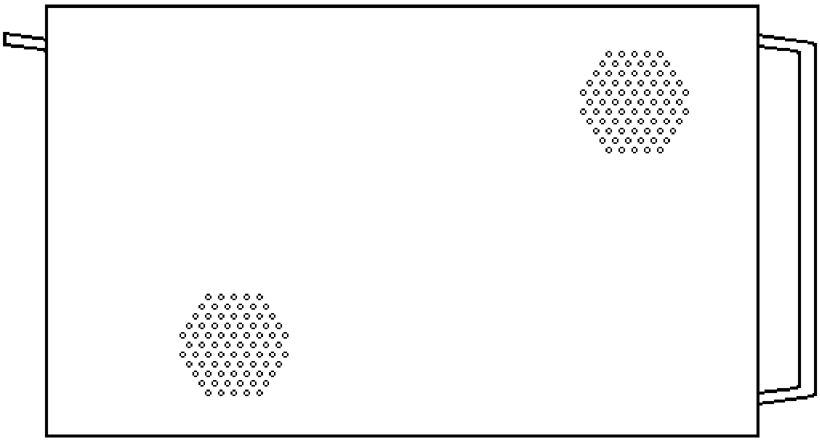


Figure 3.4. The left side of the AR550 and AR650 analyser.

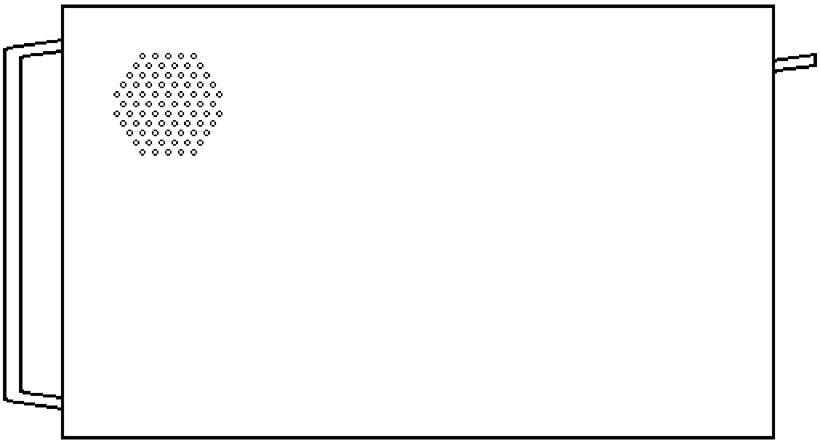


Figure 3.5. The right side of the AR550 and AR650 analyser.

3.2 Component layout, lower deck

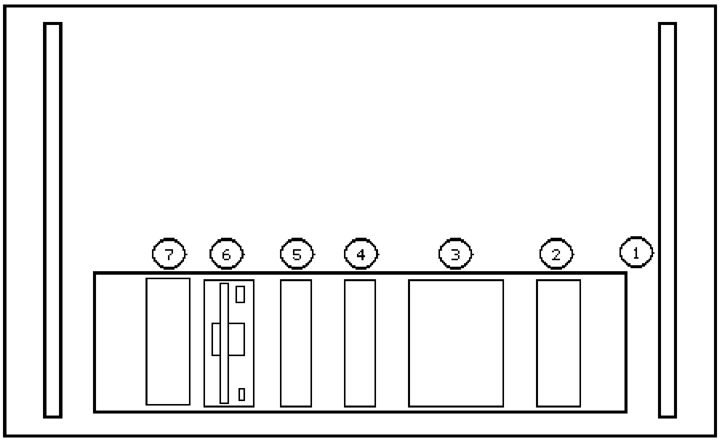


Figure 3.6. Component layout, lower deck.

Component layout AR550/AR650, lower deck			
1	Rack for euro-cards	2	Laser supply card
3	Power Module 0 - PM0	4	Power Module 2 - PM2
5	Power Module 1 - PM1	6	Floppy disk drive
7	Flash disk		

3.3 Component layout, upper deck

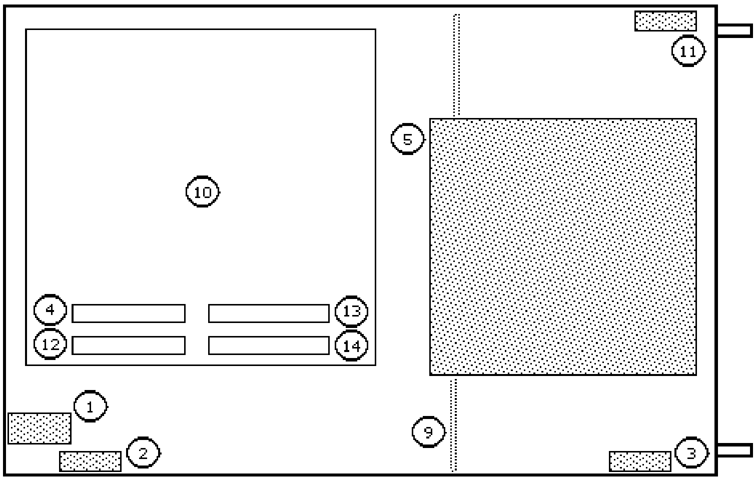


Figure 3.7. Component layout, upper deck (top view).

Component layout AR550/AR650, upper deck			
1	Mains filter	2	Fan
3	Fan	4	S/D card
5	Computer unit*		
9	Interconnection card - BP2	10	Interferometer
11	Fan	12	LF card
13	SCC card	14	SM1 card

* The computer unit includes three horizontally mounted cards:

- 29K card
- COM3, COM4
- PC main board.

Optional adapters

Analogue and digital input and output signal cards - AO 008, AI 016 resp. DI 032.

3.4 Fuses

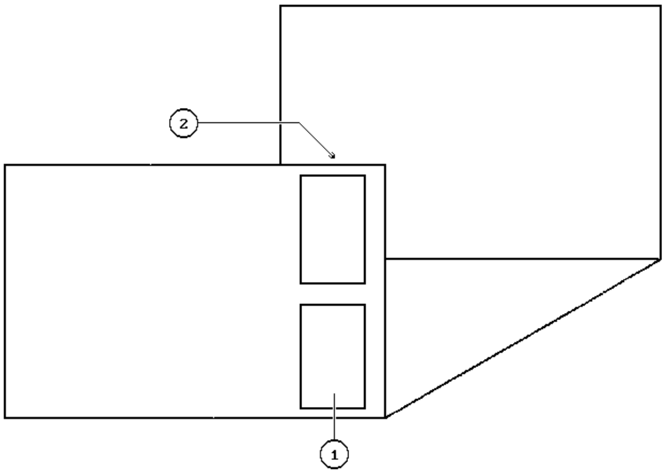


Figure 3.8. Fuse locations.

No.	**Position**	**European version (230 V_{AC}, +6 %, - 10 %)**	**US version (115 VAC, ±10 %)**
1	Fuse socket	2 × 2.5 A slow/250 V	1 × 5 A slow/250 V
2	Power module 0 - PM0	1 × 8 A slow/250 V (size 6.3 × 35 mm)	1 × 8 A slow/250 V (size 6.3 × 35 mm)
3	Power module 1 - PM1	1 × 5 A slow/250 V (size 5 × 20 mm)	1 × 5 A slow/250 V (size 5 × 20 mm)
4	Power module 2 - PM2		
	F1, F2:	1 × 2 A slow/250 V (size 5 × 20 mm)	1 × 2 A slow/250 V (size 5 × 20 mm)
	F3:	1 × 5 A slow/250 V (size 5 × 20 mm)	1 × 5 A slow/250 V (size 5 × 20 mm)

***WARNING**: For continued protection against risk of fire, replace only with fuse of the specified type and current ratings.*

***Note**: The protective housing of the instrument may only be opened by authorized service personnel.*

Safety Precautions 4

The following pages give general guidelines for managing the instrument and measurement system.

***Warning**: The keyboard and monitor comprise the only user interface with the analyser. The protective housing may be removed ONLY by authorised service personnel. The photo-multiplier/HeNe-laser and other units are powered by high voltage and any attempt to access these units may result in loss of life.*

***Warning**: Power should ALWAYS be switched off BEFORE adjusting the intensity of the light from the transmitter or connecting a new measurement path. Do not switch on power again until all adjustments have been completed. Failure to observe this precaution may result in permanent damage to the detector.*

***Warning**: DO NOT under any circumstances open or loosen doors or covers which protect the optical units. All such doors and covers are coloured yellow, or bear warning labels. Failure to observe this precaution will void the factory warranty for the instrument.*

***Warning**: Before installation, make sure the input voltage selection plug is correct (115 V or 230 V). Also check that the fuse(s) is the appropriate one(s).*

***Note**: The voltage may be changed by authorised service personnel only*

4.1 Safety precautions for the analyser

***Note**: Do not open the protective housing of the instrument. This may only be done by authorised service personnel.*

- The instrument should be connected to a 230 V_{AC} or a 115 V_{AC} external power supply. The power requirement for the analyser is approximately 110 W, and for a xenon lamp power supply, model PS150, about 220 W.
- The analyser should be installed on a flat, stable surface.
- Do not position the instrument close to radiators, heating elements or ventilation blowers. Do not expose the instrument to direct sunlight or to dust, moisture, rain or physical impact.
- Do not position the instrument in the vicinity of strong electrical or magnetic fields.

- Avoid exposing the instrument to rapid temperature fluctuations. The recommended operating temperature is +5 to +25 °C and should in no case exceed +30 °C!
- Avoid exposing the instrument to physical shocks and/or vibrations. This is particularly important when the analyser is in operation.
- Make sure to switch off electrical power *before* connecting or disconnecting cables and/or contacts. This applies to the monitor as well - but not to the keyboard.
- Make sure to switch off electrical power *before* connecting or disconnecting fibre-optic cables.
- Avoid switching on a xenon lamp, which is connected to the same mains plug as the analyser, when the analyser is running.

4.2 Safety precautions for calibration gases

The span calibration procedures require handling of gases and substances which are toxic. Good knowledge is required about their handling!

***Note**: Before handling any gas, always study the supplier's safety instructions and the regulations carefully.*

- Avoid mixing the calibration gases. Some gas blends may cause unexpected chemical reactions.
- Gas cylinders must be prevented from falling by means of chains.
- The cylinders should be stored in ventilated, specially provided, storage areas. Toxic gases should be handled preferably outside the workshop or the laboratory. Small quantities can be handled inside a building, under a well ventilated hood.
- All fitting parts must be in good condition. A pressure regulator must be inserted between the cylinder and the unit employing the gas. This function should not be performed by simply throttling the gas through a partly opened valve.

***Note**: It is important that the gas calibration system is vented to the outside! Also make sure that the gas system is free from leaks.*

Start-up and operation 5

The analyser start-up and operation instructions are described in this section. It is also necessary that the former sections and the other manuals are read and understood thoroughly prior to start-up operation.

5.1 Initial power-off inspection and preparations

To avoid instrument damage, it is important that the user perform a pre-start-up inspection of the instrument. The following items should be checked for and, if necessary, be corrected for, with the power OFF.

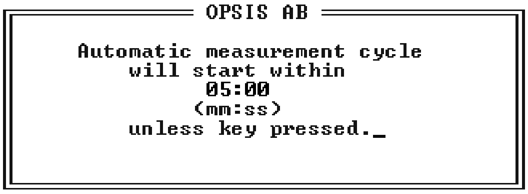
- When installing the instrument, the instructions given in section 4, Safety Precautions, should be followed. If required, the analyser should be mounted in an air temperature controlled cabinet in order to protect the instrument from a rough environment.
- Loose or missing electrical connections or circuit boards, or broken items; plugs, screws, etc.
- No loose screws, bits of wire, dirt, etc., are present.
- The correct fuse(s) (1 × 5A/250V for 115 V_{AC}, or 2 × 2.5A/250V for 230 V_{AC}) is securely in place in the fuse socket.
- Connect the cables to the keyboard, the monitor and the possible optional equipment; multiplexer, input/output signal systems, etc.
- Check that the transmitter and the receiver are correctly positioned. Connect the fibre-optic cable between the receiver and the central unit. See also the separate manual for the emitter/receiver units.

5.2 Initial power-on tests

The optimal temperature for ensuring proper operation of the computer is between +15 to +25 °C. If the instrument has been exposed to temperatures below 15 °C, allow it to warm up to room temperature before switching on the instrument.

- Plug in the analyser to a grounded power outlet of the appropriate power rating for your instrument.

- Switch on power. The fans should be heard to indicate that the power is on. Refer to the Troubleshooting section if nothing happens.
- The computer will now start. A sign-on message is displayed for about 20 seconds, after which the screen will show the following:



```
OPSIS AB

Automatic measurement cycle
will start within
05:00
(mm:ss)
unless key pressed._
```

Figure 5.1. The "warming up" message.

- If any of the installation parameters have to be changed (path length, time settings, etc.), press the spacebar and proceed into the Installation menu. All changes of the installation parameters are made via the Analyser Root Menu. If no key is pressed, the measurements will be automatically started after a warm-up period of about 5 minutes.
- Allow at least 5 minutes for warm-up before proceeding.
- Activate Optimize light in the Installation menu. The result should be a number between 0.5 and 95 %. If no value is obtained, or the value is outside the limits, first check that the opto-fibre is properly connected on the rear side and that light is reaching the analyser. If the value still is improper, proceed into the Troubleshooting section.
- Check the analyser hardware by making a System check (see section 10, System Check). If any of the five parameter values is outside the permissible limits, please refer to the Troubleshooting section.
- Before the analyser is switched into the automatic measurement mode, a reference calibration should be performed (see section 9, Calibration Procedures for details).

Measurements 6

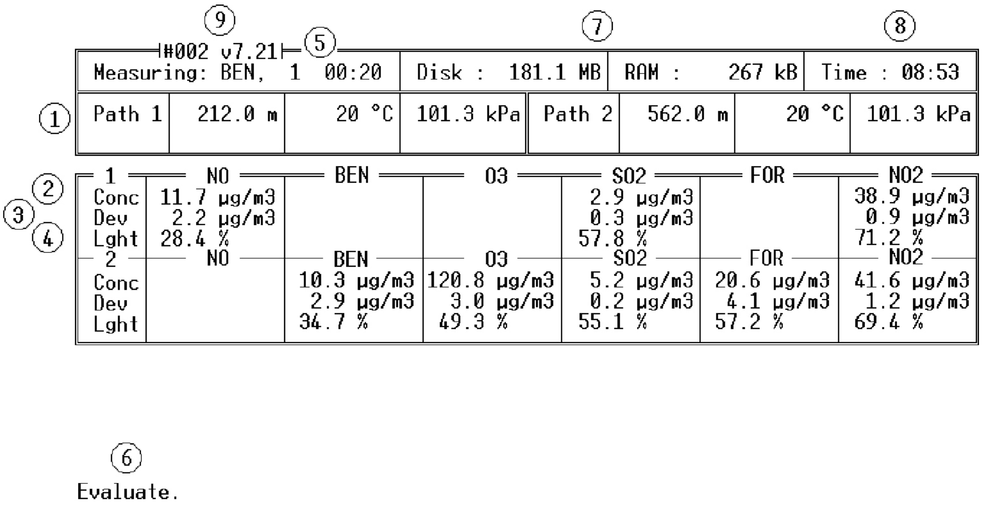
Under normal operation, the analyser shows current readings of the gas concentrations on the screen, together with other information. This is referred to as the measurement mode.

The analyser goes directly to the measurement mode after the initial five minute countdown. The measurements can also be started manually by selecting [F4] Measurements in the Analyser Root menu.

The measurement mode is aborted by pressing [Esc]. Doing so, the analyser stops all measurements as quickly as possible, and returns to the root menu. Aborting measurements can be password protected.

The analyser must be configured before the measurements can be started. This is done at the installation of the analyser. The configuration can be changed from the installation menu described in section 7, The Installation Menu.

6.1 The measurement screen



```
#002 v7.21
Measuring: BEN,  1  00:20   Disk :  181.1 MB   RAM :    267 kB   Time : 08:53
Path 1   212.0 m    20 °C   101.3 kPa   Path 2   562.0 m    20 °C   101.3 kPa

  1   NO            BEN           O3            SO2           FOR           NO2
Conc  11.7 µg/m3                                2.9 µg/m3                   38.9 µg/m3
Dev   2.2 µg/m3                                 0.3 µg/m3                   0.9 µg/m3
Lght  28.4 %                                    57.8 %                      71.2 %
  2   NO            BEN           O3            SO2           FOR           NO2
Conc                10.3 µg/m3    120.8 µg/m3   5.2 µg/m3     20.6 µg/m3    41.6 µg/m3
Dev                 2.9 µg/m3     3.0 µg/m3     0.2 µg/m3     4.1 µg/m3     1.2 µg/m3
Lght                34.7 %        49.3 %        55.1 %        57.2 %        69.4 %

Evaluate.
```

Figure 6.1. The screen during measurements.

Figure 6.1 shows an example of what the analyser presents when it is in measurement mode. The following information can be found:

1. Length, temperature and pressure used during the most recent calculation of a concentration for the path. The length is always constant, while the temperature and pressure may vary if the values come from a datalogger.
2. Results from the latest measurement. The results are corrected to normal temperature and pressure, i.e. 0 or 25 °C and 101.3 kPa, if specified. The path number is displayed above the Conc label in the menu.
3. Standard deviation in last measurement.
4. Light level in %. Zero level indicates that there is no light at all. The level should normally be between 10 and 90 % in order to obtain a valid result.
5. Gas currently being measured by the analyser. The path number is displayed after the name of the gas. Only one gas name is specified, even if more than one is evaluated at the same grating position. The seconds counting down indicates the remaining time for the spectral acquisition.
6. Operation currently performed by the computer; selecting a path, moving the grating, setting the gain of an amplifier, or evaluating a spectrum.
7. Available memory on the hard disk in megabytes, and in the primary memory in kilobytes.
8. Current time.
9. The analyser serial number and the software version number.

6.2 Scrolling the measurement screen

When the number of measurement paths and/or number of gases exceed the display capability, a window covering six gases and four paths can be slided over the table formed by the paths and gases.

All measurement data is placed in a table where the rows corresponds to the measurement paths, and the columns to the measured gases. The screen display is a window through which the table is visible. The window can be moved with the arrow keys so that any part of the table can be displayed.

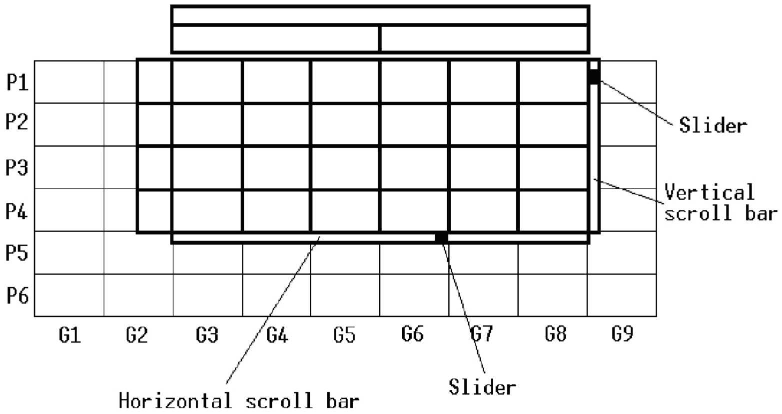


Figure 6.2. The dotted lines corresponds to the entire table. In this example, 9 gases are measured over 6 paths. The solid lines corresponds to the screen, i.e. the window the table is visible through. The window is moved with the arrow keys.

If the number of measurement paths exceeds four, a vertical scroll bar will be displayed to the right. Hidden paths can be displayed by pressing the up or down arrow keys. A slider indicates the position of the window relative to the table.

If the number of measured gases are more than six, a horizontal scroll bar will be displayed at the bottom. Hidden gases can be displayed by using the left and right arrow keys. As for the vertical scroll bar, a slider indicates the position of the window.

The arrow keys can be pressed any time during the measurements, but the window is only moved when and while the operation performed by the computer (see item 6 in figure 6.1) is Measure. In order to prevent undesired movement of the window, the arrow keys should therefore only be pressed in the Measure mode. Please note that the message Measure will not be displayed if the evaluation time exceeds the measurement time.

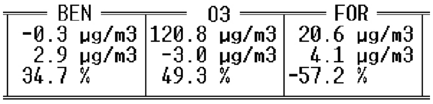
6.3 Concentration, deviation and light level

Each measurement of a gas gives not only the gas concentration, but also a deviation and a light level. The deviation is an indicator of the uncertainty of the measurement. The light level indicates the amount of light detected in the wavelength region used for evaluating the gas concentration. Hence, the light level will vary from gas to gas on the same path, depending on what wavelengths are used.

There is normally a strong relation between light level and deviation. If the light level goes down, the noise and thereby the measurement uncertainty increases, shown as an increase in deviation.

The deviation and the light levels are used for validation of the gas concentrations. See the section about data validation in section 7, The Installation Menu.

In addition to concentration, deviation and intensity of light, a number of indicators in the form of minus (-) signs are given for the interpretation of the measurement results.



```
═══ BEN ══════ 03 ═══════ FOR ═══
│ -0.3 µg/m3│120.8 µg/m3│ 20.6 µg/m3│
│  2.9 µg/m3│ -3.0 µg/m3│  4.1 µg/m3│
│ 34.7 %    │ 49.3 %    │-57.2 %    │
═════════════════════════════════
```

Figure 6.3. The minus signs.

- A concentration may be negative. In general, analysis allows for negative concentrations up to a value that is twice the value for the deviation. This is normal when the measured concentrations are very low, i.e. close to the detection limit of the analyser. Large negative concentrations indicate a serious error in analysis.
- A minus sign in front of the value for deviation indicates that the evaluation has not converged properly. The measurement value is uncertain or totally incorrect, but will still be stored. If negative values occur frequently a System check and/or a reference calibration should be performed.
- The function Data validation in the Station setup menu enables the definition of a maximum permissible deviation (see section 7, The Installation Menu). If this deviation limit is exceeded, the value obtained for light level is preceded by a minus (-) sign. However, the value is stored in the binary data file as usual.

Combinations of minus signs can of course also occur.

All measurement values are always stored and when presented in tabular form the minus signs are included.

The minus signs become important when calculating averages, when reformatting data to ascii files, and when using data collection software for data retrieval employing the Com-Vision protocol. In all cases all the negative deviation and light level values, and some of the negative concentration values will be sorted out when the integration time is set greater than zero. Negative concentrations with values up to twice the standard deviation are accepted.

Pressing the [Esc] key will interrupt the measurements and bring back the root menu. The measurements can be prevented from being interrupted with passwords.

The Installation Menu 7

The analyser must be configured before it can start measuring. The installation menu gives complete access to the configuration of the analyser. This includes definition of measurement paths and measurement times, communication, datalogger, calibration definitions, etc. The installation menu is also used to change the operation of the analyser.

The installation menu is accessed from the root menu by selecting [F1] Installation. The installation menu can be password protected.

7.1 The main installation menu

When the analyser is installed for measurements, all parameters defining the functions are entered in the different sub-menus to the Installation menu.

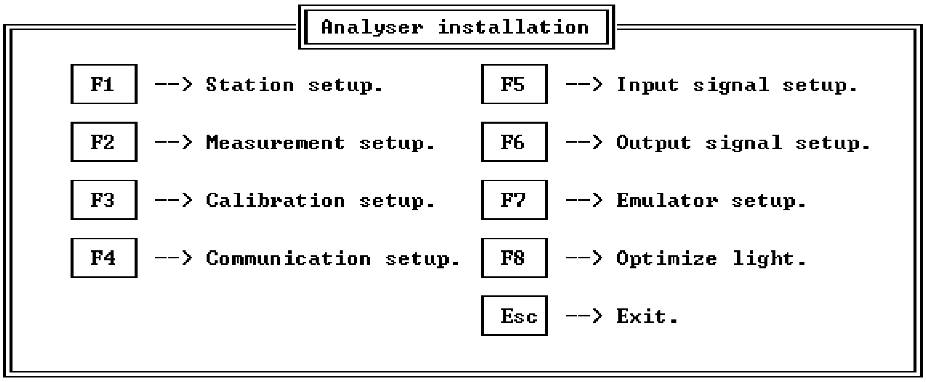


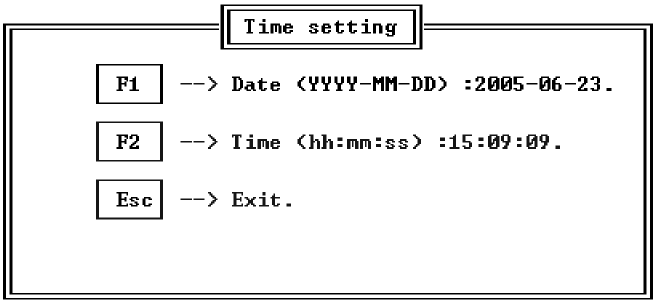
Figure 7.1. The installation menu.

- [F1] Station setup is used to set common system parameters such as station identifier, current date and time, and passwords.
- [F2] Measurement setup is used to define the measurement specifications, e.g. number of measurement paths and what pollutants to measure.
- [F3] Calibration setup is activated in order to define gas cylinders, calibration paths and calibration procedures.
- [F4] Communication setup is used to set parameters for the modem and for the direct serial communication.
- [F5] Input signal setup (option) activates external datalogger software (DL10, DL16, IO80 or IO256) and gives access to the installed logger menu.

- [F6] Output signal setup. The software IO80 and IO256 has to be installed to enable output of signals, e.g. analogue currents of 4-20 or digital status and alarm signals. [F6] gives access to a menu defining the outputs.
- [F7] Emulator setup. When the analyser is linked to an Odessa logger a DSM emulator is required to make the communication possible. The DSM emulator is installed via [F7] and is described in a separate manual. This option may also be used for other special purposes.
- [F8] Optimize light may in some cases be used in order to adjust the emitters and receivers to obtain maximum light intensity.

The above sub-menus are described in the following sections.

7.2 Station setup



```
Time setting

F1  --> Date (YYYY-MM-DD) :2005-06-23.
F2  --> Time (hh:mm:ss) :15:09:09.
Esc --> Exit.
```

Figure 7.2. The Station setup menu.

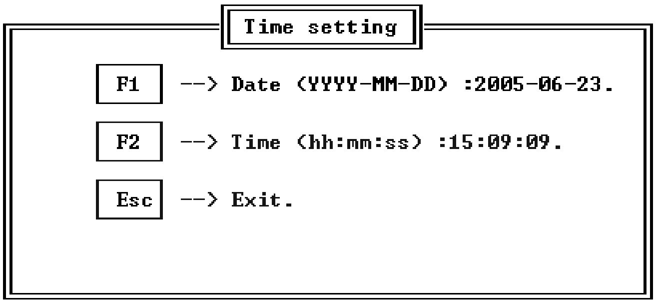
- [F1] Station name. The name must be 8 characters long, starting with an alphabetic character, and the fifth one must be a point, ".". The data are stored in month files in a packed binary format. The file name is the current year and month plus the station name. In the Data presentation menu the binary files can be converted to ascii format. It is strongly recommended that the station name is changed as soon as the monitoring configuration is changed. This gives a convenient way to separate between data obtained at different conditions, e.g. different number of monitoring paths or monitoring with and without temperature compensation.
- [F2] Location ID helps to identify the analyser when more than one is installed at a monitoring station. The ID is stored in the header of the binary file, and can be seen in the Data presentation menu.
- [F3] Date and time. Since all data generated by the analyser is marked with date and time, it is essential that the analyser clock is running correctly.
- [F4] Printer setup opens a menu where it is possible to specify and enable a printer connected to the analyser.

- [F5] Save screen can be either on or off. When the function is on, the screen is blanked about 15 minutes after the last key was pressed on the keyboard. Enabling this function protects the screen from burn-in damages.
- [F6] Password setup gives access to the definition of user names and passwords, and the access level given to each user name.
- [F7] Park is a useful function when servicing the instrument. The function disable the stepwise movement towards the measurement mode when the analyser is left in a menu other than the measurement mode.

The following sections describe the sub-menus accessed by selecting some of the above items.

7.2.1 Date and time

The analyser has a built-in real time clock which can be set by pressing [F3] Date and time at the Station setup menu. The real time clock is continuously updating the clock of the disk operating system so that the different clocks will be the same.



```
Time setting

F1  --> Date (YYYY-MM-DD) :2005-06-23.
F2  --> Time (hh:mm:ss) :15:09:09.
Esc --> Exit.
```

Figure 7.3. Menu for setting the analyser clock.

- The date is set by pressing [F1].
- The time is set by pressing [F2].

Press [Esc] to exit from the menu.

***Note**: All measurement results are stored with reference to time. It is therefore essential that the clock in the analyser is set correctly.*

***Note**: The analyser clock can be synchronised from a calling computer using the Opsis communication protocol.*

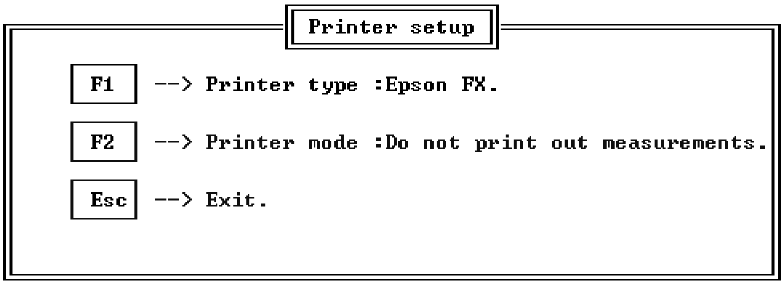
***Note**: The analyser clock may be adjusted for daylight saving time, but this may result in loss of data for the hour(s) when the clock is changed.*

7.2.2 Printer setup

A printer may be connected to the analyser using its parallel port.

__Note__: As for any other computer device, the power to the analyser must be switched off prior to connecting the printer.

Press [F4] in the Station setup menu to open the printer setup menu. Two parameters can be set for the printer.



```
Printer setup

F1  --> Printer type :Epson FX.

F2  --> Printer mode :Do not print out measurements.

Esc --> Exit.
```

Figure 7.4. The printer menu.

Press [F1] to select the appropriate printer. Five printer types are available:

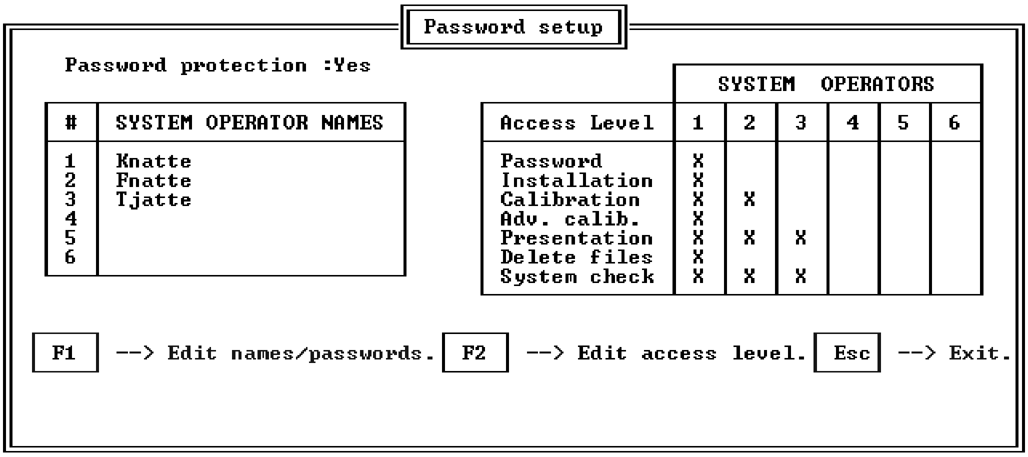
- Epson FX
- Epson JX
- Canon InkJet
- HP LaserJet, and
- HP PaintJet.

It is possible to have the result of every measurement printed as numerical values during the measurements. Press [F2] to change the printer mode. The mode can be either "Do not print out measurements" or "Print out each measurement" with obvious effect on the connected printer.

Normally, the analyser operates without any printer connected, and the printing of measurement results should then be disabled.

7.2.3 Password setup

The passwords protecting the analyser menus are set and edited by pressing [F6] in the Station setup menu.



Password setup

Password protection :Yes

#	SYSTEM OPERATOR NAMES
1	Knatte
2	Fnatte
3	Tjatte
4	
5	
6	

	SYSTEM	OPERATORS				
Access Level	1	2	3	4	5	6
Password	X					
Installation	X					
Calibration	X	X				
Adv. calib.	X					
Presentation	X	X	X			
Delete files	X					
System check	X	X	X			

F1 --> Edit names/passwords. F2 --> Edit access level. Esc --> Exit.

Figure 7.5. The password menu.

The installation of passwords is performed in two steps:

1. Establish which users (System operators) will be working with the analyser. Each system operator should be given a name and a password.
2. Define what parts of the analyser software (Access levels) each system operator should have access to.

By pressing [F1], the name and password for each system operator can be set. The password has to be written twice in order to avoid typing errors.

Typically, there is one password for the system manager, who has access to all menus in the analyser software, and one or more passwords for those who may perform a limited set of tasks at the analyser, e.g. calibration. The currently installed operator names are displayed in the left window of the menu.

The access levels are set by pressing [F2]. The following activities can be protected individually:

- Password setup: i.e. this menu. At least one operator must be given access to the password setup menu.
- Installation: the menu and sub-menus described in this section. An operator who has access to the password setup will automatically also have access to all other installation menus.
- Calibration: all menus and activities described in section 9.1, The main calibration menu.
- Advanced calibration menu: additional calibration and spectrometer performance test procedures documented in section 9.7, Advanced calibration menu. Those who have access to the advanced calibration menu automatically also have access to the standard calibration menu.
- Data presentation: the possibility to view measured data, as described in section 8, The Data Presentation Menu.

- Delete files: The sub-menu in the data presentation section enabling the removal of measurement data from the hard disk of the analyser. An operator who is able to delete files will automatically have access to all data presentation facilities.
- System check: test described in section 10, System Check, closely related to the hardware.

Press [Esc] to return to the Station setup menu.

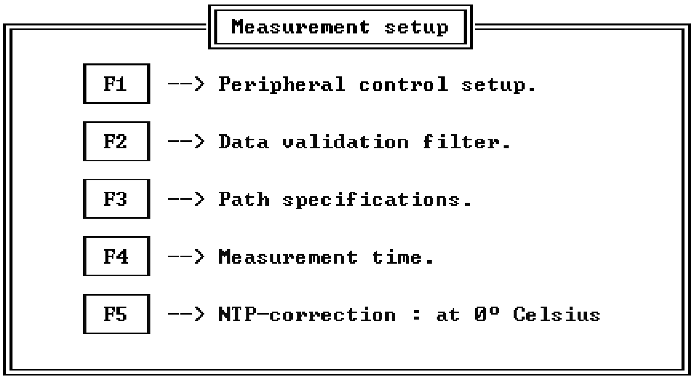
When Password protection in the upper left corner of the Password setup menu is set at "Yes", all settings in the menu are valid to provide password protection. Password protection is only activated if all defined users have both a name and a password.

The analyser prompts for an operator name and password when the user tries to reach the analyser root menu. This is possible in two situations. The first and most common one is when the measuring mode is interrupted, see section 6, Measurements. The second situation is during the start-up, before the analyser automatically starts measuring.

Once the password has been entered, access is given in accordance with the password setup menu. To avoid unauthorised use of the analyser, the user who entered the password should always force the analyser back into measuring mode before leaving the site.

7.3 Measurement setup

All information concerning how the measurements are performed is defined in the Measurement setup menu, available by pressing [F2] in the Installation menu.



Measurement setup

F1 --> Peripheral control setup.

F2 --> Data validation filter.

F3 --> Path specifications.

F4 --> Measurement time.

F5 --> NTP-correction : at 0° Celsius

Figure 7.6. The measurement setup menu.

- [F1] Peripheral control setup is used to define external devices associated with the measurements. These include multiplexer for selecting different measurement paths, movable filters for enhancing measurement performance, automatic light optimisers and automatic calibration units.
- [F2] Data validation filter defines rules for validation of measurement data. These rules can be applied when data is collected through the communication ports and when ascii files are created.

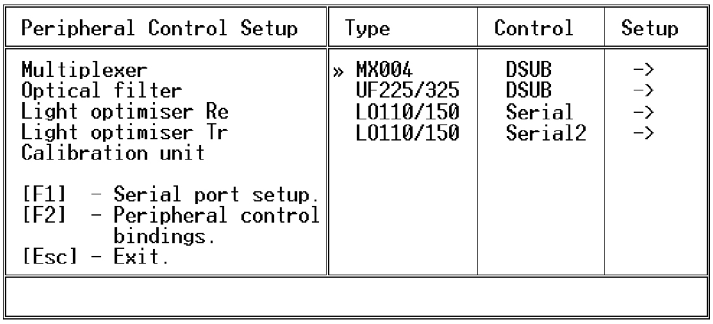
- **[F3] Path specifications** sets the number of measurement paths, and temperature, pressure and humidity corrections for each path.
- **[F4] Measurement time** gives access to a menu where the measurement time for each gas at each path may be set. The measure unit and the use of moveable filters for individual gases are also set in this menu.
- **[F5] NTP-correction** enables recalculation of gas concentrations to normalised conditions, i.e. 101.32 kPa and either 0 or 25 °C. When enabled, all gas monitoring data will be compensated for the temperature and the pressure before being stored on the hard disk. The actual temperature and pressure values are defined in the **Path specifications** menu. Also see section B, Correcting measurement results.

Press **[Esc]** to return to the **Installation** menu.

7.3.1 Peripheral control

The **Peripheral control** menu is used to configure external devices associated with the measurements or the measurement performance. These devices are

- Multiplexer, enabling measurements on two or more paths using a single analyser.
- Optical filters, enhancing measurement performance for some gases.
- Light optimiser, i.e. automatic alignment of the measurement paths.
- Calibration unit, i.e. valve control for calibration gases.



```
Peripheral Control Setup   Type         Control    Setup

Multiplexer              » MX004         DSUB       ->
Optical filter             UF225/325     DSUB       ->
Light optimiser Re         LO110/150     Serial     ->
Light optimiser Tr         LO110/150     Serial2    ->
Calibration unit

[F1]  - Serial port setup.
[F2]  - Peripheral control
        bindings.
[Esc] - Exit.
```

Figure 7.7. Peripheral control.

7.3.1.1 Multiplexers

A multiplexer is used to select one of two or more measurement paths for gas monitoring. The following models are available:

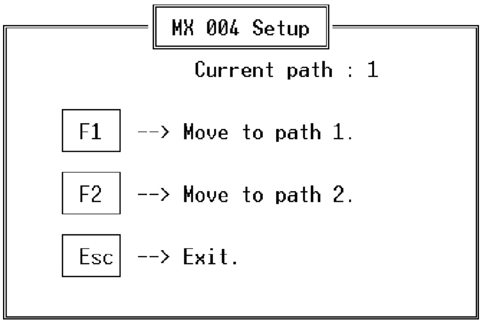
- MX004, for two monitoring paths
- MX012, for six monitoring paths
- MX024, for twelve monitoring paths, not in production anymore

- ER130, moveable transceiver unit, here treated as a multiplexer, since it operates on one of several paths at a time. Also the moveable receiver unit RE130 is installed as an ER130.

Use the up and down arrows to point at the multiplexer row, and press [Enter] to change the multiplexer Type. When the proper type is selected, go to the Setup column and press [Enter] for configuration of the selected multiplexer. Control is "DSUB" for all types, indicating the connection type between the analyser and the multiplexer. It cannot be changed.

MX004

When MX004 has been chosen, the following screen will be displayed:

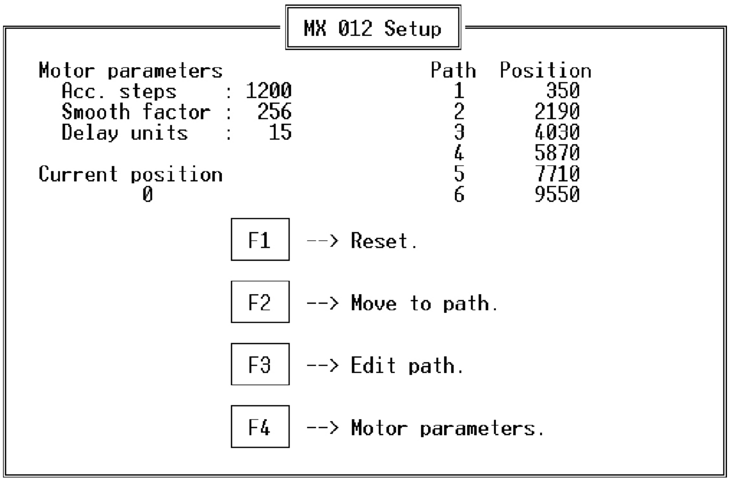


```
              MX 004 Setup
          Current path : 1

   F1   --> Move to path 1.

   F2   --> Move to path 2.

   Esc  --> Exit.
```

Figure 7.8. Installation menu for MX004.

Press [F1] and [F2] to test the functions of the MX004. If it is performing properly, return to the main installation menu by pressing [Esc]. Make sure that the physical path 1 is the one being installed as path 1 in the analyser set-up menus.

MX012 and MX024



```
                        MX 012 Setup
 Motor parameters                    Path  Position
   Acc. steps     : 1200               1       350
   Smooth factor :  256                2      2190
   Delay units   :   15                3      4030
                                       4      5870
 Current position                      5      7710
         0                             6      9550

                  F1  --> Reset.

                  F2  --> Move to path.

                  F3  --> Edit path.

                  F4  --> Motor parameters.
```

Figure 7.9. The menu for installing the MX012 multiplexer.

The menus for installing MX012 and MX024 are almost identical. The only difference is the number of paths.

A set of parameters are given on the inside of the cover of the multiplexer. These parameters refer to functions such as speed, distance between channels, etc. The values for these parameters must correspond to those defined in the menu.

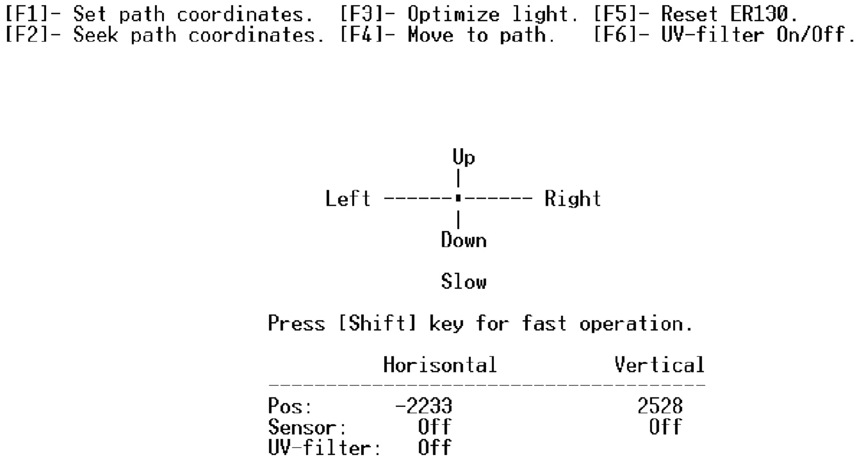
- Use [F3] to set the position parameter for each one of the 6 respective 10 paths.
- Use [F4] to set the motor parameters. They should not have to be changed from the default settings.

***Note**: Hardware failure may occur if any setting does not correspond to the text inside the cover.*

- Select [F1] Reset to test the multiplexer. The slide should then move to the start position, and the Current position value should be "0".
- Use [F2] Move to path to move to any of the installed paths. Current position should then change to the value given at Position for that path in the upper right corner of the menu.
- The accuracy may be tested for each channel by using the left and right arrow keys. The slide position is changed one step at a time for each key press. Using a light-meter LM010 the position for the maximum light transmission can be found. If necessary, the slide position can be adjusted by using the [F3] Edit path function.

ER130 and RE130

ER130 is a combined emitter and receiver, which automatically changes to the next measurement path and optimises the light. Please refer to the user's manual of ER130 for detailed instructions on handling and hardware installation. The RE130 receiver unit is basically an ER130 without the emitter optics, and it is identical to the ER130 in terms of software installation.



```
[F1]- Set path coordinates.  [F3]- Optimize light. [F5]- Reset ER130.
[F2]- Seek path coordinates. [F4]- Move to path.   [F6]- UV-filter On/Off.



                                 Up
                                 |
                   Left ------•------ Right
                                 |
                                Down

                                Slow

                      Press [Shift] key for fast operation.

                               Horisontal          Vertical
                      -------------------------------------
                      Pos:         -2233                2528
                      Sensor:        Off                 Off
                      UV-filter:     Off
```

Figure 7.10. The installation menu for the ER130.

The ER130 telescope is operated manually with the up/down and left/right arrow-keys. If [Shift] is pressed at the same time as one of the arrow keys, the operation is faster.

- [F1] is used when co-ordinates shall be defined or changed.
- [F2] is used when installing the ER130 on a path. The procedure is described below.
- [F3] is used when optimising the ER130 to a path. The telescope scans ± 20 steps horizontally and vertically in order to find the best light level within this area.
- [F4] moves the telescope to any pre-defined co-ordinates.
- [F5] resets the telescope so that both co-ordinates are set to zero.
- [F6] checks the function of the moveable UV-filter, if present.

At the bottom of the screen the current horizontal and the vertical co-ordinates are displayed. In case of power failure, the telescope has to be reset before it can find its way back to the monitoring paths.

The installation of a path is performed in the following way:

1. Turn off the control unit of the ER130. Use the handles to manually direct the telescope towards the retro-reflector. When a reflection from the retro-reflector is seen, turn on the control unit again.
2. Activate the function [F3] Optimize light. The ER130 will scan the area around the set direction for the best reflection. Check on the light level matrix, which is presented on the screen, that the reflection is properly captured. A substantial increase in light level should be detected between the first and the last steps. If not, repeat step 1.
3. Press [F2] Seek path coordinates. Enter the path number, and the ER130 will reset. The co-ordinates to the path will automatically be stored in the computer. The installation is finished.

When all paths are defined, the function of the ER130 may be checked by using [F4] Move to path. Exit from the installation menu by pressing [Esc].

***Note**: When the AR500 system is operated under the U.S. EPA Equivalency Method Designation the total cycle time must not exceed 200 seconds. Since the delay time between two measurement paths varies with the path configuration for the ER130, and is not the same as for an ordinary multiplexer, the cycle time which is indicated in the upper right corner in the Measurement Time menu may not be correct. As a final step in the installation it may therefore be necessary to check the total cycle time with a stop watch, and, whenever applicable, adjust the entered measurement times in order to not exceed 200 seconds for a full cycle when measuring.*

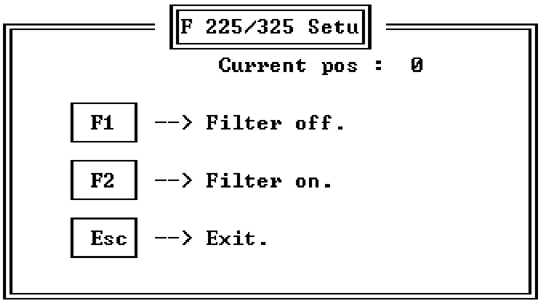
7.3.1.2 Optical filters

Moveable optical filters are used to enhance measurement performance on some gases. For instance, a UF225 filter is necessary when monitoring NO, and the UF325 filter improves measurements of some hydrocarbons. The UF425 filter combines the functions of the UF225 and UF325 filters. Physically, the moveable filters are located just in front of the fibre end in the light receiver.

Note: This menu only indicates the presence of filter(s). The actual use of an available filter must be enabled in the Measurement time menu.

UF225/UF325

The UF225 and the UF325 filters are mechanically and electrically identical, are therefore managed as the same type. The connection between the analyser and the filter device is made through the dSub connector extension at the rear, and Control is therefore always "DSUB". To verify the function of the filter, move to the Setup column and press [Enter]. This brings up the control menu for the selected filter type.



```
F 225/325 Setu
Current pos :  0

F1   --> Filter off.
F2   --> Filter on.
Esc  --> Exit.
```

Figure 7.11. Menu for testing the UF225/UF325 function.

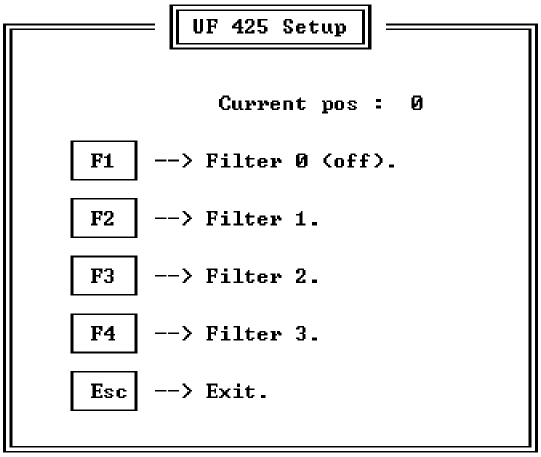
Use [F1] and [F2] to alter between filter and no filter. Press [Esc] to return to the main peripheral menu.

UF425

The UF425 filter manages up to four filter positions, of which at least one is empty and labelled "position 0". In practice, the filters are located on a wheel, which can be rotated by a stepper motor.

The connection between the analyser and the filter device is made through a serial port at the rear of the analyser, and Control is therefore always "Serial". Before the UF425 filter can be used, the [F1] Serial port setup and the [F2] Peripheral control bindings must be set up correctly. See section 7.3.1.5, Serial port setup and section 7.3.1.6, Peripheral control bindings below.

To verify the function of the filter, move to the Setup column and press [Enter]. This brings up the control menu for the selected filter type.



Current pos : 0

Figure 7.12. The menu for operating the UF425 filter.

Use [F1] through [F4] to alter between the four filter positions. Press [Esc] to return to the main peripheral menu.

7.3.1.3 Light optimisers

A light optimiser is used to automatically and regularly adjust the alignment of a measurement path. It is a convenient way to optimise the light intenisty on the path, specially if the foundation of the emitter/receiver is moving noticeably.

A light optimiser can be installed in a receiver or in an emitter. Both the emitter and the receiver on a single path can be equipped with light optimisers. Any number of paths connected to a single analyser through a multiplexer can be equipped with light optimisers.

A light optimiser is based on two stepper motors, one controlling the position of the lamp (emitter) or fibre post (receiver) in the x-direction, and one motor controlling it in the z-direction. A control algorithm, which parameters are set in the menu described below, makes sure to keep the lamp or the fibre post in the optimum position for as much light as possible to enter the analyser.

To install a light optimiser, first the operation mode must be selected or identified, then the hardware must be configured, and finally the control parameters must be set. This is described in the AQM System Installation & User´s Guide.

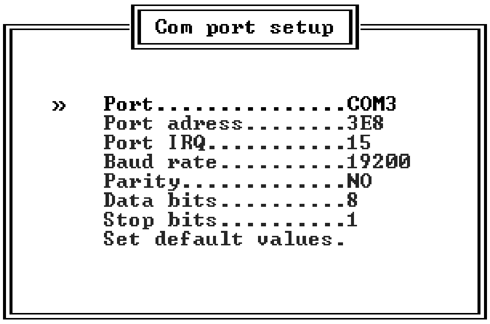
7.3.1.4 Calibration units

A calibration unit is used to control gas valves, letting calibration gas into calibration cells. It can be used either for manual control from the keyboard, or for automatic control during automatic calibrations of the analyser. In the current version of the analyser software, the basic definitions of the calibration unit is found in section 7.4, Calibration setup. The Calibration unit entry in this menu is not enabled.

Study section 7.4, Calibration setup and section 9, Calibration Procedures and the documentation of the CU004/007 calibration unit for more information.

7.3.1.5 Serial port setup

All peripheral units using Control of the type "Serial" or "Serial2" require configuration of the serial communication port. This is done by locating the cursor on a peripheral device using the serial port, and pressing [F1]. This opens a configuration menu according to figure 7.13. There is one menu for "Serial" and one menu for "Serial2", only differing in their settings.



```
Com port setup

»   Port...............COM3
    Port adress........3E8
    Port IRQ...........15
    Baud rate..........19200
    Parity.............NO
    Data bits..........8
    Stop bits..........1
    Set default values.
```

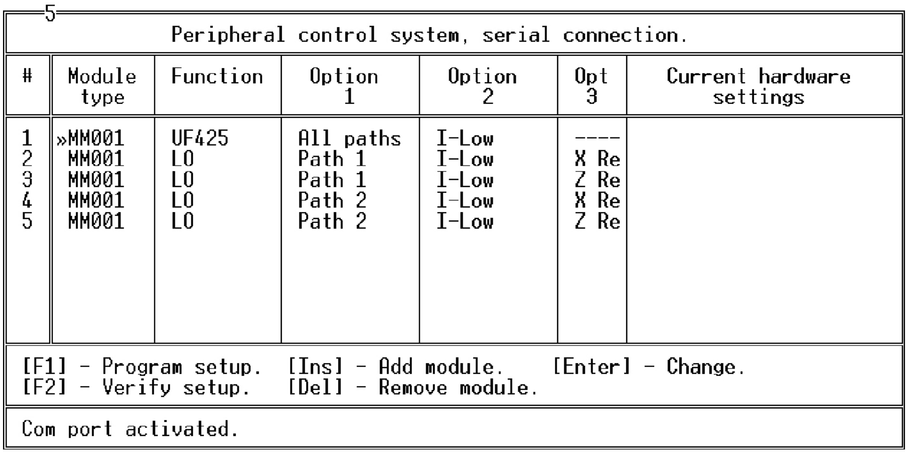
Figure 7.13. Defining the serial port for the peripheral device.

- Port defines the traditional label for the serial port.
- Port address sets the hardware address of the serial port. This address must correspond to the selected address of the serial card in use.
- Port IRQ sets the interrupt request number for the serial port. It must correspond to the hardware configuration. Please refer to the hardware documentation for proper address and IRQ settings.
- Baud rate is the transfer speed to the peripheral device. Normally, this is 19200 bps (bits per second).
- Parity should normally be "NO".
- Data bits should normally be "8".
- Stop bits should normally be "1".
- Use the "Set default values" function to set the standard Opsis parameters for the selected port (COMx).

Warning*: It is important that the port, address and IRQ number is selected correctly, and do not collide with other ports being used by the main analyser software or any other software (e.g. datalogger) in use in the analyser. The peripheral device will otherwise not work, and the function of the entire instrument may be jeopardised.*

7.3.1.6 Peripheral control bindings

Once the serial port has been defined, see the previous section, the hardware connected to the port should be defined. This is done by pressing [F2] in the peripheral control setup menu. There is one binding menu for the Control labelled "Serial", and one for the control "Serial2", if in use. Which menu is presented depends on the location of the cursor when the function key is pressed. Figure 7.14 shows the bindings menu.



```
5
            Peripheral control system, serial connection.

#   Module   Function   Option      Option    Opt   Current hardware
     type                 1           2        3        settings

1  »MM001    UF425      All paths   I-Low     ----
2   MM001    LO         Path 1      I-Low     X Re
3   MM001    LO         Path 1      I-Low     Z Re
4   MM001    LO         Path 2      I-Low     X Re
5   MM001    LO         Path 2      I-Low     Z Re

 [F1] - Program setup.  [Ins] - Add module.    [Enter] - Change.
 [F2] - Verify setup.   [Del] - Remove module.

 Com port activated.
```

Figure 7.14. The Peripheral control bindings menu. Here, one moveable filter, UF425, and two light optimisers, LO110/150, mounted on the receivers are in use.

The electronics for the UF425 and the LO110/150 are based on motor control modules MM001. The serial cable is connected to a communication unit CM001, which in its turn controls the MM001´s.

Press [Ins] to add a motor module to the list or [Del] to remove one. The total number of motor modules must correspond to the physically present modules connected to the CM001.

The following entries are available in the bindings menu:

- Module type is always "MM001".
- Function can be either "UF425", i.e. the moveable filter, or "LO", i.e. a motor for the light optimiser. A single optimiser has two motors, thus requiring two MM001s. The order in the list must correspond to the order of the MM001 modules counting from the CM001.
- Option 1 defines which paths the motor modules act on. The settings must correspond to the physical connections of the motors.
    - A UF425 can act on either a single path or on all paths. In the latter case, two or more UF425´s are connected in parallel to the same MM001, thus moving synchronously. This is possible since the analyser only measures on a single path at a time.
    - The light optimiser motor modules must be linked to a specific path.

- **Option 2** determines the current running through the motor. It can be of three different magnitudes, but should normally always be "I-Low", i.e. the lowest possible current.
- **Option 3** is only available for the light optimiser. This links each motor module to a specific location and orientation. "X Re" is the x-axis on a receiver, "Z Re" the z-axis on a receiver, "X Tr" the x-axis on an emitter and "Z Tr" the z-axis on an emitter. The setting must correspond to the physical connection of the motor modules for the light optimiser to work. Also note that the operation also depends on the **Configuration** in the **Light Optimise Setup** menu, see section 7.3.1.3, Light optimisers.

When all motor modules are defined properly, the corresponding physical devices must be programmed. This is done by pressing **[F1]**. Press **[F2]** to verify that the modules are programmed correctly. Programming codes are then shown in the **Current hardware settings** column.

7.3.2 Data validation filter

The analyser has filter functions for the gas measurements results. The filter conditions apply in two or possibly three cases:

- Presentation of data. See section 8, The Data Presentation Menu for more information. The filters are also applied when ascii files are generated as described in this chapter. The filter can be disabled by setting the integration time to zero, thereby requesting presentation of *all* data found in the data files.
- Transfer of data. The filters are applied when a calling software requests data with integration times above zero. With zero integration time, all data will be transferred, regardless of the filter limits.
- Output to IO80/IO256. The filter can be enabled to apply also when forwarding data to e.g. analogue outputs using Opsis I/O software.

Three parameters can define the filter for each measured gas:

- Deviation limit: As a stand-alone parameter, only measurement results with a deviation below the indicated one will be included in the averaging.
- Signal-to-noise limit: Adding a s/n filter limit will exclude data if the concentration is lower than the s/n limit times the deviation, adjusted for an offset at zero concentration equal to the deviation limit. Data is also excluded if the concentration is lower than minus the deviation limit. See figure 7.15.
- Light level limit: Data with light levels below the set limit will be excluded from the averaging.

Each filter parameter can be disabled by setting the corresponding limit to zero. However, a deviation limit is required to set a s/n limit.

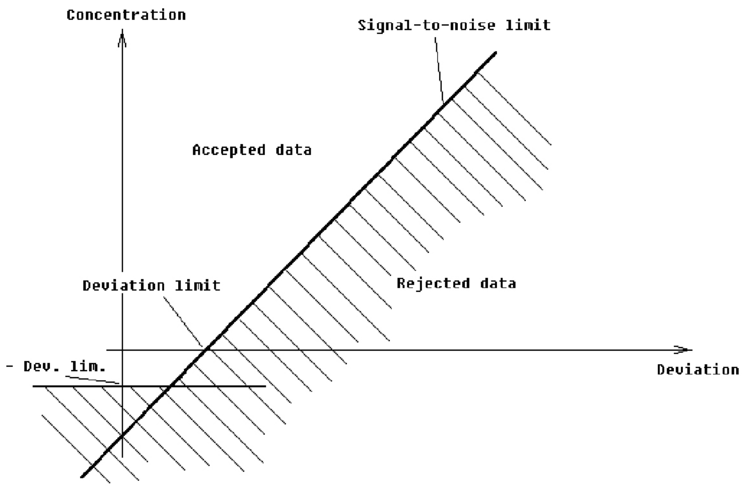
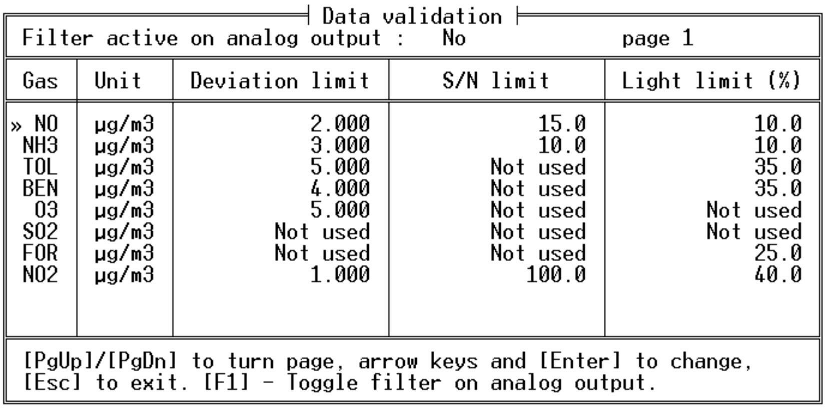


Figure 7.15. Illustration of the deviation and s/n filter rules.

Figure 7.16 shows the menu for setting the filter limits. It is accessed by selecting [F2] Data validation filter in the Measurement setup menu.



```
                     Data validation
 Filter active on analog output :   No            page 1

 Gas   Unit     Deviation limit       S/N limit       Light limit (%)

» NO   µg/m3              2.000            15.0              10.0
  NH3  µg/m3              3.000            10.0              10.0
  TOL  µg/m3              5.000        Not used              35.0
  BEN  µg/m3              4.000        Not used              35.0
   O3  µg/m3              5.000        Not used          Not used
  SO2  µg/m3           Not used        Not used          Not used
  FOR  µg/m3           Not used        Not used              25.0
  NO2  µg/m3              1.000           100.0              40.0

 [PgUp]/[PgDn] to turn page, arrow keys and [Enter] to change,
 [Esc] to exit. [F1] - Toggle filter on analog output.
```

Figure 7.16. The data validation menu.

The gases are found on different pages. Each page holds ten gases. Change page by pressing the [PgUp] or [PgDn] key. Use the up and down arrow keys to move to a specific gas on the page, and press [Enter] to change the filter limits. Press [Esc] to return to the previous menu.

The values should be entered in the displayed units, which are selected in the Measurement time menu. By entering zero as the filter value, the particular filter is disabled and the numerical value is replaced by the text "Not used".

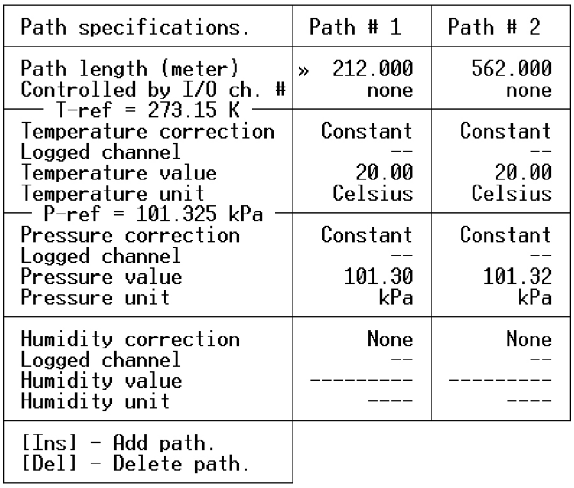
All measurement data is stored on the hard disk of the analyser, also if the filter condition excludes the value from averages. However, to indicate the failed filter conditions, the light level of the failed measurement is marked with a minus sign. This minus sign is shown when studying data which has been requested with zero integration time.

Pressing [F1] toggles between having the filter applied when forwarding data to outputs or not. If enabled, only concentrations passing the filter will forwarded. The current status is shown at "Filter active on analog output".

__Note__: It is generally better to leave the filters disabled in the analyser, and instead do the filtering in presentation software like Opsis EnviMan ComVisioner. Data should be transferred using zero integration time, guaranteeing the calling computer to get a mirror image of the data found on the hard disk of the analyser. The filter function is mainly present for backwards compatibility.

7.3.3 Path specifications

In order to define the measurement path or paths, [F3] Path specifications should be selected in the Measurement setup menu. If more than one path will be used, a multiplexer must first be installed. The installation of multiplexers is described in section 7.3.1, Peripheral control.



```
Path specifications.        Path # 1    Path # 2

Path length (meter)      »  212.000     562.000
Controlled by I/O ch. #        none        none
─── T-ref = 273.15 K ───
Temperature correction     Constant    Constant
Logged channel                   --          --
Temperature value             20.00       20.00
Temperature unit            Celsius     Celsius
── P-ref = 101.325 kPa ──
Pressure correction        Constant    Constant
Logged channel                   --          --
Pressure value               101.30      101.32
Pressure unit                   kPa         kPa

Humidity correction            None        None
Logged channel                   --          --
Humidity value            ---------   ---------
Humidity unit                  ----        ----

[Ins] - Add path.
[Del] - Delete path.
```

Figure 7.17. Path specifications menu with two paths defined.

Up to 10 paths can be defined, numbered from 1 to 10.

- A new path is added by pressing the [Ins] key. The new path will always be placed last among the already defined paths.
- A path is removed by pressing the [Del] key. It is always the last path which will be removed.

The cursor is moved with the arrow keys. When more than four paths are defined the paths outside the display are indicated with double arrows. The display is rolling when the left and right arrow keys are used.

Path length and control

- At Path length, the length is entered. The unit is metres, with up to 6 decimals. All decimals are used in the calculations, although not all are displayed.
- The measurement at a specific path may be switched on and off from outside through a datalogger input. The datalogger channel number is specified at Controlled by I/O ch. #. Measurement is allowed if the analyser finds a digital high value in the specified channel. The function is disabled by entering 0 as the channel number, giving the text "none" in the menu.

7.3.3.1 Correction of data

Compensation can be performed with respect to three parameters; temperature, pressure and humidity (water vapour). The gas concentration and deviation will be corrected to the temperature set in the Measurement setup menu, and to the pressure 101.325 kPa (1 atm.).

Temperature correction

Temperature correction can be performed based either on a "Constant" or a "Logged" value.

- "Constant" can be used when the temperature is expected to be fairly constant. A Temperature value should be entered.
- "Logged" means that a dynamic correction is used, based on temperature readings provided by a datalogger. The datalogger channel number for the temperature should be entered at Logged channel. The current reading is shown at Temperature value.

The Temperature unit is either Celsius (°C), Fahrenheit (°F) or Kelvin (K).

Pressure correction

Pressure correction is in the same way either Constant or Logged.

- When set to "Constant" a Pressure value has to be entered.
- When set to "Logged", a dynamic correction is used based on pressure readings provided by a datalogger. The Logged channel number has to be specified. The current reading is presented at Pressure value.

The Pressure unit is either Pa, hPa, kPa or inches mercury (in.Hg).

When no temperature or pressure correction should be done, the temperature respective the pressure should be set Constant with the temperature value 0 °C (32 °F) and pressure value 101.325 kPa, i.e. the reference values at NTP correction to 0 °C.

Humidity correction

Humidity correction is used to provide the measured concentrations on a dry basis, instead of on a wet basis, which is standard.

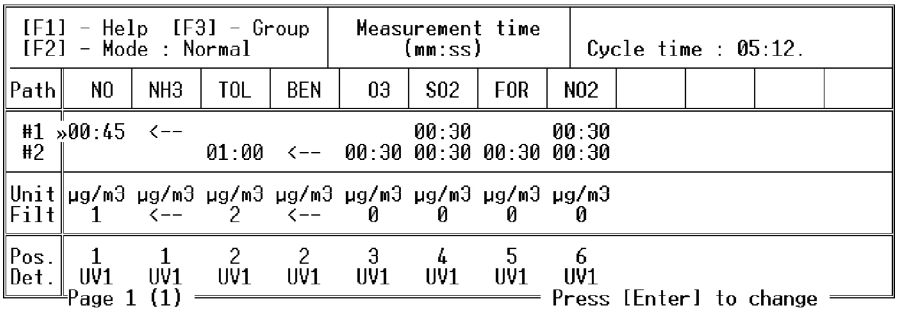
- When the correction is "None", the concentrations are presented as weight per wet cubic metres, i.e. the humidity correction is not in use.
- "Constant" humidity correction is used if the water vapour level is constant and well-known. The level is entered at Humidity value. The unit may be either % or g/m^3.
- A "Logged" humidity correction grabs a measured water vapour level from the logger input area. The logger channel number representing the water vapour is entered at Logged channel. As for the constant correction, the unit can be either % or g/m^3.

When the water vapour concentration is provided by the gas analyser itself, the measured value must first be directed to an output channel of the IO80/IO256 interface and then looped back internally in the IO80/IO256 software to a channel in the input area.

For obvious reasons, the measurement result for water vapour cannot be corrected for water vapour.

7.3.4 Measurement time

The measurement parameters for each gas and each path have to be defined before the measurements can start. The menu is displayed when [F4] Measurement time is selected in the Measurement setup menu.



```
[F1] - Help  [F3] - Group   Measurement time
[F2] - Mode : Normal              (mm:ss)         Cycle time : 05:12.
Path   NO    NH3    TOL    BEN    O3     SO2    FOR    NO2
 #1 »00:45   <--                        00:30         00:30
 #2                 01:00   <--   00:30  00:30  00:30  00:30
Unit µg/m3  µg/m3  µg/m3  µg/m3  µg/m3  µg/m3  µg/m3  µg/m3
Filt   1     <--     2     <--     0      0      0      0
Pos.   1      1      2      2      3      4      5      6
Det.  UV1    UV1    UV1    UV1    UV1    UV1    UV1    UV1
     Page 1 (1)                        Press [Enter] to change
```

Figure 7.18. The Measurement time menu.

The menu can display up to 12 gases. If the number of gases exceeds 12, the [PgUp] or [PgDn] keys should be used to turn pages. The cursor is moved with the arrow keys.

The Measurement time menu gives important information on how the analyser performs the measurements.

Gases

The gases are displayed in the same order as they are normally measured by the analyser. However, the measurement and presentation order can be modified as described below, using the [F2] and [F3] function keys.

- At the line Pos, the grating position for the measurement of each gas is shown as a number from 1 and upwards. The same number for two or more components means that they are being monitored in parallel, as is the case with NO and NH_3, and with TOL and BEN in the above figure.
- At the line Det., the detector type for a specific gas is shown. A standard AR500 analyser is provided with only one UV detector ('UV1'), whilst an AR620 can be equipped with a 'UV1' and an 'IR1' detector.
- The gases measured at the same grating position and with the same detector may be divided into groups. Each group specifies the evaluation procedure for the gases in the group. The same spectrum can therefore be evaluated in different ways for different gases. The groups are indicated by the lack of delimiters between the gas names. For instance, TOL and PXY are often evaluated simultaneously, while BEN will be evaluated on its own, even if the measured spectrum (the grating position) is the same for all three gases.

Measurement times

Measurement times are set individually for each monitoring path.

- Move the cursor to the selected gas and path and press [Enter]. The time is written in the format "MM:SS", M means minutes and S seconds.
- Measurement times are only set for each grating position. For the gases measured in parallel only the time for the first gas has to be set. The times for the other gases will be indicated by arrows.
- By entering the measurement time 0 (zero), the measurement and/or evaluation of the gas is disabled.
- The total cycle time is displayed in the upper right corner of the menu.

Unit

The Unit for the gas can be selected individually for each gas. The results are also corrected to the reference temperature T_0 and reference pressure P_0.

- Use [Enter] to turn to the appropriate unit.
- Possible units are the absolute units ng/m^3, $\mu g/m^3$, mg/m^3 and g/m^3, and the volume-ratio units ppt, ppb, ppm and %.
- The selected unit affects all menus in the software, i.e. the measurement mode, the data presentation menu, the calibration menu, etc.
- Independent of the selected unit the results are always stored on the hard disk memory in the unit $\mu g/m^3_n$.

The pollution concentrations are measured in the absolute unit µg/m^3. Corrections are automatically made with respect to the temperature T_0 and the pressure P_0 prior to data storage and presentation, providing that the function is enabled, see section 7.3. Section B, Correcting measurement results includes a detailed discussion concerning temperature and pressure corrections as well as conversions into different units.

Filters

As discussed in the peripheral control section , filters are required when measuring some gases. A filter is activated for an individual gas by setting the appropriate filter number at the line "Filt". "Filter 0" means no filter in front of the fibre end in the receiver. "Filter 1" means filter in position for UF225/325, and the first filter in position for UF425. "Filter 2" and "Filter 3" are the second and third filters on a UF425, and can only be used in combination with this filter unit. The setting is valid for all gases measured at the corresponding grating position.

Help screen

Press [F1] to display a help screen for the Measurement time settings.

Measurement mode

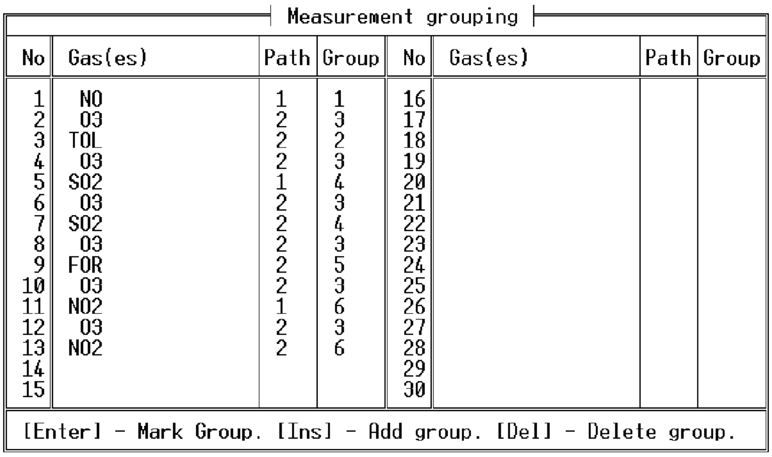
Press [F2] to change the measurement mode.

- "Normal" means that the gas concentrations are calculated and shown immediately after the spectral acquisition has finished for the individual gas (group, actually).
- "Concurrent" is used to calculate and show data for all gases at the same time, after the complete measurement cycle for all gases on all paths is ready. This mode may be preferred in some situtations.

"Normal" is the preferred operation mode.

Measurement grouping

Pressing [F3] opens a sub-menu where the order of gas measurements can be modified. A typical use is to measure one gas and/or path often, and the other gases and/or paths less frequent, for instance for regulatory reasons.



```
                       Measurement grouping
No  Gas(es)            Path Group  No  Gas(es)            Path Group
 1   NO                 1    1     16
 2   O3                 2    3     17
 3  TOL                 2    2     18
 4   O3                 2    3     19
 5  SO2                 1    4     20
 6   O3                 2    3     21
 7  SO2                 2    4     22
 8   O3                 2    3     23
 9  FOR                 2    5     24
10   O3                 2    3     25
11  NO2                 1    6     26
12   O3                 2    3     27
13  NO2                 2    6     28
14                                 29
15                                 30
 [Enter] - Mark Group. [Ins] - Add group. [Del] - Delete group.
```

Figure 7.19. Changing group sequence.

When entering the menu for the first time, the group order is the same as the enabled gases set in the main Measurement time menu. It is now possible to select a group by putting the cursor in front of it, and pressing [Enter].

The selected group can now be copied and inserted in other positions among the groups. This is done by moving the cursor to the group which the gas is to be inserted before, followed by pressing the [Ins] key.

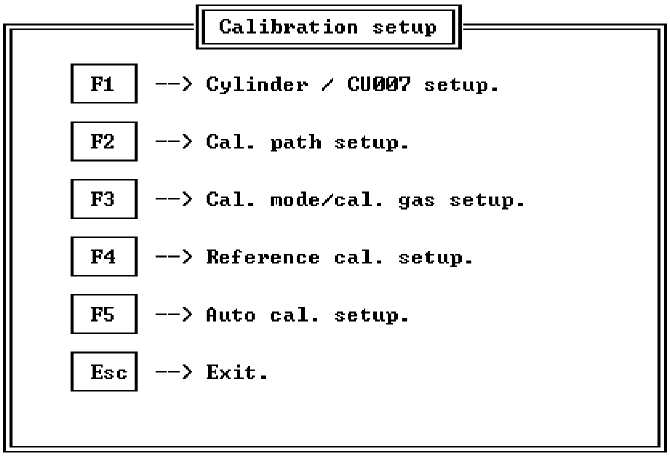
A copied group can be removed by moving the cursor to it and pressing the [Del] key. It is not possible to remove any of the original groups. To remove a gas from the list completely, set the measurement time to zero in the main Measurement time menu.

In figure 7.19, the group holding O3 on path 2 has been copied and inserted in every second position. Every second measurement result produced by the analyser is therefore ozone on path two. The ozone concentration is therefore updated frequently, while the other gases are measured "inbetween".

***Note**: It is only groups that can be added or modified in this menu. If two or more gases are measured in the same group, all those gases will be modified in the same way.*

7.4 Calibration setup

The information required for enabling calibration is entered in the Calibration setup menu, available by pressing [F3] in the Installation menu.



```
Calibration setup

F1  --> Cylinder / CU007 setup.

F2  --> Cal. path setup.

F3  --> Cal. mode/cal. gas setup.

F4  --> Reference cal. setup.

F5  --> Auto cal. setup.

Esc --> Exit.
```

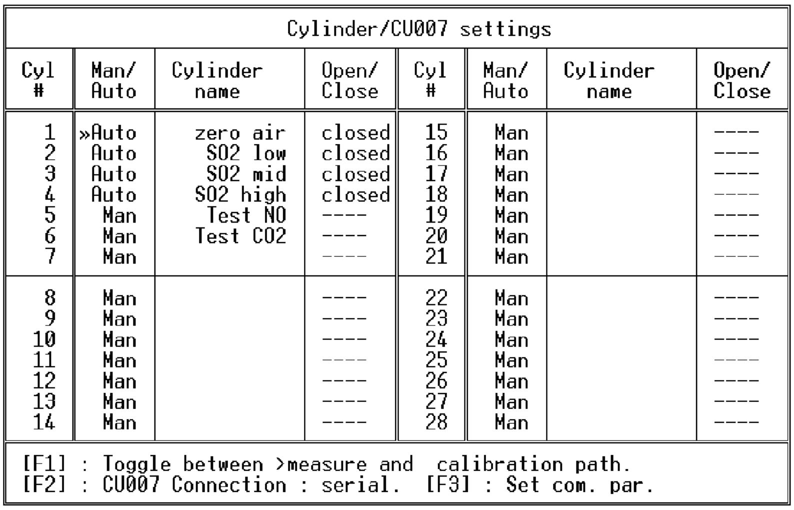
Figure 7.20. Calibration setup menu.

The configuration of calibrations is performed in the following steps:

1. The gas cylinders which are used when calibrating the analyser are defined by selecting [F1] Cylinder/CU007 setup.
2. The calibration paths have to be defined. This is done in the menu opened with [F2] Cal. path setup.
3. By selecting [F3] Cal. mode/cal. gas setup, calibrations based on measurements of known gas concentrations can be defined. The result of these calibrations are span and offset factors which may be used to correct the measurement results produced by the analyser.
4. Selecting [F4] Reference cal. setup, a menu opens where the procedures for recording reference spectra are set.
5. Finally, each of the defined calibration procedures can be activated from outside by trig signals, or by the analyser itself at times separated by fixed intervals. These possibilities can be set up when selecting [F5] Auto cal. setup.

7.4.1 Gas cylinders/CU004/CU007

In the menu [F1] Cylinder/CU007 setup in the Calibration setup menu, the different gas cylinders to be used in the calibrations are defined. The menu is used both for manual management of gas cylinders and for automatic handling using the CU004 or CU007 calibration units. The seven-valve CU007 is mentioned in the text below, but it may just as well be a CU004, managing four valves.



```
                          Cylinder/CU007 settings
 Cyl | Man/ | Cylinder  | Open/ | Cyl | Man/ | Cylinder  | Open/
  #  | Auto |   name    | Close |  #  | Auto |   name    | Close

   1 |»Auto |  zero air |closed |  15 |  Man |           |  ----
   2 | Auto |   SO2 low |closed |  16 |  Man |           |  ----
   3 | Auto |   SO2 mid |closed |  17 |  Man |           |  ----
   4 | Auto |  SO2 high |closed |  18 |  Man |           |  ----
   5 |  Man |   Test NO | ----  |  19 |  Man |           |  ----
   6 |  Man |  Test CO2 | ----  |  20 |  Man |           |  ----
   7 |  Man |           | ----  |  21 |  Man |           |  ----

   8 |  Man |           | ----  |  22 |  Man |           |  ----
   9 |  Man |           | ----  |  23 |  Man |           |  ----
  10 |  Man |           | ----  |  24 |  Man |           |  ----
  11 |  Man |           | ----  |  25 |  Man |           |  ----
  12 |  Man |           | ----  |  26 |  Man |           |  ----
  13 |  Man |           | ----  |  27 |  Man |           |  ----
  14 |  Man |           | ----  |  28 |  Man |           |  ----

 [F1] : Toggle between >measure and  calibration path.
 [F2] : CU007 Connection : serial.  [F3] : Set com. par.
```

Figure 7.21. The menu for setting up the gas cylinders.

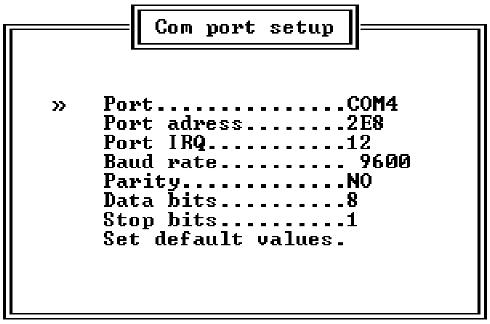
- Up to 28 gas cylinders can be defined. The gas cylinders are labelled with numbers from 1 to 28. Each gas cylinder should always be given a name, in the Cylinder name field. The name should be unique and describe the gas cylinder so that it easily can be identified. The names will be used during the calibrations initiated in the calibration menu, see section 9, Calibration Procedures.
- At least one of the defined gas cylinders should be a zero-air cylinder. It is recommended that the zero-air cylinder is placed as cylinder no. 1. If there actually *is* a gas cylinder containing zero-air (or N_2) or if it is just a connection to clean purge air does not matter.
- When one or more CU007 auto-calibration units is used, the gas cylinders may be defined to be opened by this unit. Since a CU007 has seven separate valves, the gas cylinders are identified in groups of seven. Cylinders 1 to 7 belong to CU unit no. 1, cylinders 8 to 14 to no. 2, etc.
- The field Man/Auto controls if the valve is opened by the CU, or if the user should be prompted to connect the gas cylinder during calibration. If the field says "Auto", the control is given to the auto-calibration unit.
- The function of a CU004 or CU007 can be tested by moving the cursor to the field Open/Close, and pressing [Enter]. The selected valve should then open. Pressing [Enter] one more time closes the valve.

Two or three function keys are available in the menu:

- [F1] can be used to switch between measurement path(s) and calibration paths(s), providing that the emitter/receiver hardware is equipped with this kind of mechanics, and that a CU004/007 is in use. The switching is made either by moving the fibre end in the receiver by a motor (ER070 and ER080), or by flipping a mirror (ER060/062). The bracket indicates the current status of the switch signal.
- [F2] is used to select the connection method to the CU007. Elder CU007 are controlled using a special digital card in the analyser. The CU007 connection should

then be "digital". CU004 and new CU007 use a serial port for controlling the valves. Connection should then be "serial".

- If a serial connection is used for the CU004/007, the port must be configured using the [F3] option. The menu for the port configuration is identical to the peripheral control ports. See section 7.3.1.5, Serial port setup for more information.



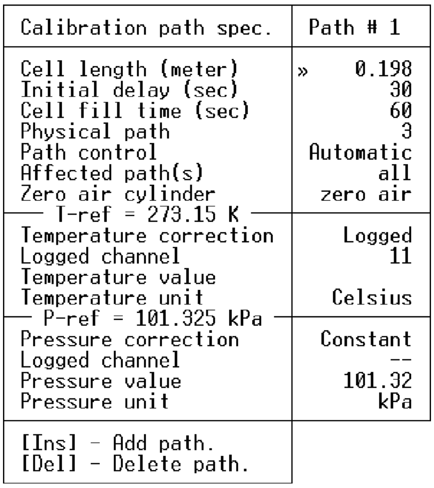
```
Com port setup

»   Port...............COM4
    Port adress........2E8
    Port IRQ...........12
    Baud rate.......... 9600
    Parity.............NO
    Data bits..........8
    Stop bits..........1
    Set default values.
```

Figure 7.22. Serial port setup for the calibration unit.

***Warning**: Make sure not to select a serial port used for other purposes. Improper use of the serial port may result in instrument malfunction.*

7.4.2 Calibration paths

The calibration path information is entered when selecting [F2] Cal. path setup in the Calibration setup menu.



```
Calibration path spec.      Path # 1

Cell length (meter)       »     0.198
Initial delay (sec)                30
Cell fill time (sec)               60
Physical path                       3
Path control                Automatic
Affected path(s)                  all
Zero air cylinder            zero air
── T-ref = 273.15 K ──
Temperature correction         Logged
Logged channel                     11
Temperature value
Temperature unit              Celsius
── P-ref = 101.325 kPa ──
Pressure correction          Constant
Logged channel                     --
Pressure value                 101.32
Pressure unit                     kPa

[Ins] - Add path.
[Del] - Delete path.
```

Figure 7.23. The calibration path setup.

The definition of calibration paths is similar with the ones for the measurement paths, with a few exceptions.

Usually, one calibration path is sufficient for performing all necessary calibrations. There are however situations where different path lengths are required. Legislation may also require more than one calibration path. For these purposes up to six calibration paths can be defined. Four of them are visible on the screen simultaneously.

The calibration paths are labelled with numbers from 1 and upwards. A new calibration path is inserted when the [Ins] key is pressed. The new path is always added last among the other paths. By pressing [Del], the last calibration path is removed.

The cursor is moved around in the fields by using the arrow keys. If there are more calibration paths than those shown on the screen, double arrows to the left or to the right of the path numbers are shown. By trying to move the cursor outside of the visible paths, the temporarily hidden paths will be shown.

Path specifications

- The length of each calibration path is entered in metres at Cell length. Up to 6 decimals can be used, even though not all of them are shown on the screen.
- Initial delay is used in dual systems, where two different Opsis analysers, usually an AR600 and an AR650, share the same path. When one instrument decides to start a calibration sequence, the other must be stopped. This is done by transferring a calibration status signal from the first instrument to the second instrument's path control input (section 7.3.3, Path specifications). However, it may take a while for the second instrument to stop its measurements. For this reason, an initial delay can be set in the first instrument, allowing the second wan to terminate gracefully before switching to a calibration path and/or starting to fill a calibration cell with gas. The delay is entered in the unit seconds.
- Cell fill time defines the time between when a gas cylinder is connected to the calibration cell and when the analyser starts measuring the concentration. It should be given in seconds. The time depends on the available flow from the gas cylinder and the size of the cell. The time should always be adjusted so that the concentration has time to stabilise before the analyser starts measuring.
- Physical path defines the position of the multiplexer (if any) during the calibrations. If an ER070 or an ER080 is used for calibration, the physical path should be the same as the measuring path for the emitter/receiver. In those cases, the analyser will automatically switch to the calibration path inside the ER070/080 units. Using a stand-alone calibration path connected to a multiplexer input, the separate input number should be given. Possible values are 1 to 10.
- When the operator wants to manually connect the calibration path to the analyser Path control should be "Manual". The user will be asked to connect the fibre prior to the calibration. The multiplexer will still move to the path defined at Physical path. If Path control is "Automatic", the user will *not* be prompted to connect the fibre, even if the calibration is initiated manually.
- New span and offset factors are produced as a result of gas calibrations. If desired (see below) the new factors can automatically replace the old ones, thus enabling a self-calibrating analyser. The analyser holds one set of span and offset factors for

each *measurement* path. At Affected path(s), it is defined for what measurement path(s) the span and offset factors should be adjusted.

  - Using one single calibration path, the affected paths should be "All".
  - Using ER070/080, the result of the calibration should only affect the factors of physical measurement path for which the unit is defined. Affected path should therefore normally be the same as the path number at Physical path.
  - At the moment, there is no obvious situation where the physical path should differ from the affected path, unless the latter is "All".

- At Zero air cylinder, the name of the cylinder providing zero air for the calibration path should be defined. There are two situations during calibration where the analyser has to know how to connect zero air to the calibration cell.
  - The first is after finishing a gas calibration. If the last gas cylinder during the calibration is not the zero gas cylinder, the analyser will automatically flush the cell with the gas from the Zero air cylinder. In this way reactive gases will always be washed out of the calibration cell, preventing corrosion.
  - The second situation is during reference calibrations, where it is critical that the calibration cell does not contain any traces of calibration gases, but just pure zero air.

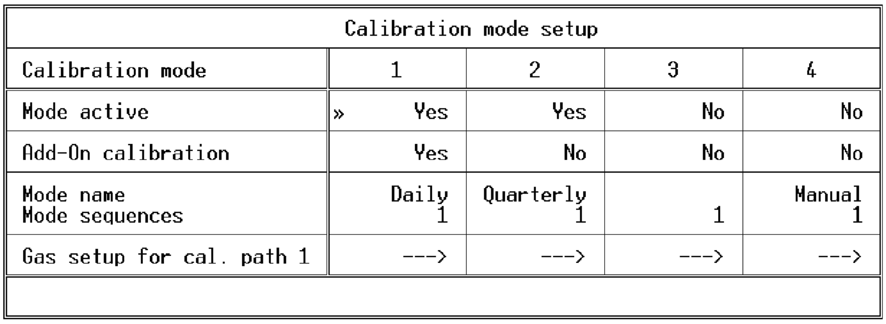
Correction of data

The path should be set up with a Temperature correction and a Pressure correction, in order to obtain the measurement results at standardised temperature (0 or 25 °C and pressure (101.32 kPa) The possibilities and procedures for doing this are identical to those for the measurement paths. A description is found in section 7.3.3, Path specifications. See also section B, Correcting measurement results.

Press [Esc] to leave the menu.

7.4.3 Calibration modes/calibration gases

When gas cylinders and calibration paths have been defined the calibration procedures can be entered. When selecting [F3] Cal. mode/cal. gas setup, the gas calibrations can be defined.



Calibration mode setup				
Calibration mode	1	2	3	4
Mode active	» Yes	Yes	No	No
Add-On calibration	Yes	No	No	No
Mode name	Daily	Quarterly		Manual
Mode sequences	1	1	1	1
Gas setup for cal. path 1	--->	--->	--->	--->

Figure 7.24. Calibration mode setup.

Gas calibrations are performed in different *modes*. A mode defines a specific calibration procedure, including which gases to calibrate and which gas cylinders to use. More than one calibration path can be defined, and each mode covers them all. When starting a gas calibration, the calibration mode has first to be selected. Up to four modes can be defined.

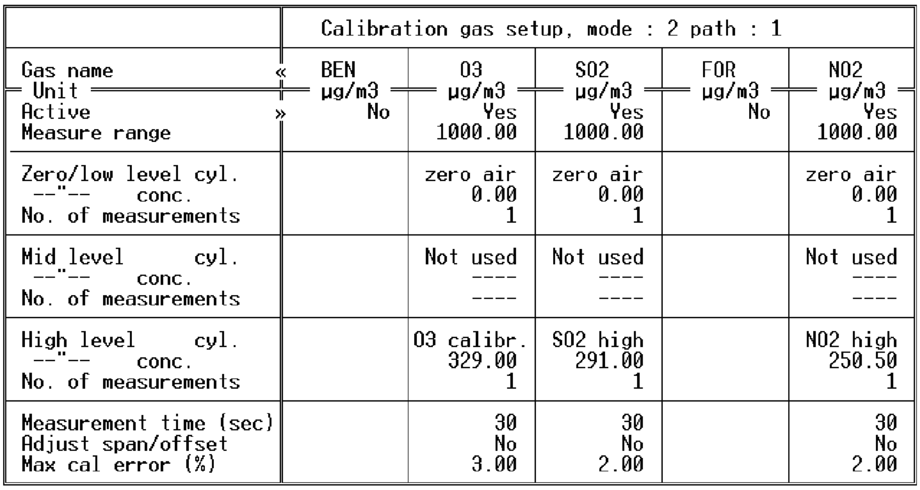
Thanks to the modes, sets of different calibration sequences can be defined. In figure 7.24 there is one mode describing how a daily calibration is performed, one mode for a quarterly calibration with specifications other than the daily calibrations, and finally one mode for manual calibrations which may be changed from time to time depending on occasional needs and requirements.

The cursor in the menu is moved with the arrow keys.

- Mode active indicates whether the mode is active. Move the cursor to the selected mode and press [Enter] to change between the two states "Yes" and "No".
- Add-on calibration can be active or not. This is an important setting and influences the entire performance of the calibration. In an add-on calibration, a known concentration is measured on top of an unknown, but measurable background level. In a normal calibration, there is no background, and absolute concentrations can be measured. The description below first discusses the latter case, and necessary modifications for the add-on case are introduced at the end of the text.
- Each mode must have a unique name. The name should describe the purpose of the calibration mode, since the name is used when selecting which calibration to perform. The name is entered by moving the cursor to the fields next to Mode name and pressing [Enter].
- Legislation may require that the entire calibration procedure is repeated a number of times. At Mode sequences, the number of repetitions is defined.
- Gas setup for... gives access to a menu described below, where the details of the calibration of each gas at the selected calibration path are defined. The appearance of the menu depends on whether add-on calibrations are chosen or not.

Press [Esc] to leave this menu.

The procedure for calibrating a specific gas can be set up individually for each calibration mode and each calibration path. By moving the cursor to one of the arrows in the calibration mode setup menu, and pressing [Enter], the following menu is displayed:



```
                          Calibration gas setup, mode : 2 path : 1

Gas name                « BEN        O3         SO2        FOR        NO2
Unit                      µg/m3      µg/m3      µg/m3      µg/m3      µg/m3
Active                  »      No       Yes        Yes         No        Yes
Measure range                       1000.00    1000.00               1000.00

Zero/low level cyl.                 zero air   zero air              zero air
  --"--     conc.                      0.00       0.00                  0.00
No. of measurements                       1          1                     1

Mid level      cyl.                 Not used   Not used              Not used
  --"--     conc.                       ----       ----                  ----
No. of measurements                     ----       ----                  ----

High level     cyl.                 O3 calibr. SO2 high              NO2 high
  --"--     conc.                    329.00     291.00                250.50
No. of measurements                       1          1                     1

Measurement time (sec)                   30         30                    30
Adjust span/offset                       No         No                    No
Max cal error (%)                      3.00       2.00                  2.00
```

Figure 7.25. The gas calibration setup. The content of this menu is specific for each calibration mode and for each calibration path.

The menu has one column for each gas. The cursor is moved to different fields using the arrow keys. A field is edited by pressing [Enter]. Five gases are presented at a time. When the analyser is calibrated for more than five gases, this is indicated by double arrows to the right or to the left of the gas names. Use the left and right arrow keys to move the window.

- The calibration of each gas can be switched on or off by pressing [Enter] in the fields to the right of Active. If calibration is active, the field says "Yes", otherwise "No". Once a gas is activated, the calibration procedure for this gas can be set up. A number of reference concentrations are defined further down. The unit for the concentrations is the same as has been selected in the measurement setup, see section 7.3.4, Measurement time.
- When evaluating the result of a gas calibration, a measurement range may be required as a reference. Since the analyser does not have a measurement range in the conventional meaning, it has to be defined in the menu. This is done at Measure range. The range does not affect the measurements. The value is often specified by legislation, e.g. depending on the highest expected concentrations.

Normal span/offset calibration

- Each gas, for each calibration mode and each calibration path, can be calibrated with three different concentrations. These concentrations are called Zero/low level, Mid level and High level. Each level is characterised by its gas cylinder and the concentration of the specific gas in the gas cylinder.
  - The cyl. name defines which cylinder will be used during the calibration at the specific level. When the calibration at this level is disabled the field will show the text "Not used".

  - If the level is used, the concentration of the selected gas in the specified gas cylinder should be given at conc.
  - The number of measurements is defined at No. of measurements. If more than one measurement is performed, the calibration result is the mean value of the results at that level.
- At Measurement time, the time for each measurement at each level is specified. The time should be given in units of seconds. More than one measurement may be performed at each level, see above.
- Finally, we can let the analyser evaluate the result of the calibration measurements, and adjust the corresponding span and offset factors automatically. The automatic adjustment is switched on or off at Adjust span/offset. If the corresponding field says "Yes", the adjustments are allowed. The details of the corrections are described in section 9, Calibration Procedures.
- In order to prevent errors due to wrong gas concentrations in the cylinders or hardware failures, there is a maximum permitted calibration error to be defined. Here is where the measure range and the concentrations in the gas cylinders comes in. The calibration error *CE* is calculated as

$$CE = \frac{C_m - C_c}{r} \cdot 100\,\% \qquad (7.1)$$

  C_m = measured concentration, C_c = cylinder concentration, r = measurement range

  If the calibration error exceeds the value defined at Max cal error, the calibration has failed, and no adjustments on the span and offset factors will be performed based on the measurement.

Add-on calibration

***Note**: Add-on calibrations are primarily intended for ambient air quality monitoring. The function is currently only available in the UV-DOAS analysers, i.e. the AR500 and AR600 series.*

An add-on calibration is based on a known gas concentration filling a cell present in the ordinary measurement path. As a result, the analyser should report a step-like increase of the background gas concentration. To compensate for the background concentration, zero air is used to fill the cell before and after the calibration gas, and background measurements are made before and after the measurement of the ‘step’ concentration. See figure 7.26.

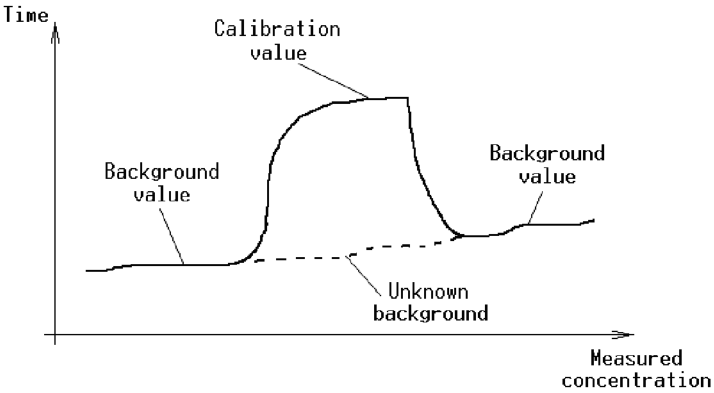


Figure 7.26. Add-on calibration.

The calibration result is the measured calibration error, subtracted by the average of the background values before and after the calibration. By using the average, we make a reasonable assumption of the unknown gas concentration in the background during the time the cell is filled with calibration as and the analyser reports an increased concentration.

The calibration error, *CE*, is calculated as

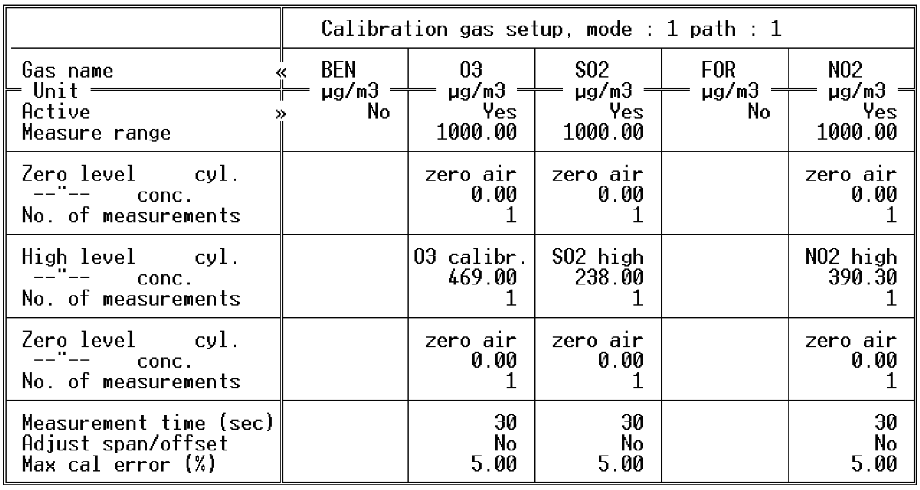
$$step = C_m - \frac{b_1 - b_2}{2} \tag{7.2}$$

C_m = measured concentration, b_1 = background value 1, b_2 = background value 2

$$CE = \frac{step - C_c}{r} \cdot 100\ \% \tag{7.3}$$

C_c = cylinder concentration, r = measurement range

When enabling add-on calibration (see figure 7.24), the gas setup menu changes slightly to look as shown in figure 7.27.



	Calibration gas setup, mode : 1 path : 1				
Gas name «	BEN	O3	SO2	FOR	NO2
Unit	µg/m3	µg/m3	µg/m3	µg/m3	µg/m3
Active »	No	Yes	Yes	No	Yes
Measure range		1000.00	1000.00		1000.00
Zero level cyl.		zero air	zero air		zero air
--"-- conc.		0.00	0.00		0.00
No. of measurements		1	1		1
High level cyl.		O3 calibr.	SO2 high		NO2 high
--"-- conc.		469.00	238.00		390.30
No. of measurements		1	1		1
Zero level cyl.		zero air	zero air		zero air
--"-- conc.		0.00	0.00		0.00
No. of measurements		1	1		1
Measurement time (sec)		30	30		30
Adjust span/offset		No	No		No
Max cal error (%)		5.00	5.00		5.00

Figure 7.27. The gas calibration setup menu when add-on calibrations are enabled.

- Each gas, for each calibration mode and each calibration path, is calibrated in three steps. First, a background measurement is made, when the calibration cell in the ordinary measurement path is filled with zero air. This corresponds to the first Zero level. Then the measurement is made on the known calibration gas, specified as High level. Finally, the second background measurement is made, corresponding to the second Zero level entry. All three levels must be specified for the add-on calibration to be complete.
  - Select the cylinder to the corresponding cylinder name from the cylinder configuration menu.
  - Set the concentration of the zero levels to 0, and the concentration of the high level to the expected step increase in gas concentration, taking cylinder concentrations and path and cell lengths into account. Normally, the two zero levels use the same zero air gas cylinder.
  - Set No. of measurements to the requested number. If more than one measurement is performed, the calibration result is the mean value of the results at that level.
- Measurement time specifies the time spent on each measurement.
- The span factor (only, not the offset) can be adjusted automatically as a result of the add-on calibration. This is enabled by setting Adjust span/offset to "Yes." To prevent calibration errors, a maximum allowed calibration error (*CE*, as specified above) can be set at Max cal error. If the calibration error exceeds this limit, no span adjustment is made.

Order of measurements

The measurement order in a calibration mode is not necessarily the same as the order of the gases in the menu. Instead, the procedure is optimised to preserve calibration gas. For instance, the zero air gas cylinder is normally used for the zero (background) level for all gases. To avoid unnecessary flush time, all zero levels for all gases are measured at the same time, requiring only a single flush time delay. In the same way, ‘mixed’ gas bottles may be used for more than one gas to reduce the number of required gas cylinders and the total calibration time.

The order of the gas cylinders in the cylinder setup (see section 7.4.1, Gas cylinders/ CU004/CU007) determines the calibration sequence. The software starts with the gas cylinder with the highest number, and continues backwards to the first cylinder, which normally is the zero gas cylinder. In this way, the calibration cells are flushed with zero air at the same time as the zero (background) measurements are made.

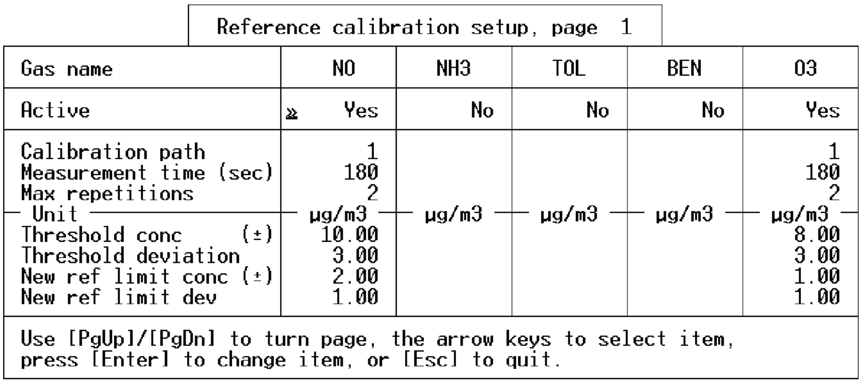
> ***Hint**: In some add-on cases, calibrating several gases, the time between the initial and final background measurements can become unacceptably long. The calibration can then be divided in two or more modes.*

Press [Esc] to return to the previous menu.

7.4.4 Reference calibration

> ***Note**: Reference calibration is not used on all gases. Particularly, IR-DOAS instruments (AR550, AR650) do normally not require reference calibrations.*

Reference calibration means checking and recording the reference spectrum for each wavelength region the analyser uses when measuring. The setup is accessed by selecting [F4] Reference cal. setup in the Calibration setup menu.



```
                  Reference calibration setup, page  1
Gas name                  NO      NH3      TOL      BEN       O3
Active                  »  Yes       No       No       No      Yes
Calibration path            1                                    1
Measurement time (sec)    180                                  180
Max repetitions             2                                    2
 Unit                   µg/m3    µg/m3    µg/m3    µg/m3    µg/m3
Threshold conc     (±)  10.00                                 8.00
Threshold deviation      3.00                                 3.00
New ref limit conc (±)   2.00                                 1.00
New ref limit dev        1.00                                 1.00
Use [PgUp]/[PgDn] to turn page, the arrow keys to select item,
press [Enter] to change item, or [Esc] to quit.
```

Figure 7.28. The menu for setting up reference calibrations.

Use the arrow keys to move the cursor between the menu fields. Press [Enter] to edit the content of the field the cursor is positioned at. The menu is divided into pages. Each page holds information about reference calibration of five gases. If the analyser is calibrated for more than five gases, press [PgUp] or [PgDn] to turn pages.

- Reference calibration can be defined for each measurement group. The calibration is turned on and off in the Active fields. If the field says "Yes", reference calibration is enabled for this group. An arrow in the field marks that the enabling of calibration is done at another gas in the group.

Some gases in the are sometimes evaluated without the presence of a reference spectrum. Reference calibration can therefore not be made for these gases. In that case, the Active field is marked "undef".

- There is only one lamp spectrum for each gas, even if the gas is measured at several paths. At Calibration path, the path used for registering the lamp spectrum is specified. Any of the defined calibration paths could be used. Since there should be no difference between the lamp spectra in the calibration paths, the same path could be used for all gases, even if there are more than one calibration paths available.

The reference calibration starts by filling the calibration path with gas from the zero air cylinder. A measurement is then performed for the specific gas or gases in the group. The measurement result is compared with allowed levels, and suitable actions are taken based on the result of the comparison.

- Measurement time defines for how long the test measurement of the gas should last. The value should be given in seconds.
- At Max repetitions, the maximum number of attempts to read a new reference spectrum is entered. This is a precaution taken in order to prevent the analyser from not being able to exit the reference calibration procedure during an automatic calibration.

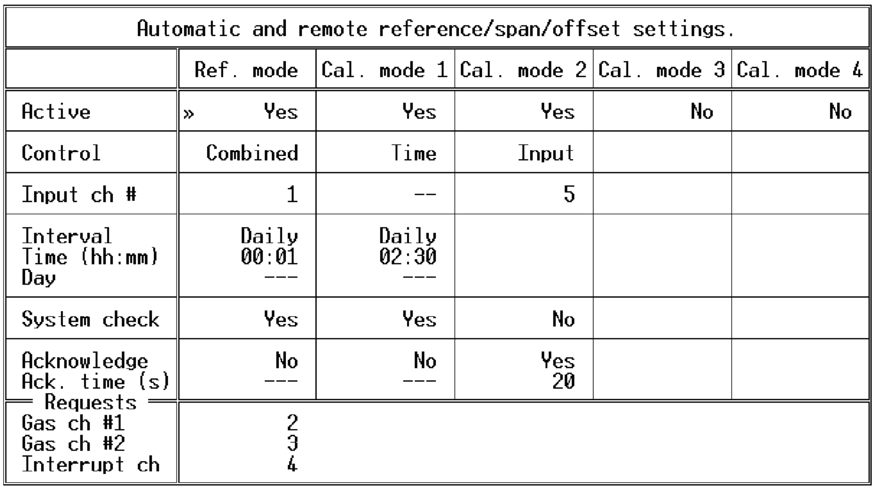
  The Max repetitions parameter should be set to

  - 0 (zero) if reference calibrations are performed manually.
  - 1 (one) or higher if the reference calibration is started automatically.

  See section 9, Calibration Procedures for more information.
- The measured concentration(s) and deviation(s) are first of all compared with the levels at Threshold conc and Threshold deviation. If the absolute value of the measured concentration exceeds the threshold concentration, or the measured deviation exceeds the threshold deviation, the measurement has failed, and the reference calibration of the gas is terminated. In this way, the analyser is prevented from registering a reference spectrum which is not valid. This can happen for instance when the zero air in the calibration cell is contaminated.
- If the measured results pass the threshold tests, they are compared with New ref limit conc and New ref limit dev. If the absolute value of the measured concentration is below the new reference limit concentration, and the measured deviation is below the new reference limit deviation, the existing reference spectrum is considered to be in order, and a new spectrum will therefore not be registered. This terminates the calibration of the gases in the current group.
- If the measurement results is between the Threshold and the New reference limit values the spectrum is registered as a new reference. If a new reference is not accepted within the Max repetitions times, the original spectrum is restored and the calibration of the gases in the group is terminated. During manual reference calibration, the user can force a new spectrum into the analyser regardless of the obtained measurement results.

7.4.5 Automatic calibrations

Gas calibration modes and reference calibrations can be started either from the menus (section 9, Calibration Procedures) or automatically. The latter case is either controlled by a timer inside the analyser or from outside through a digital input channel. The menu accessed by selecting [F5] Auto cal. setup in the Calibration setup menu defines the automatic calibrations. Automatic calibrations are only available if an CU004/007 autocalibration unit is connected to the analyser.



Automatic and remote reference/span/offset settings.

	Ref. mode	Cal. mode 1	Cal. mode 2	Cal. mode 3	Cal. mode 4
Active	» Yes	Yes	Yes	No	No
Control	Combined	Time	Input		
Input ch #	1	--	5		
Interval Time (hh:mm) Day	Daily 00:01 ---	Daily 02:30 ---			
System check	Yes	Yes	No		
Acknowledge Ack. time (s)	No ---	No ---	Yes 20		
Requests Gas ch #1 Gas ch #2 Interrupt ch	 2 3 4				

Figure 7.29. Auto calibration setup menu.

The reference calibration procedure and the gas calibration modes have their own column in the menu. As before, the arrow keys move the cursor in the menu, and a field is edited by pressing [Enter].

- Active is either "Yes" or "No", and sets whether the mode is tested for automatic initialisation.
- Control can be "Time", "Input" or "Combined".
    - If control is "Input", Input ch # defines which logger channel controls the calibration mode. Any datalogger channel could be used. Note that the datalogger software has to be set up to transfer the calibration signal from outside the analyser to the input interface.
    - If control is "Time", Interval tells how often the calibration is started. Possible intervals are "Daily", "Weekly" and "Monthly", with obvious meanings. The time of day for the calibrations should always be given at Time, expressed in hour and minute with a colon in between. A weekly calibration requires the Day to be set to one of the weekdays. A monthly calibration requires Day to be set to a date in the month.
    - "Combined" allows calibration control from both "Input" and "Time".
- The start of a calibration may be preceded by a system check, see section 10, System Check. This is selected at System check. The system check is enabled if "Yes" has been selected. The result of the system check can be monitored as an output.

- The analyser may acknowledge that a specific calibration procedure (mode) is finished. The acknowledge is turned on and off at Acknowledge. The signalling is performed by the output software IO80 or IO256.
- When acknowledge is activated, the duration of the acknowledge being sent out is set in units of seconds at Ack. time.
- Requests are defined when the calibration procedure shall be started via an external serial signal using, for instance, the Cactus protocol. Two start signals can be set, and the input channel numbers have to be entered. A request signal contains a five digit number:

Digit No.	Meaning	Result
1	Calibration mode (1 - 4)	Starts the calibration for the specified mode with all gases that are active in that mode. Mode1 = 1, mode 2 = 2, etc.
2	Path (0 - 9)	All paths = 0, path 1 = 1, path 2 = 2, etc.
3, 4	Gas number (0 - 99)	The gases are numbered in the order they are presented in the menu. For a typical CEM system NO = 01, SO_2 = 02, NO_2 = 03. All gases = 00.
5	Level (0 - 3)	All levels = 0, Low level = 1, mid level = 2, high level = 3.

Since there are two independent request channels available it is possible to activate, for instance, the calibration of NO and NO_2 individually, one gas in each channel. Examples of request signals for a CEM system are:

Ch. 1	Ch. 2	Results
11020	00000	Mode 1, path 1, gas SO_2, all levels
12033	00000	Mode 1, path 2, gas NO_2, high level
10000	00000	Mode 1, all paths, all gases, all levels
20010	20020	Mode 2, all paths, gases NO and NO_2, all levels

The request signal must be sent to the analyser only once. The analyser should be running as a slave and the DAS should thus be the master.

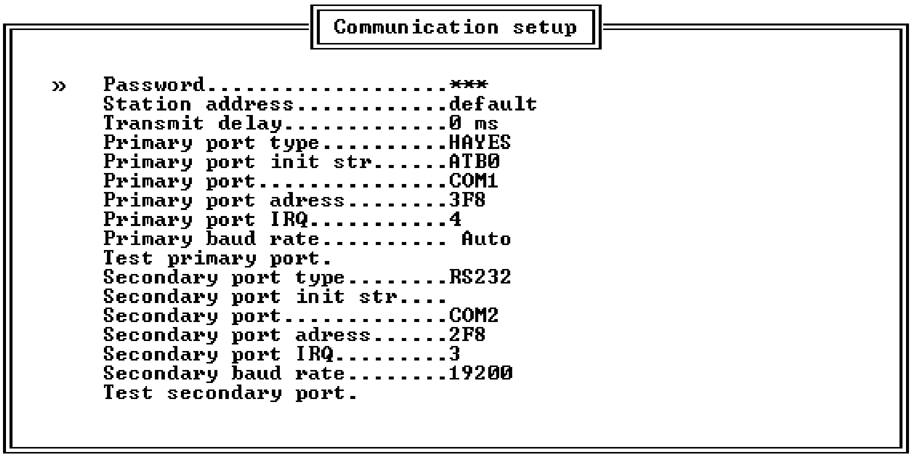
In case the calibration procedure has to be interrupted the channel number for an interrupting signal can be defined at Interrupt ch. When the interrupt signal is set at the value 1.0 the ongoing calibration will be terminated as soon as possible, i.e. when the cells are flushed with zero air, etc.

7.5 Communication setup

The analyser is normally equipped with a modem for transmission of data by telephone. The modem is Hayes-compatible, which enables telecommunication according to the following standards: Bell 103/212A in the US and CCITT V.21 and V.22 in Europe. The modem is asynchronous and operates at standard modem speeds. It is also possible to use a second communication port for direct transfer of data to another computer through a permanently connected (leased) line.

The communication is based on the Opsis ComVision/ComView protocol, see further section A, The ComView protocol

Press **[F4] Communication setup** at the **Installation** menu to access the communication configuration menu.



```
                       Communication setup

 »   Password...................***
     Station address............default
     Transmit delay.............0 ms
     Primary port type..........HAYES
     Primary port init str......ATB0
     Primary port...............COM1
     Primary port adress........3F8
     Primary port IRQ...........4
     Primary baud rate.......... Auto
     Test primary port.
     Secondary port type........RS232
     Secondary port init str....
     Secondary port.............COM2
     Secondary port adress......2F8
     Secondary port IRQ.........3
     Secondary baud rate........19200
     Test secondary port.
```

Figure 7.30. Menu for the settings of the communication parameters.

To change the settings for these parameters, use the arrow-keys to highlight and press **[Enter]**.

- Each analyser may be protected by a **Password** used during communication, which prevents unauthorised access to the analyser through the telephone line. The corresponding password must then be defined in the software of the calling computer.
- The **Station address** is used in certain situations where several analysers share the same serial line to a calling computer. The station address is a number between 0 and 9, and the corresponding value must be set in the software of the calling computer. **Default** value is "0".
- The **Transmit delay** forces the specified delay between receiving a request from a calling computer, and transmitting the answer. The delay may be necessary when radio equipment is used somewhere along the communication line, and there is a delay time in this equipment when switching between receiving and transmitting data. Examples of such equipment are radio modems and some types of cellular (mobile) phones. The transmit delay parameter may also be useful when making overseas calls, where satellite communication introduce delays along the line. A corresponding delay should usually also be specified in the calling computer.
- In most cases, the transmit delay should be set to zero. However, if a lot of communication errors occur, it may be worthwhile trying to set a certain delay time, especially if radio equipment is known to be involved in the communication hardware. Try setting the delay to 30 ms on both sides, and check if the errors disappear. If not, increase the delay in steps of 30, until an improvement is noticed.
- The delay should normally not exceed 100 ms, since the net data transfer speed then becomes noticeable lower than optimum. Check the communication equipment if a higher delay is required, and see if it is possible to enable some "quick reply" mode.

- There is a primary and a secondary serial port. Port is either of "COM1" through "COM4". In some versions of the analyser software, the corresponding port address and interrupt request number can be explicitly set. The usage of the ports vary from one analyser to the other, depending on which other serial communication based devices are in use.

***Warning**: Make sure not to use serial ports reserved for other purposes. Failure to do so may result in malfunction of the analyser. Please refer to the system documentation for listings of available serial ports.*

- Port type should be "Hayes" for a port connected to a Hayes compatible modem, and "RS232" otherwise. Setting the type to "Hayes" forces the analyser to send certain modem initialisation codes when the analyser is started or when leaving the communication configuration menu.
- Port init string is additional information required by the modem for initialisation. The string should follow the Hayes AT standard. A common string is "ATB0".
    - "AT" is the attention code. It clears the buffer and informs the modem of the baud rate, data format and parity. Any command or command line must be preceded by AT.
    - "B0" switches the modem to CCITT V21, V22 protocol, the European standard.
    - "B1" switches the modem to Bell 103/212A protocol, the American standard.

  Note that the protocol should be the same for both the dialling and the answering computer.

    - "Sr=n" changes the register r to the value n. The following registers can typically be changed:
    - "S0" ring to answer on, i.e. the number of rings to go through until the modem answers. Range: 0 - 255, default value is "0".
    - "S10" carrier lost time. An increased value will decrease the sensitivity for short drop-outs, e.g. when the lines are bad or when a mobile telephone is used. Range: (1 - 255) * 0.1 seconds, default value is "60". The value should normally not be changed.

  Example: "ATB0S0=1". "ATB0" is the setting for Hayes, European standard. "S0=1" means that the modem will answer after the first signal.

***Note**: Other initialisation codes may be in use depending on modem types and line conditions. Refer to the modem documentation for more information.*

- Port address and Port IRQ are to be set according to the hardware specifications. Normally, "COM1" and "COM2" uses fixed addresses and IRQs, but the settings for "COM3" and "COM4" may vary. Always refer to the system documentation for specifications. The address and IRQ may not be adjustable in some versions of the analyser software.

Warning*: Do not change the address or IRQ settings unless you know what you are doing. Setting these parameters wrong may result in malfunction of the analyser. Please refer to the system documentation.*

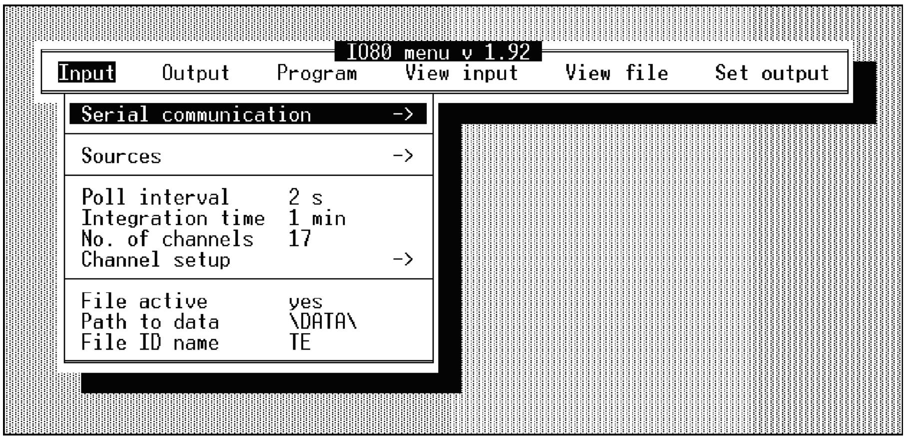
- Baud rate sets the transmission speed and should correspond to the settings in the calling computer.

  When the baud rate is set at "Auto" the modem will set the baud rate in accordance with the dialling modem. However, the analyser modem then must be capable of at least 9600 bits per second and the data compression and error correction of the modem must be disabled, since those functions are handled by the software. The initialisation codes of the Opsis modems are factory set to disable data compression and error correction. Please refer to the modem manual for information.
- Test port is used to check the response from the device connected to the port. Any character typed on the keyboard will be sent out on the serial port. Any received character will be shown on the screen. Press [Esc] to exit the test mode.

7.6 Input signal setup

In many applications there is a datalogger connected to the analyser. There are four different models available: DL010, DL016, IO80 and IO256. A datalogger consists of hardware for reading the data and software for the calculations of mean values and the data storage. The datalogger software must interact with the analyser software in order to store data permanently. The analyser software may also use results from the datalogger e.g. for temperature compensations.

The correct datalogger type must be installed in the analyser software. Select [F5] Input signal setup in the Installation menu and answer [Y] (yes) or [N] (no) to the questions until the correct datalogger type turns up. Once the datalogger is installed, the menu for setting up the datalogger can be accessed. The description of the datalogger menus are found in the respective manual for the dataloggers.



```
Poll interval     2 s
Integration time  1 min
No. of channels   17

File active       yes
Path to data      \DATA\
File ID name      TE
```

Figure 7.31. The menu for setting up the inputs in an IO80 datalogger.

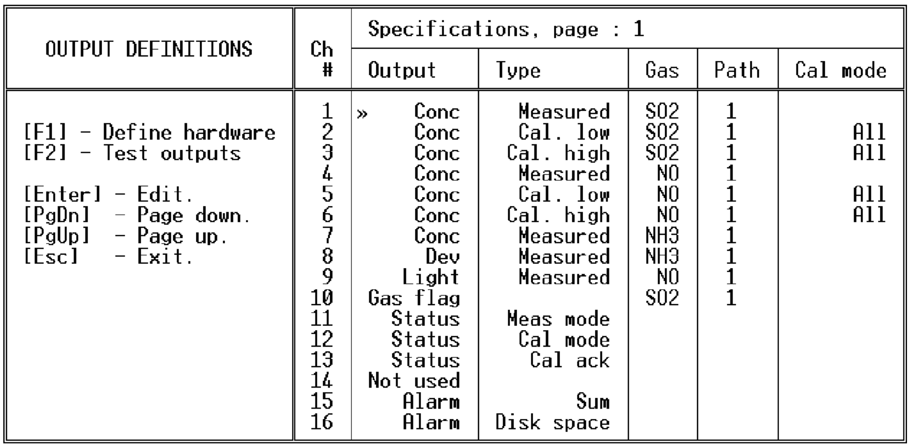
7.7 Output signal setup

In addition to the standard communication using the ComVision/ComView protocol, the analyser is also prepared for providing measurement results and status signals through the standardised software IO80 and IO256. IO80 and IO256 can be set to control analogue and digital outputs, and also to transfer data to other computers by various communication protocols. New hardware or communication protocols can therefore easily be added by extending the IO software.

The IO software can simultaneously be used as a datalogger, see section 7.6, Input signal setup.

The interaction between the analyser and the IO80/IO256 takes place through a software interface. For the outputs, the software interface consists of 80 or 256 memory positions, or channels. The analyser can write values into these channels, and the IO80/IO256 can read the written values an do whatever it has been programmed to do with them.

The way the analyser uses the 80/256 channels is set up by selecting [F6] Output signal setup in the Installation menu.



OUTPUT DEFINITIONS

[F1] - Define hardware
[F2] - Test outputs

[Enter] - Edit.
[PgDn] - Page down.
[PgUp] - Page up.
[Esc] - Exit.

Specifications, page : 1

Ch #	Output	Type	Gas	Path	Cal mode
1	» Conc	Measured	SO2	1	
2	Conc	Cal. low	SO2	1	All
3	Conc	Cal. high	SO2	1	All
4	Conc	Measured	NO	1	
5	Conc	Cal. low	NO	1	All
6	Conc	Cal. high	NO	1	All
7	Conc	Measured	NH3	1	
8	Dev	Measured	NH3	1	
9	Light	Measured	NO	1	
10	Gas flag		SO2	1	
11	Status	Meas mode			
12	Status	Cal mode			
13	Status	Cal ack			
14	Not used				
15	Alarm	Sum			
16	Alarm	Disk space			

Figure 7.32. Configuration of outputs.

The output channels are numbered from 1 and upwards. 16 channels are displayed on each page of the menu. The other channels are available on other pages by pressing [PgUp] or [PgDn]. The contents of the menu fields are changed by using the arrow keys to move the cursor to a field, and then pressing [Enter].

- By pressing [F1], the IO software starts, and the hardware or protocol which IO80/ IO256 uses can be defined.
- Pressing [F2], the outputs can be set by manually filling in values in the output channels.

The IO80 and IO256 software are described in separate manuals.

- In the Output column, the output parameter is defined. Available outputs are "Concentration", "Deviation" and "Light level", which are results of the measurements performed by the analyser, and "Status", "Alarm" and "Gas flag" which are flags that may be set by the analyser software during operation.
- Each output has a set of different Types, which are described below.

The values placed in the interface channels are the actual values of the concentrations, deviations and light levels as they are measured, after compensation for temperature etc. The units for concentrations and deviations are those defined in the measurement setup menu. The unit for light levels is always %.

The values for status, alarm and gas flags are either 1.000 (active) or 0.000 (not active). If any information for a specific channel in the output setup is changed, the actual output value for that channel is set to zero initially.

7.7.1 Concentration, deviation and light level

Five types available for these outputs: "All", "Measured", "Cal. low", "Cal. mid" and "Cal. high".

- "Measured" means that the concentration, deviation or light level result of a normal measurement is placed in the output channel. The gas name is selected in the column Gas, and the measurement path in the column Path.
- "Cal. low", "Cal. mid" and "Cal. high" means that the concentration, deviation or light level result obtained during a gas calibration at the corresponding level is forwarded to the output channel. The gas name is selected in the Gas column, the calibration path in the Path column, and the calibration mode in the Cal mode column. The calibration mode is either a specific mode, defined by its number, or "All", meaning that the result from all calibration modes where the gas and path are active will be placed in the same output channel whenever and however the gas calibration is activated. This is useful in combination with the calibration acknowledge status flag described further down. Note that the result of a gas calibration measurement will be placed in the output channel only if this has been enabled in the gas calibration menu.
- "All" means that every measurement result for the specified gas and path will be placed in the output channel, no matter if the result was obtained during a normal measurement or during a gas calibration. This is useful in combination with the calibration status flag, described below.

7.7.2 Status

Status is either of eight types:

- "Meas mode", measurement mode, is active as long as the analyser is performing normal measurements. As soon as the menu is entered, the flag is deactivated.
- "Cal mode", calibration mode, is activated when a gas or reference calibration is performed, activated either manually or automatically. By monitoring the measurement mode and calibration mode flags, it can be determined if a true measurement value or a calibration result is located in an output channel.
- "Syst check", System check flag is raised during the performance of a system check. The three flags "Meas mode", "Cal mode" and "System check" can thus never be active at the same time.
- "Neg dev", negative deviation is a warning flag which is set as soon as the analyser has performed a measurement which results in a negative deviation. Negative deviations are discussed in section 6, Measurements.
- "Cal ack", Calibration acknowledge may be set to indicate that a reference calibration or a gas calibration mode has been carried out. By monitoring the calibration acknowledge flag, it can be determined which calibration result is currently present in an output channel, if "Cal mode" for a gas has been set to "All".
- "Path nn on" indicates for each one of the measurement paths if the analyser is currently measuring on it or not.
- "Meas valid", measurement valid, is raised when a full measurement cycle is completed.
- "Gas valid", gas valid, is indicating when a specified gas concentration is available. The result is valid when the following three conditions are fulfilled:

- | standard deviation | < deviation limit
- | light level | > light level limit
- concentration ≠ -999.0 µg/m^3.

The gas valid signal is zero until a measurement result is approved. The flag is also reset when the measurements are interrupted.

7.7.3 Alarm

Alarm can be either "Sum", "Disk space", "Modem", "MX", "Sys. chk.", "Program" or "186card n".

- "Sum alarm" is activated if any other alarm is activated.
- "Disk space" alarm is set when the available memory on the hard disk gets below 500 kB.
- "Modem" alarm is set if the built-in modem fails, thus disabling communication through the telephone line connected to the analyser.
- "MX" alarm flag is raised if the analyser detects an error in a connected multiplexer.
- "System check" alarm is flagged if a system check of the hardware failed for one reason or another. See section 10, System Check for more information.
- "Program" alarm is set if the analyser software is interrupted unexpectedly.
- "186card n" is activated if the analyser detects an error in the electronics controlling the spectrometer and the detectors.

The last two alarms are mainly intended for factory testing.

7.7.4 Gas flag

The "Gas flag" signal consists of 8 bits and is therefore intended for serial communication only, for instance using the Cactus protocol. The signal is defined for a specified gas at a specified path and gives information on what is going on in the analyser at the moment. The 8 bits have the following indications, starting on the most significant one.

Bit No.	Pattern	Interpretation
7,6	00	Calibration mode 1
	01	Calibration mode 2
	10	Calibration mode 3
	11	Calibration mode 4
5,4	00	Normal measurement mode
	01	Calibration, low level
	10	Calibration, mid level
	11	Calibration, high level
3	0	|Channel shift| ≥ 6
	1	Warning: |channel shift| > 6

Bit No.	Pattern	Interpretation
2	1	Calibrating
1	1	Idle, no measurement result is available
0	0	Result is OK
	1	Result is bad, see below

The value of the last bit is set as follows. The result is considered bad if any of the following three conditions are true:

- |standard deviation| > deviation limit
- |light level| < light level limit
- concentration or deviation < 0 at the same time as |conc.| > 2* |deviation|.

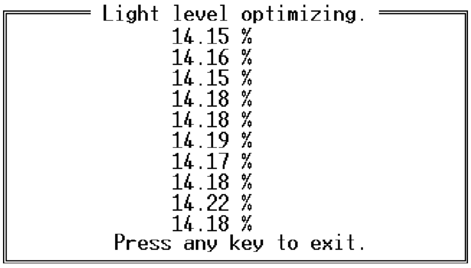
7.8 Emulator setup

In some applications, additional software is used to mimic the serial protocols of other types of data sources, like other brands of dataloggers. The configuration of such communication routines, or emulators, is accessed by pressing [F7] Emulator setup in the Installation menu. The configuration is described in separate manuals. An error message is displayed if no emulator is installed in the analyser.

7.9 Optimize light

High quality measurements can only be obtained if there is enough light coming into the spectrometer. The light levels should therefore be monitored regularly, and adjustments should be made to the emitters and receivers as soon as the light levels tend to fall. The adjustment procedures are described in the emitter/receiver manuals.

The light level is preferably adjusted with the help of an LM010 light meter and a short fibre connected to the receiver. If an L010 is not available, the maximum light level may instead be found by reading the values presented when selecting [F8] Optimize light in the Installation menu.



```
Light level optimizing.
      14.15 %
      14.16 %
      14.15 %
      14.18 %
      14.18 %
      14.19 %
      14.17 %
      14.18 %
      14.22 %
      14.18 %
 Press any key to exit.
```

Figure 7.33. The light intensity in percent is shown continuously when selecting the Optimize light function.

The values are given in percent, where 0 % means no light at all, and 100 % means that the detector is saturated. The levels cannot be compared with the light levels obtained during regular measurements. The function does not select a specific light path, but simply uses the path which is currently connected to the analyser. If more than one measurement path is used, the correct path can be selected from the multiplexer installation menu before entering the Optimize light function.

Optimize light is only available in UV-DOAS instruments, and it is not available in an analyser using a fixed grating. See section 10, System Check for details.

The Data Presentation Menu 8

The Opsis analyser has built-in functions for presenting gas data and datalogger data both in numerical and graphical formats. The functions are accessed from the root menu by selecting [F2] Data presentation.

The presentation menu are available in the analyser mainly as a service for on-site inspections. Normally, data are collecting using various communication software and studied in other locations.

The analyser gas measurements will be stopped while data is presented.

8.1 Introduction

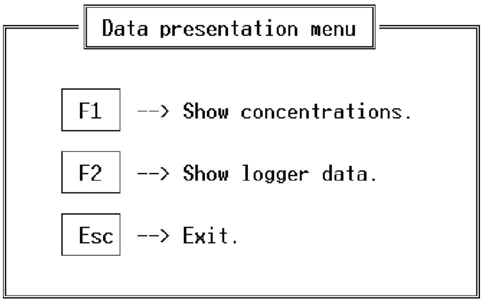


Figure 8.1. The data presentation menu.

The data presentation menu is shown in figure 8.1. Select:

- [F1] Show concentrations to present gas measurement results.
- [F2] Show logger data to display data acquired by the built-in datalogger, if present.

Press [Esc] to return to the root menu.

All measurement values are stored in binary files on the hard disk of the analyser. If converting data into ascii format, the entered integration time is an important parameter.

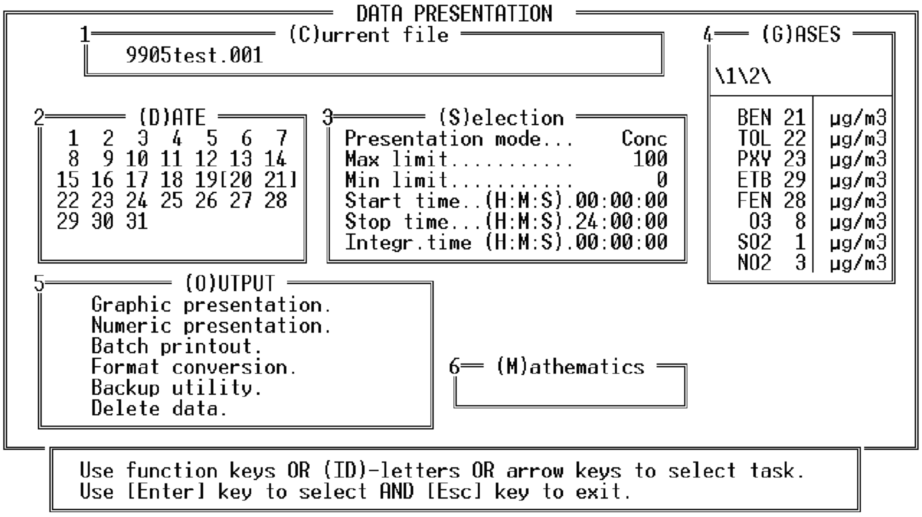
All measurement values can be presented and reformatted if the integration time is set at zero. Also the possible minus (-) signs are kept after reformatting.

If the integration time is greater than zero, e.g. for calculation of average hourly values, the marked values are not included in the data presented (except the negative concentrations with an absolute value less than twice the deviation). If a file containing such values is converted, the marked values will not be present in the new file (see also section 8.3, Presentation of datalogger data).

These criteria are only valid for gas measurement data. Datalogger data cannot be filtered.

8.2 The gas presentation menu

Press [F1] Show concentrations to obtain the following display:



```
                         DATA PRESENTATION
     1 (C)urrent file                                  4 (G)ASES
       9905test.001                                    \1\2\

  2 (D)ATE                  3 (S)election                BEN 21  µg/m3
    1  2  3  4  5  6  7      Presentation mode...   Conc  TOL 22  µg/m3
    8  9 10 11 12 13 14      Max limit..........     100  PXY 23  µg/m3
   15 16 17 18 19[20 21]     Min limit..........       0  ETB 29  µg/m3
   22 23 24 25 26 27 28      Start time..(H:M:S).00:00:00 FEN 28  µg/m3
   29 30 31                  Stop time...(H:M:S).24:00:00  O3  8  µg/m3
                             Integr.time (H:M:S).00:00:00 SO2  1  µg/m3
                                                          NO2  3  µg/m3
  5 (O)UTPUT
      Graphic presentation.
      Numeric presentation.
      Batch printout.
      Format conversion.           6 (M)athematics
      Backup utility.
      Delete data.

   Use function keys OR (ID)-letters OR arrow keys to select task.
   Use [Enter] key to select AND [Esc] key to exit.
```

Figure 8.2. The data presentation menu for gas data.

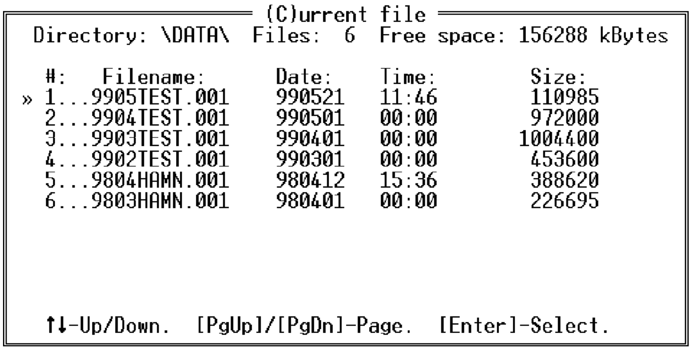
Key to the Data presentation menu:

- [F1] (C)urrent file indicates the data file currently being presented including the location ID entered in the Station setup menu.
- [F2] (D)ate shows the days of the month for which data can and will be presented.
- [F3] (S)election is used to set integration time and scales for graphic presentation.
- [F4] (G)ases selects the compounds and the paths for which data are being presented.
- [F5] (O)utput indicates how the data are to be presented and whether they are to be reformatted to ascii format.
- [F6] (M)athematics is used if the data have to be adjusted with a constant factor.

Use the function keys or the letter within the parentheses to select menu. It is also possible to use the arrow keys to move the highlighted frame and then press [Enter] at the appropriate menu. To exit from this menu, press [Esc].

8.2.1 Selecting a data file

Gas data are stored in files named "YYMMABCD.EFG", where "YYMM" are year and month and "ABCD.EFG" is the station name defined in the Install station menu. A new data file is thus generated for each month. Data from any month can be presented. When (C)urrent file is selected, the following display will appear:



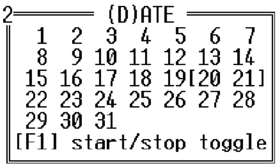
```
══════════════════════ (C)urrent file ══════════════════════
 Directory: \DATA\  Files:  6   Free space: 156288 kBytes

   #:   Filename:       Date:    Time:        Size:
 » 1...9905TEST.001     990521   11:46        110985
   2...9904TEST.001     990501   00:00        972000
   3...9903TEST.001     990401   00:00       1004400
   4...9902TEST.001     990301   00:00        453600
   5...9804HAMN.001     980412   15:36        388620
   6...9803HAMN.001     980401   00:00        226695





   ↑↓-Up/Down.  [PgUp]/[PgDn]-Page.  [Enter]-Select.
```

Figure 8.3. Selecting a data file.

All binary files containing data will be shown. To select data for a specific month, use the arrow-keys to highlight your selection and then press [Enter]. If data are stored in more than 10 files, the additional files can be displayed by pressing [PgUp] or [PgDn]. To return to the Data presentation menu, press [Esc].

8.2.2 Selecting dates

If (D)ate is selected, a period of 1 to 31 days can be defined. Use the arrow-keys to move the brackets, and press [Enter] or [F1] to alternate between the left and the right bracket. Only the dates containing data are highlighted. To return to the Data presentation menu, press [Esc].

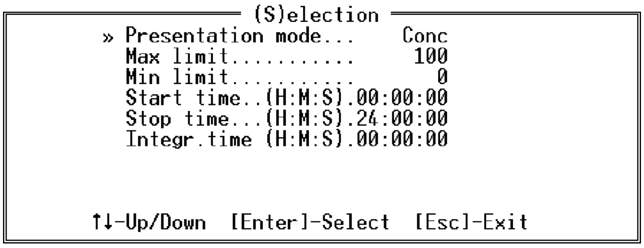


```
2═════ (D)ATE ══════
  1  2  3  4  5  6  7
  8  9 10 11 12 13 14
 15 16 17 18 19[20 21]
 22 23 24 25 26 27 28
 29 30 31
[F1] start/stop toggle
```

Figure 8.4. Selecting dates.

8.2.3 Changing scales and integration time

Select sub-menu 3, (S)election in order to change integration time or the scales for graphic presentation.



```
                  (S)election
      » Presentation mode...    Conc
        Max limit..........      100
        Min limit..........        0
        Start time..(H:M:S).00:00:00
        Stop time...(H:M:S).24:00:00
        Integr.time (H:M:S).00:00:00


   ↑↓-Up/Down  [Enter]-Select  [Esc]-Exit
```

Figure 8.5. The Selection menu.

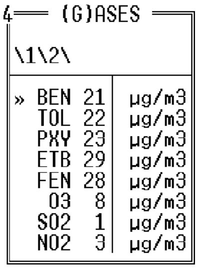
Use the arrow-keys to highlight the parameter to be changed and then press [Enter].

- Presentation mode sets which gas parameter to display in the graph. It is either "Conc", which will show only concentrations, or "Combined", which will show both concentration, standard deviation and light level for the selected gas(es).
- Max and Min limit set the scale on the y-axis on the graph, but do not affect numerical presentation.
- Start and Stop time define the time interval for any operation in the Data presentation menu, also for the Format conversion and Mathematics functions.
- Integration time defines the size of the time frame. As an example, the integration time should be set at 60 minutes to obtain a presentation of results as average hourly values. If integration time is set at zero, all results will be shown in the form of a curve. If the integration time is greater than zero, the results will be presented as a bar graph, where values marked with minus signs have been sorted out. The Integration time also affects the Format conversion function.

To return to the Data presentation menu, press [Esc].

8.2.4 Selecting substances and paths

Use sub-menu 4, (G)ases to select substances and measurement paths. To select a substance or a light path, use the arrow-keys to highlight the desired item and then press [Enter]. To exclude a substance or a path, repeat this procedure. The highlighted paths and substances will be shown when presenting the data.



```
4 (G)ASES
\1\2\

» BEN 21  µg/m3
  TOL 22  µg/m3
  PXY 23  µg/m3
  ETB 29  µg/m3
  FEN 28  µg/m3
   O3  8  µg/m3
  SO2  1  µg/m3
  NO2  3  µg/m3
```

Figure 8.6. Selecting gases and paths.

To return to the Data presentation menu, press [Esc].

8.2.5 Presentation of measurement results

Use sub-menu 5, (O)utput to show measurement results numerically or graphically on the monitor or obtain a printout. Data files can also be converted to text-file format, copied to a diskette, or erased. Use the arrow-keys to highlight the selection.

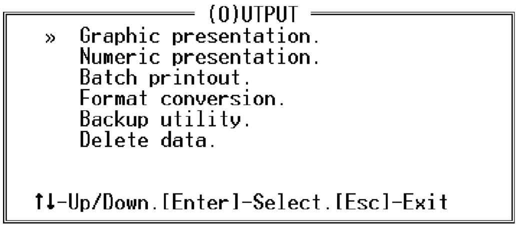
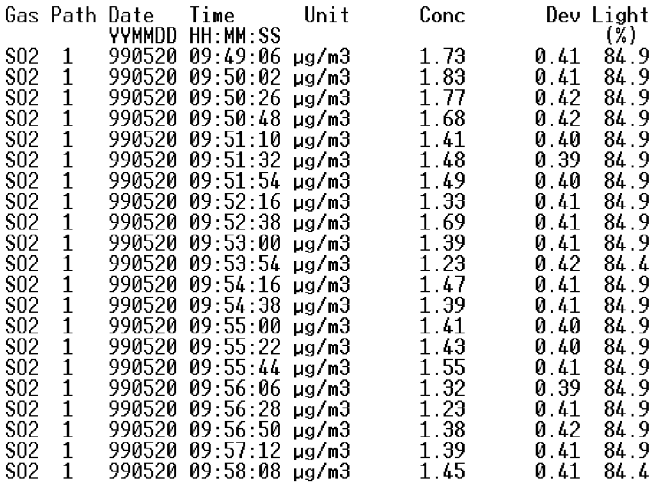


Figure 8.7. The Output menu.

To display the values on the monitor, select Graphic presentation or Numeric presentation. The diagrams on the next pages illustrate the significance of the Integration time setting.

- Graphic presentation generates a graph, either a curve or a histogram The type is dependent on the Integration time setting. The time scale is defined by the Date interval and the Start and Stop time settings. The concentration scale is defined by the Max and Min limit settings. To make a printout of the graph, press [P].
- Numerical presentation generates a table. The table is defined by the Date, the Integration time, and the Start and Stop time settings. To turn pages on the screen, press the [Space] bar. To make a printout, answer [Y] to the question at the end of the table.
- If a number of days are to be printed out individually, Batch printout can be used. After the selection of gases, dates, etc., a printout will automatically be made, one for each selected day, and the printouts will be either graphic ([G]) or numerical ([N]).
- For Format conversion, see section 8.4, Converting data files to ascii format for a detailed description.
- Backup utility enables copying of binary or ascii files to the 3 1/2" diskette station. A formatting function for diskettes is also provided by Backup utility. See section 8.5, Copying data files for the details.
- Delete data provides the possibility of removing data files from the hard disk. See section 8.6, Removing data files for details.

To return to the Data presentation menu, press [Esc].



```
Gas Path Date    Time      Unit       Conc       Dev Light
         YYMMDD  HH:MM:SS                             (%)
SO2  1   990520 09:49:06 µg/m3      1.73      0.41  84.9
SO2  1   990520 09:50:02 µg/m3      1.83      0.41  84.9
SO2  1   990520 09:50:26 µg/m3      1.77      0.42  84.9
SO2  1   990520 09:50:48 µg/m3      1.68      0.42  84.9
SO2  1   990520 09:51:10 µg/m3      1.41      0.40  84.9
SO2  1   990520 09:51:32 µg/m3      1.48      0.39  84.9
SO2  1   990520 09:51:54 µg/m3      1.49      0.40  84.9
SO2  1   990520 09:52:16 µg/m3      1.33      0.41  84.9
SO2  1   990520 09:52:38 µg/m3      1.69      0.41  84.9
SO2  1   990520 09:53:00 µg/m3      1.39      0.41  84.9
SO2  1   990520 09:53:54 µg/m3      1.23      0.42  84.4
SO2  1   990520 09:54:16 µg/m3      1.47      0.41  84.9
SO2  1   990520 09:54:38 µg/m3      1.39      0.41  84.9
SO2  1   990520 09:55:00 µg/m3      1.41      0.40  84.9
SO2  1   990520 09:55:22 µg/m3      1.43      0.40  84.9
SO2  1   990520 09:55:44 µg/m3      1.55      0.41  84.9
SO2  1   990520 09:56:06 µg/m3      1.32      0.39  84.9
SO2  1   990520 09:56:28 µg/m3      1.23      0.41  84.9
SO2  1   990520 09:56:50 µg/m3      1.38      0.42  84.9
SO2  1   990520 09:57:12 µg/m3      1.39      0.41  84.9
SO2  1   990520 09:58:08 µg/m3      1.45      0.41  84.4
```

Figure 8.8. Presentation of data in tabular form. All measurement values within the selected time interval are displayed. Integration time is zero.

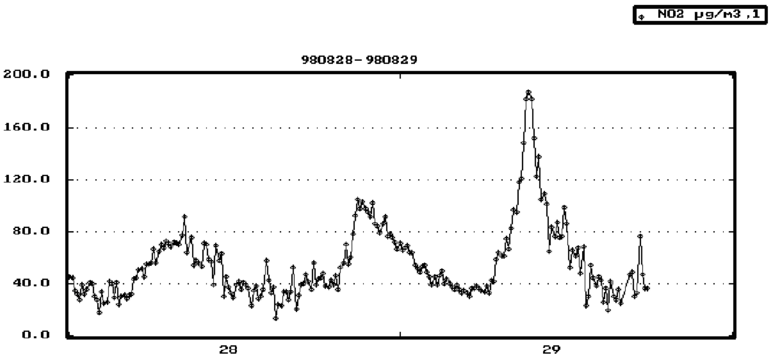


Figure 8.9. A graphic presentation. Integration time has been set at zero. All measurement values are shown. The scale on the y-axis is decided by Max and Min limit in the Selection frame.

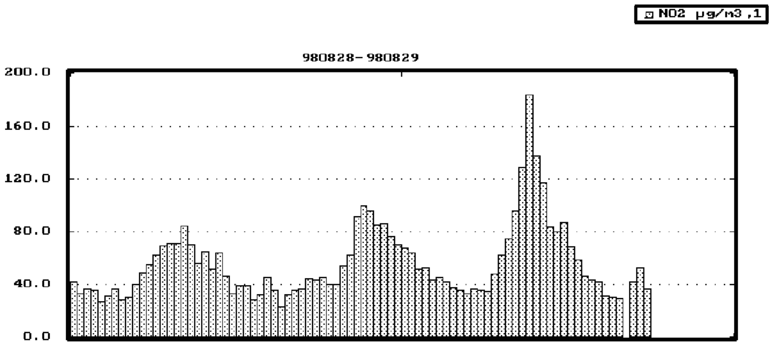
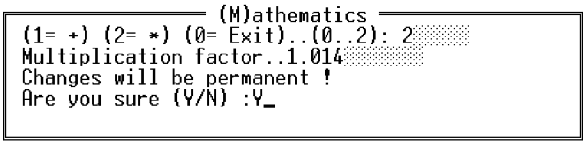


Figure 8.10. A graphic presentation with an integration time of 30 minutes. The data is filtered with respect to negative values.

8.2.6 The Mathematics function

The function (M)athematics is used when the values in a data file are to be adjusted with a constant factor. The factor can either be added to the values or be used as multiplying factor. This may be appropriate if e.g. the length of the measurement path has been incorrectly entered.

The change affects only the measurement values between the Start and the Stop time settings for the marked dates and gases.



```
                    (M)athematics
(1= +) (2= *) (0= Exit)..(0..2): 2
Multiplication factor..1.014
Changes will be permanent !
Are you sure (Y/N) :Y_
```

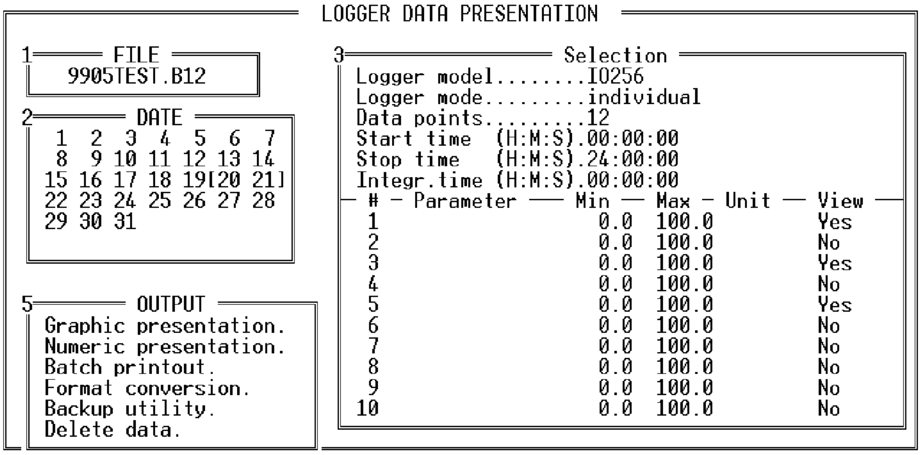
Figure 8.11. "1" means addition, "2" means multiplication.

- The added constant should be expressed in the unit which is specified for the gas in the Gases frame. The unit is defined in the Measurement time menu, see Section 7, The Installation Menu. Only the concentration values are changed. Subtraction is the same as adding a negative constant.
- Multiplication is made on both the concentration and the deviation values.

***Warning**: The changes in measurement values are permanent. This means that the Mathematics function should be used with extreme care.*

8.3 Presentation of datalogger data

To display logger data on the monitor, press [F2] Show logger data. This menu is structured in the same way as the menu which presents concentrations.



```
LOGGER DATA PRESENTATION

1 FILE
  9905TEST.B12

2 DATE
   1  2  3  4  5  6  7
   8  9 10 11 12 13 14
  15 16 17 18 19[20 21]
  22 23 24 25 26 27 28
  29 30 31

5 OUTPUT
  Graphic presentation.
  Numeric presentation.
  Batch printout.
  Format conversion.
  Backup utility.
  Delete data.

3 Selection
  Logger model........I0256
  Logger mode.........individual
  Data points.........12
  Start time   (H:M:S).00:00:00
  Stop time    (H:M:S).24:00:00
  Integr.time  (H:M:S).00:00:00
 # - Parameter -- Min -- Max - Unit -- View
  1                0.0  100.0          Yes
  2                0.0  100.0          No
  3                0.0  100.0          Yes
  4                0.0  100.0          No
  5                0.0  100.0          Yes
  6                0.0  100.0          No
  7                0.0  100.0          No
  8                0.0  100.0          No
  9                0.0  100.0          No
 10                0.0  100.0          No
```

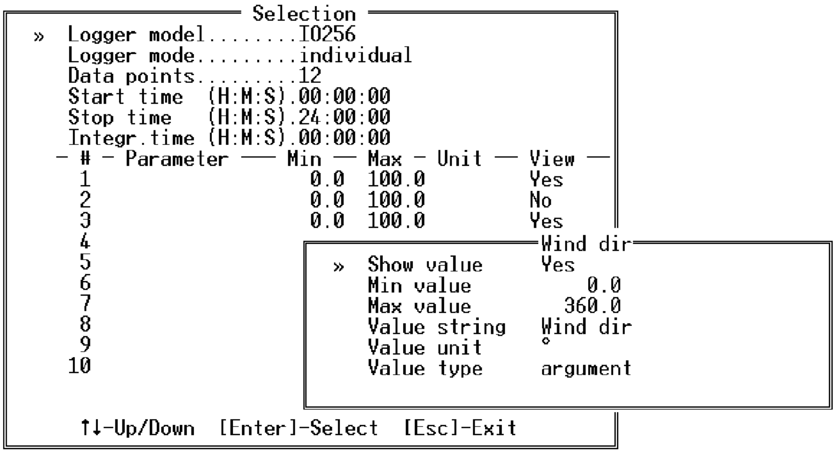
Figure 8.12. Datalogger data presentation menu.

- [F1] File is used to select the data file for presentation. Datalogger files have the extension ".Bnn", where nn indicates the number of sensor signals. A file from a datalogger which is defined as a wind-station has always the extension ".B06".
- [F2] Date is used to select days in the current month. Only the dates for which data exists are highlighted. Use [Enter] to toggle between the two brackets.
- [F3] Selection is used to select type of sensors, scales and integration time. See section 8.3.1, Selection menu for datalogger data.
- [F5] Output. The menu is next to identical with the corresponding one for gas monitoring data. However, the y-axis is always scaled from 0 to 100 %, since parameters with different units may share the same diagram. 0 % correspond to the Min value defined in the Selection menu, and 100 % is thus the Max value, see section 8.3.1, Selection menu for datalogger data.

To return to the Data presentation menu, press [Esc].

8.3.1 Selection menu for datalogger data

The selection menu for datalogger data has several items in common with the corresponding menu for gas monitoring data. However, there are some significant differences.



```
                      Selection
  »  Logger model........I0256
     Logger mode.........individual
     Data points.........12
     Start time  (H:M:S).00:00:00
     Stop time   (H:M:S).24:00:00
     Integr.time (H:M:S).00:00:00
   - # - Parameter ── Min ── Max - Unit ── View ──
     1                  0.0  100.0         Yes
     2                  0.0  100.0         No
     3                  0.0  100.0         Yes
     4                                      Wind dir
     5                     »  Show value     Yes
     6                        Min value         0.0
     7                        Max value       360.0
     8                        Value string   Wind dir
     9                        Value unit     °
     10                       Value type     argument

      ↑↓-Up/Down  [Enter]-Select  [Esc]-Exit
```

Figure 8.13. The datalogger selection menu.

- The Logger model toggles between DL010, DL016, IO80 and IO256, and should be set to the correct model when the data file has been selected.
- Logger mode indicates whether the datalogger is configured as a windstation, or with individual definitions on the sensors. The setting must be the appropriate one, otherwise the presented values may not be correct.
- Data points indicates the number of channels used on the datalogger, and must be the same as the number in the file name extension.
- The Start and Stop time and the Integration time settings have the same function as for the gas monitoring data.

- To obtain the correct presentation of the datalogger data the Parameter definitions must be set according to the logger setup. When one of the items is selected a new menu is presented:
    - Show value indicates whether the parameter is to be presented or not.
    - Min and Max value settings define the presented range.
    - Value string should be an appropriate name of the parameter.
    - Value unit indicates the measurement unit of the parameter.
    - Value type, finally, should be set according to the parameter type. "Scalar" is the normal setting. "Abs. value" is used for vector parameters, for instance wind vector. "Argument" is used for parameters which measure an angle, for instance wind direction. The Max value should then be set to "360" (°).

8.4 Converting data files to ascii format

Measurement results are stored on the hard disk as binary files and formatted so that the measurements for each month comprise a separate file. This format can be converted to ascii code (logger format) by selecting Format conversion in the Output menu. There is one formatting function in each presentation menu, one for gas data and one for datalogger data.

Three questions should be answered before the reformatting is performed:

- Convert file to logger format? (Y/N)
- Include seconds? (Y/N)
- Enter 2 ID-letters:XX

The ascii format is dependent on whether seconds are included in the time information, or not. The different ascii formats are described below. The two ID letters should be unique for the file. Information on year and month is always included in the file name, just as for the binary files. The extension is defined by the file format. Example: 9504PR.OPS.

The conversion is made according the settings in the Date, Gas, and Selection menus. In the Selection menu the Integration time and the Start and Stop time settings are the important parameters. The Integration time not only enables measurement data to be converted to, for instance, hourly mean values, but also defines the filtering criterion.

- If the integration time is set to zero, all measurement values will be reformatted.
- If the integration time is greater than zero, some gas measurement values will not be included in the conversion. The omitted values are the ones marked with a minus sign at the concentration, the deviation and/or the light level. See also section 6, Measurements. Gas measurement data will be omitted if:
    - the concentration is negative and is more than twice the maximum permissible standard deviation.

- the standard deviation exceeds the maximum permissible standard deviation (marked with a minus at the light level).
- the standard deviation is marked with a minus sign, which shows that evaluation of the measurement value has not converged.

Please note that no datalogger values are filtered.

The following formats are available for gas and datalogger data:

standard gas data	xx.OPS
gas data including seconds	xx.SEC
wind-station data	xx.WND
variable datalogger data	xx.Ann
datalogger data including seconds	xx.Snn

"xx" is the ID name entered when formatting. "nn" is the number of datalogger channels used, and is the same as in the binary file name extension.

In the following five tables, the ascii file formats are described. Examples of the format of the lines are given after each table.

Table 8.1: Standard ascii file for gas data, xx.OPS.

Position	No. of char.	Interpretation
1-2	2	Gas number, see section B.4, Conversion factors.
5-12	8	Month/day/year
15-19	5	Hour:minute
21-22	2	Monitoring path number
24-30	7	Concentration in $\mu g/m^3$
32-38	7	Deviation in $\mu g/m^3$
40-41	2	Light level in %
42-43	2	Carriage Return + Line Feed
Example: 27 05/21/99 14:00 02 1.23E+1 1.23E-1 62		

Table 8.2: Gas data file including seconds, xx.SEC.

Position	No. of char.	Interpretation
1-2	2	Gas number, see section B.4, Conversion factors.
5-12	8	Month/day/year
15-22	8	Hour:minute:second
24-25	2	Monitoring path number
27-33	7	Concentration in $\mu g/m^3$
35-41	7	Deviation in $\mu g/m^3$
43-44	2	Light level in %
45-46	2	Carriage Return + Line Feed
Example: 22 05/21/99 15:00:00 01 1.23E+1 1.23E-1 66		

Table 8.3: A wind station is a logger which is configured with six channels: four wind parameters and two temperatures. File Name: xx.WND.

Position	No. of char.	Interpretation
1-2	2	ID number
5-12	8	Month/day/year
15-19	5	Hour:minute
21-27	7	Wind velocity in m/s
29-35	7	Wind vector in m/s
37-43	7	Wind direction in degrees (0-360)
45-51	7	Standard deviation of wind direction in degrees
53-60	8	Temperature 1 in °C
62-69	8	Temperature 2 in °C
70-71	2	Carriage Return + Line Feed
Example: 99 05/21/99 12:00 1.23E+0 1.23E+0 1.23E+2 1.23E+1 1.234E+1 1.234E+1		

*Table 8.4: Generic datalogger data, xx.Ann. n = number of sensors, x = (n-1)*11 + 21.*

Position	No. of char.	Interpretation
1-2	2	ID number
5-12	8	Month/day/year
15-19	5	Hour:minute
21-30	10	Value 1
32-41	10	Value 2
43-52	10	Value 3
...	...	...
x-(x+9)	10	Value n
x+11	1	Carriage Return
x+12	1	Line Feed
Example: 01 05/21/99 07:15 1.2345E+01 1.2345E+02 1.2345E+03...		

*Table 8.5: Logger data incl. seconds, xx.Snn. n = number of sensors, y = (n-1)*11 + 22.*

Position	No. of char.	Interpretation
1-2	2	ID number
4-11	8	Month/day/year
13-20	8	Hour:minute:second
22-31	10	Value 1
33-42	10	Value 2
44-53	10	Value 3
...	...	...
y-(y+9)	10	Value n
y+11	1	Carriage Return
y+12	1	Line Feed
Example: 01 05/21/99 07:15:00 1.2345E+01 1.2345E+02 1.2345E+03...		

8.5 Copying data files

The measurement data files stored on the hard disk in the analyser can be of four types. They can be distinguished by their file names.

- The gas measurement binary file names contain 12 characters, of which the first four indicate the year and month during which measurements were made. The following four + three characters are defined at the installation. Example: 9504PUST.069.
- A reformatted measurement data file has a 2-letter ID and the extension "OPS" or "SEC", depending on whether seconds are excluded or included. Example: 9504PU.OPS.
- Binary datalogger files have the same four first characters as the corresponding gas data file, but have the extension "Bnn". "nn" is the number of channels used on the logger. A wind-station always has the extension "B06". Example: 9504PUST.B06
- Datalogger files that has been converted to ascii format may have the extensions "WND", "Ann" or "Snn". Example: 9506PU.WND.

Data files can be copied by invoking the Backup utility in the Output menus.

- Select a [B]inary or a [A]scii format file to copy. After the type of file has been selected, a list of all the files stored in this format will be shown.
- If the diskette in the diskette drive is not formatted. it can be formatted by pressing [F1]. The [F2] key is used to select the appropriate floppy drive, i.e. either A: or B:. The built-in floppy drive (if any) is the B-drive, unless otherwise marked on the drive or specified in the instrument documentation.
- To start copying, move the cursor to the appropriate file name and press [Enter].

If the file is larger than the diskette size, the file will be backed up to more than one diskette. The analyser will ask for a new diskette when the former one is full until the whole file is backed up. Old data on the diskettes will be deleted. It is important to keep the diskettes in the proper order.

To restore the data file from the diskettes to another computer, the DOS command RESTORE should be used. For more information, see the DOS manual.

8.6 Removing data files

As data is stored on the hard disk of the analyser, the available disk space decreases. In order to avoid problems due to lack of free disk space, old data files have to be removed from the hard disk. The amount of free disk space is shown in the measurement menu, see figure 6.1. It is recommended that the available disk space is checked regularly, at least once a month. It is also possible to activate an alarm for nearly full hard disk, see section 7, The Installation Menu.

Note: *It is strongly recommended that the original binary files are always backed up before they are deleted from the analyser hard disk.*

Copying files is discussed in the former section.

Data files can be removed from the hard disk by invoking the Delete data function in the Output menus.

- Select a [B]inary or a [A]scii format file to delete. After the type of file has been selected, a list of all the files stored in this format will be shown.
- To start deleting, move the cursor to the appropriate file and press [Enter].
- Press [Y] to confirm that the selected file should be removed.

Warning: *Once a file has been removed from the hard disk, it cannot be recovered. Therefore use the Delete data function with extreme care.*

Calibration Procedures 9

Opsis analysers, just as well as any other types of instruments, need calibration to ensure that the reported gas concentrations are valid. All procedures for verifying adjusting the instrument calibration are found in the calibration menu.

This section describes the software aspects of the calibration procedures and related functions. Additional important information about calibration is found in QAQC manuals of the Opsis analysers.

9.1 The main calibration menu

To display the calibration menu, select [F3] Calibration in the Analyser Root menu.

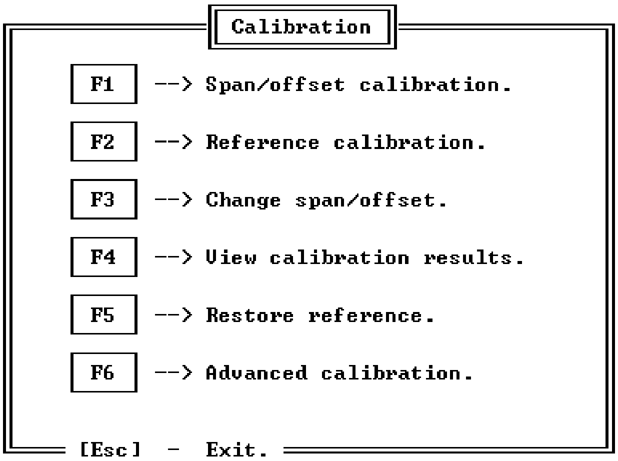


Figure 9.1. The Calibration menu.

- [F1] Span/offset calibration is used to start single or multi-point span calibrations for the activated gases.
- [F2] Reference calibration is used to start reference calibrations.
- [F3] Change span/offset enables manual adjustments of the factors for each gas.
- [F4] View calibration results opens a text file where information on all results from the calibrations are listed.
- [F5] Restore reference enables the previous reference spectrum to be re-activated.

- [F6] Advanced calibration includes recording of an oxygen spectrum and recalculation of measurement results, as well as other advanced routines affecting the measurement results.

Pressing [Esc] makes the software return to the root menu.

It is advisable to perform a system check before starting the span/offset or reference calibration procedures. See section 10, System Check for more information.

9.2 Span/offset calibration

A span and offset calibration means that the instrument response is compared with a calculated, well-known concentration. A daily check can consist of a single calibration point only. A full span and offset calibration should consist of at least three equally spaced calibration points. Based on the results the span and offset factors for each gas can be adjusted.

Span and offset calibrations of the Opsis analyser can be made either using the ordinary measurement mode or the special calibration utilities in the analyser software. The first method is described in detail in the QA/QC Manual. This section will therefore only include the calibration techniques based on the analyser calibration utilities.

The analyser calibration utilities support both manual and automatic span/offset calibrations. A manual calibration gives the operator full control of selection of paths, gas cylinders and gases to be calibrated. Automatic calibrations can be made at pre-set time intervals and be initiated by external signals. Several definitions has to be made in the calibration set-up menus prior to the start. The set-up menus are described in section 7.4, Calibration setup.

9.2.1 Preparations

The following entries must be prepared before the calibration can start:

In the Calibration paths menu (section 7.4.2)

- The physical parameters for at least one calibration path must be defined.
- The Path control setting "Manual" or "Auto" indicates whether the calibration path is connected manually or automatically.

In the Gas cylinders/CU007 menu (section 7.4.1)

- The available standard gas cylinders, and to which gas port on the CU004 or CU007 unit respective cylinder is connected, should be entered.

- The Man/Auto setting indicates whether the cylinder should be connected manually or automatically when calibrating.

In the Calibration mode setup menu (section 7.4.3)

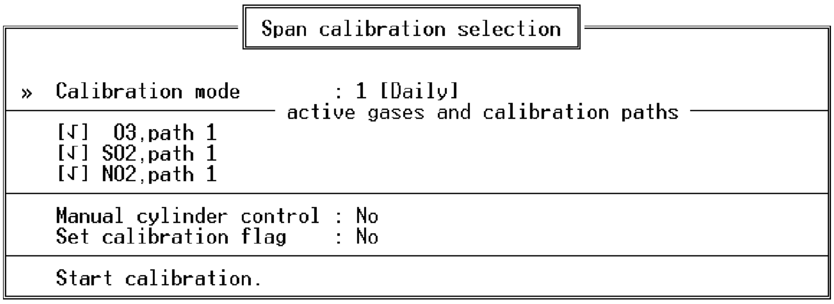
- At least one mode for at least one calibration path should be active.

In the Calibration gas setup menu (section 7.4.3)

- The gas or gases to be calibrated should be active.
- The settings for the each standard gas cylinder should be interconnected with the settings in the Gas cylinder menu above.
- The measurement time and range for each gas.
- The number of measurements at each level. The result at each level is the arithmetic mean value of the measurements.
- Automatic span/offset adjustments, yes or no.
- The maximum calibration error (CE).

9.2.2 Span/offset calibration performance

1. The calibrations are activated by selecting [F1] Span/offset calibrations in the Calibration menu. The following menu is presented.



```
Span calibration selection

» Calibration mode        : 1 [Daily]
                              active gases and calibration paths
  [√]  O3,path 1
  [√] SO2,path 1
  [√] NO2,path 1

  Manual cylinder control : No
  Set calibration flag    : No

  Start calibration.
```

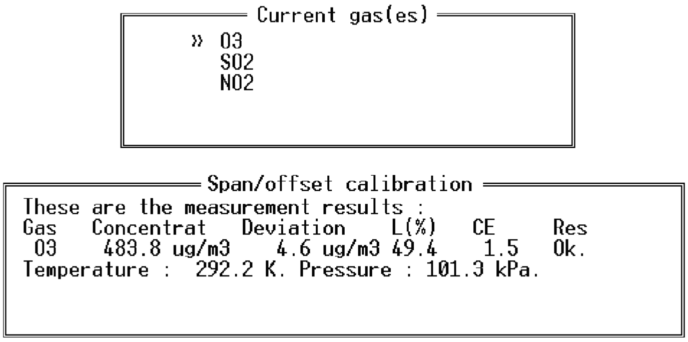
Figure 9.2. Start menu to the span/offset calibrations.

2. Select the appropriate active Calibration mode at the top line. A list of the active gases is presented in the frame below.
3. The gases can be selected one by one by ticking them with "ϑ".
4. Manual cylinder control can be "Yes" or "No".
    - When "Manual cylinder control" is selected, i.e. "Yes" is entered, the operator is requested to connect the first standard gas cylinder to the cell (if the Gas cylinder control is set to "Manual"). The second request is to connect the calibration path to the analyser (if Path control is set at "Manual"). Each

step is similarly preceded with a request and the message "Press any key or [Esc] to quit". By pressing **[Esc]** one or more steps can be ignored.

- When automatic control is selected the entire procedure is run through without interruptions, and no interaction with the operator is required. The command is equivalent with the automatic calibrations initiated either by the internal clock or by an external signal. The **Path control** and the **Gas cylinder controls** have to be set at "Automatic".

5. The **calibration flag** is a status output which normally should be set off.
6. The results from each step in the calibration procedure are presented on the screen, see the figure below. The results include information on concentration, deviation, light level and whether the calibration error, **CE**, is within the permissible limit. This is indicated with the message "Ok" or "Fail" at **Res** to the very right, see section 7.4.3, Calibration modes/calibration gases for a discussion concerning the settings. All results are also stored in a calibration text file so that they can be reviewed with the **View calibration results function**, see section 9.5, Calibration results.
7. The procedure can be terminated by pressing **[Esc]**.



```
Current gas(es)
» O3
  SO2
  NO2

Span/offset calibration
These are the measurement results :
Gas   Concentrat   Deviation    L(%)   CE     Res
 O3    483.8 ug/m3    4.6 ug/m3 49.4    1.5   Ok.
Temperature :  292.2 K. Pressure : 101.3 kPa.
```

Figure 9.3. Information on the calibration results after a span/offset calibration.

When a successful calibration has been run through the results can be used to calculate new span and offset factors for each gas and, if required, on each path. Normally the factors are the same for all paths, see figure 9.5.

Depending on the number of concentration levels the new span and offset factors is calculated in somewhat different ways. In either case the calculations can be illustrated with a diagram where the analyser response is plotted against the calibration concentrations, see figure 9.4.

The new span is calculated from the slope *k* of a straight line, and the offset from the intercept *b* with the Y-axis.

$$\text{new span} = \frac{1}{k} \tag{9.1}$$

$$\text{new offset} = -b \tag{9.2}$$

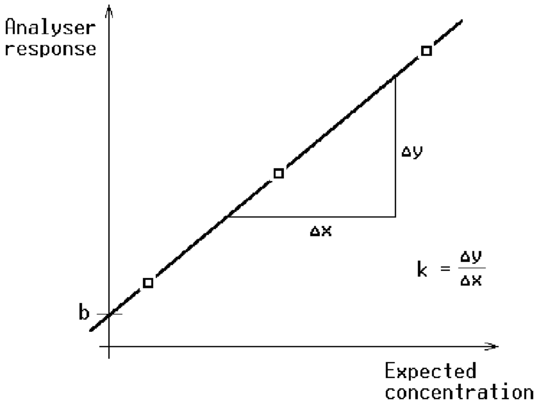


Figure 9.4. Calibration diagram.

- When one calibration level is used a straight line is extended through the zero point. The span is calculated from the slope, see above, whilst the offset factor will always be zero.
- When two calibration levels are used a straight line is drawn through the points, and the span and offset factors are determined in accordance with the equations above.
- When using three calibration levels a straight line is fitted to the points with a least-squares fit. The span and offset factors are calculated as above.

***Note**: Only the concentration levels where the result of the calibration error test was Ok will be included in the calculations.*

The span and offset factors will automatically be updated only if the following three conditions are fulfilled:

1. The mode was started automatically or from the keyboard with automatic control.
2. The Adjust span/offset function in the Calibration gas setup menu is "Yes".
3. All calibration errors are within the Max cal. error.

The setting at Affected path in the Calibration path menu defines whether "All" or only one specified path will be affected concerning the new span and offset factors. The new factors can always be entered via the keyboard in the Change span/offset menu, see section 9.4.

9.3 Reference calibration

***Note**: Reference calibration may not be available for some gases.*

Reference calibration means checking and recording the reference spectrum for a wavelength region used by the analyser during measurements. The setup of the reference calibration procedure is described in section 7.4.4, Reference calibration.

Reference calibration can be performed from the menu in two ways, manually or automatically. A manual calibration gives the operator full control of selection of reference light, zero air and gases to be calibrated. An automatic reference calibration is performed without any interaction from the operator, as if it had not been started from the menu but at a specific time or by an external signal (see section 7.4.5, Automatic calibrations).

9.3.1 Preparations

The following settings have to be entered:

In the Calibration paths menu (section 7.4.2):

- The physical parameters for at least one calibration path must be defined.
- By setting the calibration path length to same as (one of) the actual measurement paths the results from the reference calibration are easier evaluated.
- When no zero air source is required, for instance when the reference calibration is made without a cell, the Cell flush time can be set at zero.
- The Path control setting "Manual" or "Auto" indicates whether the calibration path is connected manually or automatically.

In the Gas cylinders/CU007 menu (required only for automatic reference calibrations, see section 7.4.1):

- To which gas port on the CU004/007 unit the zero air source is connected.
- The Man/Auto setting indicates whether the zero air source should be connected manually or automatically when calibrating.

In the Reference calibration setup menu (section 7.4.4):

- All parameters for all gases to be reference calibrated must be set.

When performing automatic reference calibrations the Gas cylinder control at the zero air source, and the Path control must be set at "Automatic". Fully automatic calibrations require an ER070 or an ER080 unit, or that a separate calibration path is installed via a multiplexer.

9.3.2 Reference calibration performance

1. The calibrations are activated by pressing [F2] Reference calibration in the Calibration menu. An entrance menu which is similar with the one in figure 9.2 is presented.
2. Calibrate all gases can be "Yes" or "No".

- When "Yes" a new reference will be recorded for all gases thus overriding all conditions which are entered in the setup menus.
- When "No" a list of the active gases is presented in the frame below. Each gas can be selected/deselected by positioning the cursor in front of the gas and pressing [Enter].

3. Manual cylinder control can be "Yes" or "No".
    - When "Manual cylinder control" is selected, i.e. "Yes" is entered, the operator is requested to connect the zero air source to the cell. The second request is to connect the calibration path to the analyser. Each step is similarly preceded with a request and the message "Press any key or [Esc] to quit". By pressing [Esc] one or more steps can be ignored. "Manual control" allow the operator to force the analyser to register a new reference.
    - When "No" is entered the entire procedure is run through without interruptions, and no interaction with the operator is required. The Path control and the Gas cylinder controls have to be set at "Automatic".

The calibration flag is a status output which normally should be set off.

Reference calibration step by step

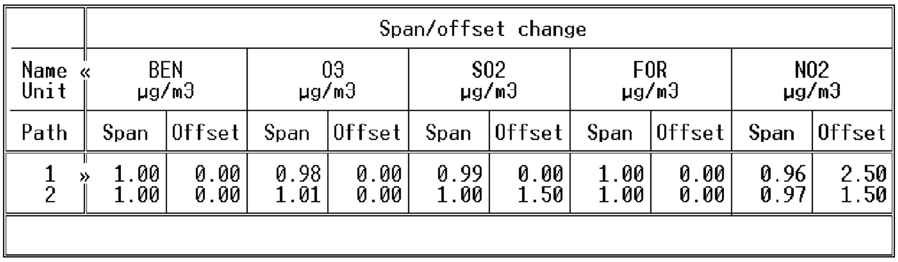
1. The first recording is compared with the old reference spectrum.
    - In case the concentration and the deviation are higher than the Threshold values (see section 7.4.4, Reference calibration) the result is "Fail" and the procedure is terminated. The zero air source, the calibration light source, etc., should then be checked for possible causes to the failure.
    - In case the concentration and deviation values are better than the New ref. limit values the result is "Ok". The procedure is terminated, since no new reference is required.
    - When the concentration and deviation values are within the range between the New ref. limit and Threshold values the result is "New", and a second recording is made.
2. The new recording is compared with the first one. When the new concentration and deviation values are better than the New ref. limit values the reference result is "Ok", and the second recording is stored as a new reference. When outside the New ref. limit values the result is "New" and another is made. The number at Max repetitions set the total number of trials.
3. In case no new reference is good enough, the procedure is terminated and the original reference is restored.

The results from each step in the reference calibration procedure are presented on the screen. The results include information on concentration, deviation, light level and whether the new reference is accepted or not. All results can be reviewed View calibration results function, see section 9.5, Calibration results.

9.4 Manual change of span and offset

The gas calibration is resulting in span and offset factors for each gas, which are used to correct the primary measurement results produced by the analyser. One span and one offset factor can be set for each gas on each measurement path. The gas concentrations which are presented on screen and stored on the hard disk are first multiplied with the span factor, and then added with the offset factor.

All factors can be viewed and changed when selecting [F3] Change span/offset in the Calibration procedures menu. The span and offset factors can also be adjusted automatically, see section 7.4.3, Calibration modes/calibration gases and section 9.2, Span/offset calibration.



Span/offset change

Name « Unit	BEN µg/m3		O3 µg/m3		SO2 µg/m3		FOR µg/m3		NO2 µg/m3	
Path	Span	Offset	Span	Offset	Span	Offset	Span	Offset	Span	Offset
1 »	1.00	0.00	0.98	0.00	0.99	0.00	1.00	0.00	0.96	2.50
2	1.00	0.00	1.01	0.00	1.00	1.50	1.00	0.00	0.97	1.50

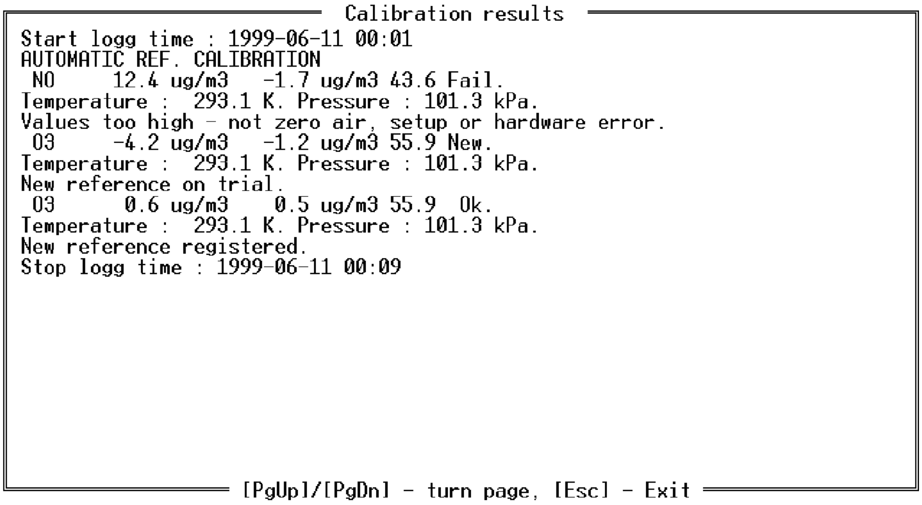
Figure 9.5. Menu for changing span and offset factors.

Use the arrow keys to control the cursor. Press [Enter] for the parameter to change, and type the new value.

***Note**: The span has no unit whilst the offset factors should be entered in the same unit as defined in the Measurement time setup menu (section 7.3.4, Measurement time).*

9.5 Calibration results

All calibration results are stored in a text file which can be reviewed by selecting [F4] View calibration results.



```
Start logg time : 1999-06-11 00:01
AUTOMATIC REF. CALIBRATION
 NO     12.4 ug/m3   -1.7 ug/m3 43.6 Fail.
Temperature :  293.1 K. Pressure : 101.3 kPa.
Values too high - not zero air, setup or hardware error.
 O3     -4.2 ug/m3   -1.2 ug/m3 55.9 New.
Temperature :  293.1 K. Pressure : 101.3 kPa.
New reference on trial.
 O3      0.6 ug/m3    0.5 ug/m3 55.9  Ok.
Temperature :  293.1 K. Pressure : 101.3 kPa.
New reference registered.
Stop logg time : 1999-06-11 00:09
```

Figure 9.6. All calibration results are listed in a text file.

The information is the same as being presented on the screen at each step of the calibration procedures. To view the information, a start date should be entered. If there is more information for the selected day than is displayed on the screen, it can be viewed by pressing the [PgUp] and [PgDn] keys.

Use the [Esc] key to return to the calibration menu.

9.6 Restore reference

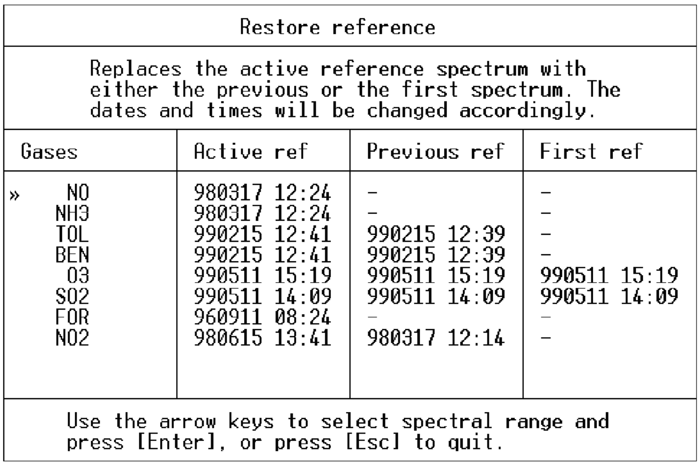
***Note**: Reference calibration may not be available for some gases.*

When doing a reference calibration the currently active reference spectrum is compared with the just recorded one. Based on pre-defined conditions the analyser determines whether the new spectrum is better than the currently existing reference.

During manual reference calibrations a new reference can always be forced to be accepted. This is necessary for instance when the conditions are not set properly, or if the active reference spectrum is bad. However, it also increases the risk of recording a bad spectrum.

A bad reference spectrum is often causing evaluation failures, indicated by negative deviations, see section 6, Measurements. If a bad reference spectrum has been accepted by the analyser, a new reference should be recorded. However, in many cases it would be safer to restore the previously active spectrum prior to recording a new one. The ordinary comparison could then be used to indicate whether the new spectrum is acceptable or not.

An old reference can be restored by selecting [F5] Restore reference in the Calibration menu.



```
                    Restore reference

        Replaces the active reference spectrum with
        either the previous or the first spectrum. The
        dates and times will be changed accordingly.

 Gases            Active ref       Previous ref     First ref

»    NO           980317 12:24     -                -
   NH3            980317 12:24     -                -
   TOL            990215 12:41     990215 12:39     -
   BEN            990215 12:41     990215 12:39     -
    O3            990511 15:19     990511 15:19     990511 15:19
   SO2            990511 14:09     990511 14:09     990511 14:09
   FOR            960911 08:24     -                -
   NO2            980615 13:41     980317 12:14     -

      Use the arrow keys to select spectral range and
      press [Enter], or press [Esc] to quit.
```

Figure 9.7. Selecting which reference to restore.

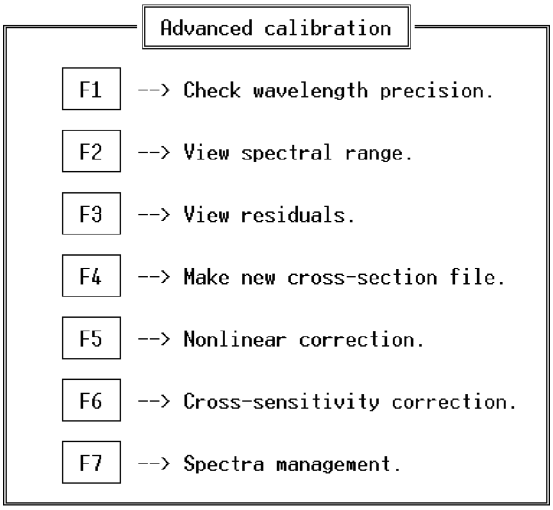
All gases which the analyser is calibrated for are listed in the window. Each row corresponds to a group, i.e. one or more gases measured and evaluated in parallel. Since there is only one reference spectrum per group, the reference for all gases in the same group will be changed simultaneously.

- Select which group to restore the reference for with the arrow keys, and press [Enter].
- Select whether the previous, [P], or the first, [F], reference should be restored. The first reference was recorded when the instrument was assembled.
- In order to avoid mistakes, the analyser asks "Are you sure?" before replacing a spectrum. Answer [Y] or [N]. There is no undo function.

9.7 Advanced calibration menu

__Warning__: Make sure you fully understand the function of the different procedures found in this menu before you use them. Improper use may result in analyser malfunction and complete loss of calibration.

The Advanced calibration menu is accessed through the Calibration menu and is opened by pressing [F6]. The menu can be protected with a password.



Advanced calibration

F1 --> Check wavelength precision.

F2 --> View spectral range.

F3 --> View residuals.

F4 --> Make new cross-section file.

F5 --> Nonlinear correction.

F6 --> Cross-sensitivity correction.

F7 --> Spectra management.

Figure 9.8. The Advanced calibration menu.

- [F1] Check wavelength precision is used to check the wavelength setting of the analyser. A mercury lamp CA004 is required.
- [F2] View spectral range displays the light source spectrum on the screen.
- [F3] View residuals starts re-calculations of the activated components. This function can be used for instance to check the result when a new reference has been recorded.
- [F4] Make a cross-section file is used when a new oxygen spectrum is to be recorded. Oxygen is only interfering with some components being monitored in ambient air.
- [F5] Nonlinear correction gives a possibility to correct for a non-linear response at the high end of the measurement range.
- [F6] Cross-sensitivity correction is an advanced function for compensating for cross-sensitivities between gases, in particular when one gas is present in very high concentrations.
- [F7] Spectra management is used to activate continuous storage of measurement spectra, and to move spectra for viewing.

Press [Esc] to exit the menu.

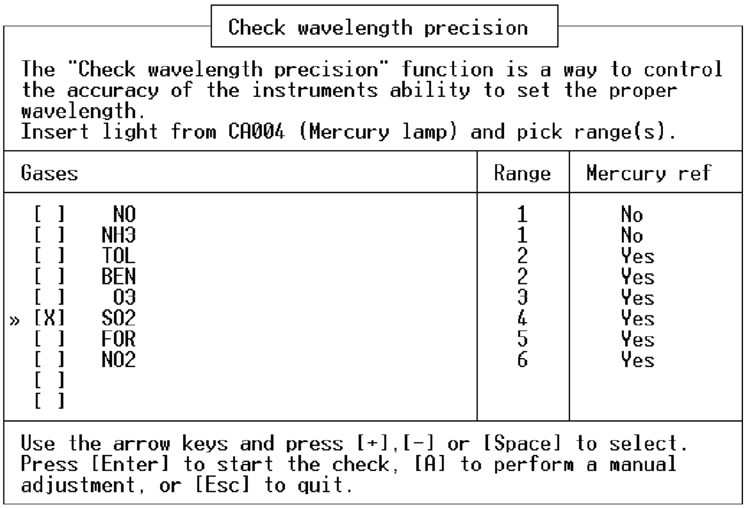
9.7.1 Check wavelength precision

Note: This function is only available in the UV-DOAS instruments.

The accurate setting of the grating to a wavelength window is performed in three steps (assuming the grating is not fixed):

1. **Resetting**. The grating rotates almost a full revolution. The function is checked by parameters 1 and 2 in System check.
2. **Resetting, part 2**. The grating is moved so that the 0:th order of interference (the reflected image) is centred onto the detection system. The peak should be positioned at channel no 500 within ± 50 channels. Parameters 3, 4 and 5 in System check provide information about this function. It can also be checked using the sub-menu View spectral range.
3. **Setting**. The grating is then moved to the position where the measurements are made. A wavelength window with a width of typically 40 nm is projected onto the detector, and the accuracy of the grating position must be within ± 10 channels. This can be checked by using the Check wavelength precision function.

When the instrument was manufactured, mercury spectra for most of the measurement components was recorded. The precision of the grating setting can then be checked by recording a new mercury spectrum and comparing the position of mercury peaks with the old ones. An Opsis mercury lamp CA004 is required.



```
Check wavelength precision

The "Check wavelength precision" function is a way to control
the accuracy of the instruments ability to set the proper
wavelength.
Insert light from CA004 (Mercury lamp) and pick range(s).

Gases                                Range   Mercury ref

  [ ]   NO                             1        No
  [ ]  NH3                             1        No
  [ ]  TOL                             2        Yes
  [ ]  BEN                             2        Yes
  [ ]   O3                             3        Yes
» [X]  SO2                             4        Yes
  [ ]  FOR                             5        Yes
  [ ]  NO2                             6        Yes
  [ ]
  [ ]

Use the arrow keys and press [+],[-] or [Space] to select.
Press [Enter] to start the check, [A] to perform a manual
adjustment, or [Esc] to quit.
```

Figure 9.9. The setup menu for the Check wavelength function.

Several components may have the same Range indication. They are then evaluated in the same wavelength window, and are thus using the same mercury spectrum. Use the [+], [-], or [Space] keys to select components. Only the components for which a mercury reference exists can be checked (indicated with "Yes" in the last column).

Prior to the check is started the computer asks for a measurement time. 30 seconds is usually sufficient.

Press [A] to make a manual adjustment of the wavelength setting.

Check wavelength precision procedure

The procedure is as follows:

1. Connect the CA004 cable to the multiplexer port on the analyser.

2. Connect an opto-fibre (2 to 5 metres long) between the CA004 and the analyser.
3. Switch on the CA004 by pressing the black button gently. The green diode on the aluminium box should give light.
4. Select components to check, set the times, and press [Enter].

When the recording of the mercury spectrum is finished, the result is presented in two ways. First as a graph, where the original spectrum is shown together with the new one. When pressing [Esc], the channel shift is calculated and presented together with an accuracy factor. The accuracy factor is the correlation between the two spectra within an interval of ± 50 channels. The factor can be between 0 and 1, and is here expressed in %. Normally the accuracy is 90 % or higher. The factor is used to confirm that the comparison is made with the correct mercury spectrum, i.e. the mercury lamp functions well and the analyser operates correctly.

The channel shift must not exceed ± 10 channels. The result will otherwise be a negative deviation when the component is evaluated. However, if necessary, a correction of the shift can be made. This correction should be made if the shift is more than 5 channels. It can only be done when the shift is less than 50 channels, and when the accuracy is better than 50 %.

- If a correction is desired, press [Y]. Otherwise, press [Enter] or [N].
- Always repeat the wavelength check when an adjustment has been made.

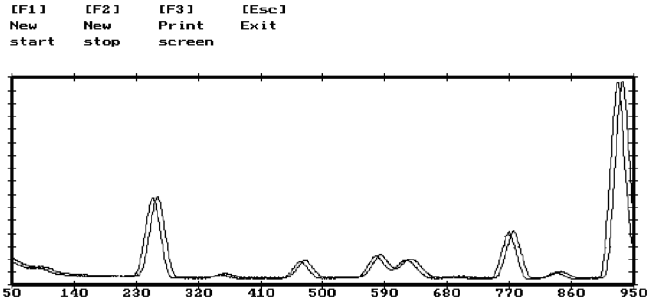


Figure 9.10. Check of the grating precision of ozone, using mercury spectrum. New start and stop channels can be selected with the [F1] and [F2] keys. [F3] is used to generate a printout.

9.7.2 View spectral range

Two possibilities are offered in this submenu:

1. Check of the 0:th order (the same for all gases, UV-DOAS only).
2. Check of the lamp spectrum for an activated gas on a selected measurement path.

When activating View spectral range any light source can be used. A recording time of 30 seconds is normally sufficient. To study a selected lamp spectrum, press any key to continue. To study the 0:th order, press [Z].

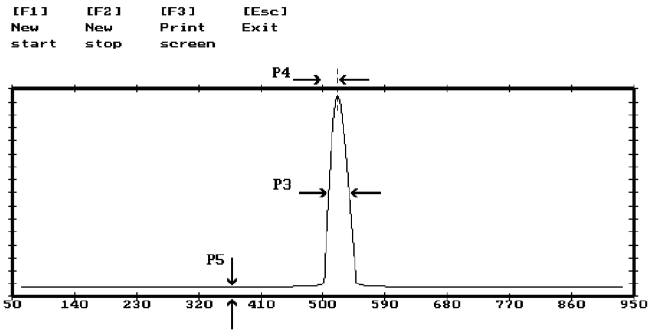


Figure 9.11. Check of the 0:th order. A comparison with the System check is possible (P3, P4 and P5 in the diagram).

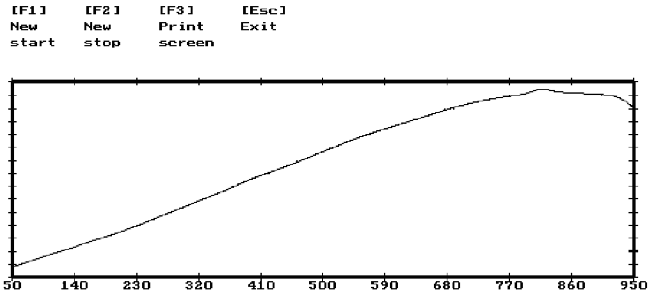


Figure 9.12. Recording of the lamp spectrum in the wavelength window where ozone is measured.

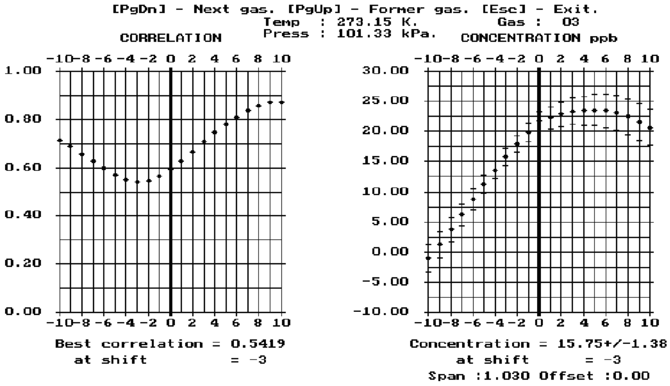
The lamp spectrum should always look the same for each gas. However, small differences in the slope may sometimes be detected, for instance in the window for NO and NH3 when the wrong type of lamp or fibre is used.

9.7.3 View residuals

In a buffer memory, the ten last measurement spectra for each gas from each path are stored. Spectra from the calibration procedures are also stored. These spectra can be retrieved and re-calculated using the View residuals function. This function is important, for instance when the result from a reference calibration is to be checked.

When activating View residuals the gas to be investigated is selected. Use the [+] , [-] , or [Space] keys. Press [Enter] or [M] to view measurement spectra or [C] for calibration spectra.

The last ten measurements for the selected component are listed on the screen. If results from more than one path exists, the path can be changed with the and [←] and [→] keys. Use the [↑] and [↓] keys to select a measurement, and press [Enter] again.



```
Temp  : 273.15 K.        Gas :  O3
Press : 101.33 kPa.
Best correlation = 0.5419
  at shift       = -3
Concentration = 15.75+/-1.38
      at shift       = -3
  Span :1.030 Offset :0.00
```

Figure 9.13. Graphic presentation of the calculations. When pressing [Esc] the result is presented in numbers. Press [P] for a printout. Not available in IR-DOAS.

The correlation is calculated by comparing the fitted spectrum with the recorded spectrum. The presented correlation factor p has a minimum where the spectrum shows the best fit. The results are calculated 21 times, one for each channel within the interval ± 10 channels. To the left the correlation factor p is presented as a function of the shift. The right diagram shows the variation of the concentration together with the standard deviation, the error bars, for each value.

- The correlation curve to the left has a distinct minimum only when there is a gas concentration present. The channel shift for that minimum is a direct measure of the grating setting accuracy. The more centred, the better.
- When measuring on zero air the correlation curve should be as flat, and as close to 1, as possible.
- If no minimum is found, the curve is a continuous slope, the evaluation will fail, leading to a negative standard deviation.

9.7.4 Make a new cross-section file

***Note**: This function is only available in the UV-DOAS instruments, and is primarily intended for use in ambient air quality monitoring.*

In the wavelength window where most of the hydrocarbons are evaluated, oxygen is the major interfering substance. Oxygen is present with a concentration of about 20 %, and the amount of light absorption is only dependent on the path length. However, the oxygen absorption is many times stronger than the absorption from the other pollutants. It is therefore necessary to fit the size of the oxygen spectrum in the evaluation as closely as possible to the one in the monitoring path.

With the function Make new cross-section file it is possible to record an oxygen spectrum for each one of the monitoring paths, and by those means optimising the evaluation of the hydrocarbons.

Equipment

For the performance, the following equipment is required:

- Analyser, calibrated for hydrocarbons.
- Measurement path for which oxygen spectrum is to be recorded. If the lamp in the emitter is ozone generating, the emitter must be provided with a fan.
- A calibration setup CB100, see the section for reference calibrations in the hardware manual.
- A mercury lamp CA004.

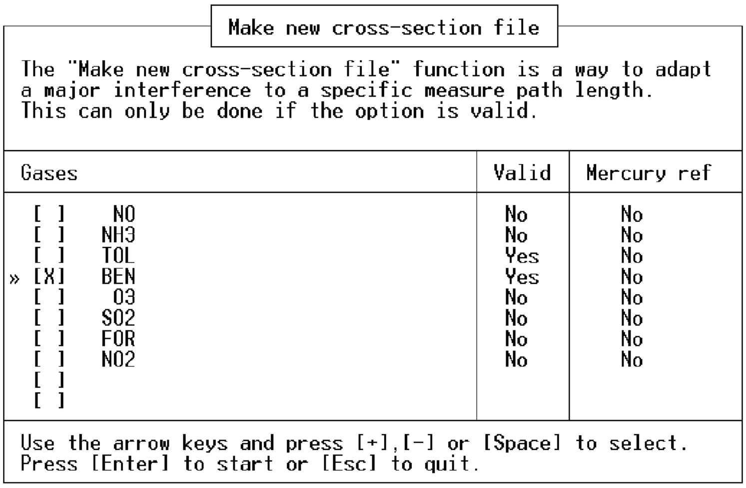
Performance

The performance is made in three steps.

1. First, the atmosphere spectrum is to be recorded. It is therefore important to select a day when the pollution levels are low in order to minimise the offsets of the pollutants.
2. Secondly, a reference spectrum must be recorded, so that the differential absorption can be calculated.
3. The last step is to determine the shift of the spectrum to make it overlap the original calibration spectra. For that purpose a mercury spectrum should be recorded. The final oxygen spectrum is then perfectly fitted to the monitoring path, from which it was recorded. When no CA004 lamp is available the fitting can be made with respect to the previous oxygen spectrum.

The procedure can be repeated for all paths at the monitoring station.

The oxygen spectra are stored as files on the hard disk of the analyser, with the extensions ".App", "pp" indicates the path number. If a certain ".App" file is not found when evaluating, the original oxygen spectrum will be used instead. This file has the extension ".AIR". The ".App" files can thus be deleted without destroying the evaluation (however with great care!).



```
Make new cross-section file

The "Make new cross-section file" function is a way to adapt
a major interference to a specific measure path length.
This can only be done if the option is valid.

Gases                                       Valid     Mercury ref

  [ ]   NO                                  No        No
  [ ]  NH3                                  No        No
  [ ]  TOL                                  Yes       No
» [X]  BEN                                  Yes       No
  [ ]   O3                                  No        No
  [ ]  SO2                                  No        No
  [ ]  FOR                                  No        No
  [ ]  NO2                                  No        No
  [ ]
  [ ]

Use the arrow keys and press [+],[-] or [Space] to select.
Press [Enter] to start or [Esc] to quit.
```

Figure 9.14. Oxygen spectra can only be recorded where the option is valid.

9.7.4.1 New cross-section file performance

1. Adjust the emitter, the receiver, and possibly the multiplexer so that the light level is optimised. The better light level, the better result.
2. Make a System check, and check the wavelength precision with the mercury lamp to make sure that the analyser is running properly.
3. Prepare the calibration light source. The light spot from the fibre end must be smooth, and the light level should be in the order of 60 to 70 %. Check with the analyser in the automatic measurement mode, and adjust the light by adjusting the calibration unit.
4. Activate the component, and set the measurement time to 5 min.
5. Insert the light from the current monitoring path, and enter the path number under which it is defined in the Install station menu.
6. Activated the recording. When finished, move the opto-fibre at the receiver to the CB100 setup so that the same fibre is used as when measuring at the open path. Record the reference spectrum.
7. Finish by recording the spectrum from the CA004 lamp. 30 seconds is a sufficient recording time.

Check the result by measuring from the monitoring path. The deviations of the hydrocarbons should have improved compared with the original evaluation, and the concentrations should be in the same order as the deviations. A final adjustment of the offset is necessary, since the hydrocarbon levels which were present when recording the oxygen spectrum are included in the oxygen correction.

***Note**: Oxygen backgrounds in hydrocarbon gas measurements are discussed further in the Opsis QA/QC Manual for ambient air quality monitoring.*

9.7.5 Non-linear correction

In certain applications, for instance when very long measurement paths are installed, the analyser response in not perfectly linear at the high end of the measurement range. This shows up when performing a multi-point gas calibration using standard gas with high concentrations and/or long calibration cells.

The non-linear response can be corrected for by applying a polynomial of the second degree in the evaluation. The polynomial is determined by the analyser based on the result of a multi-point span calibration. The calculated concentration and the analyser response should be entered in the Nonlinear correction menu for at least three calibration points.

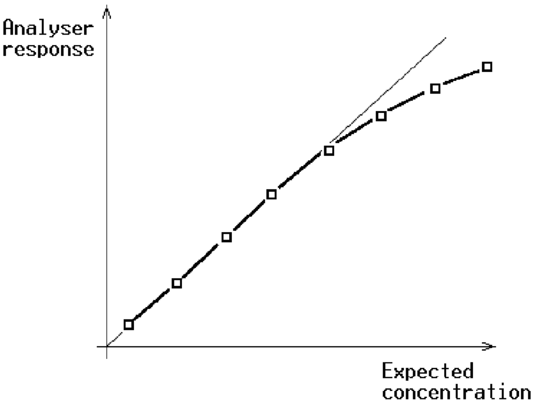
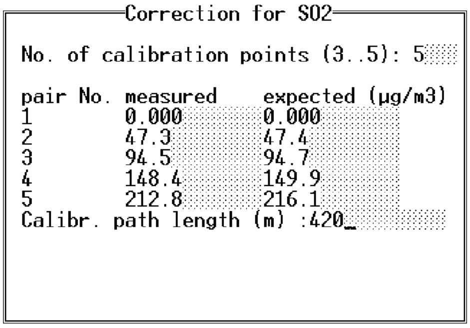


Figure 9.15. Non-linear corrections can compensate for high concentration saturation.

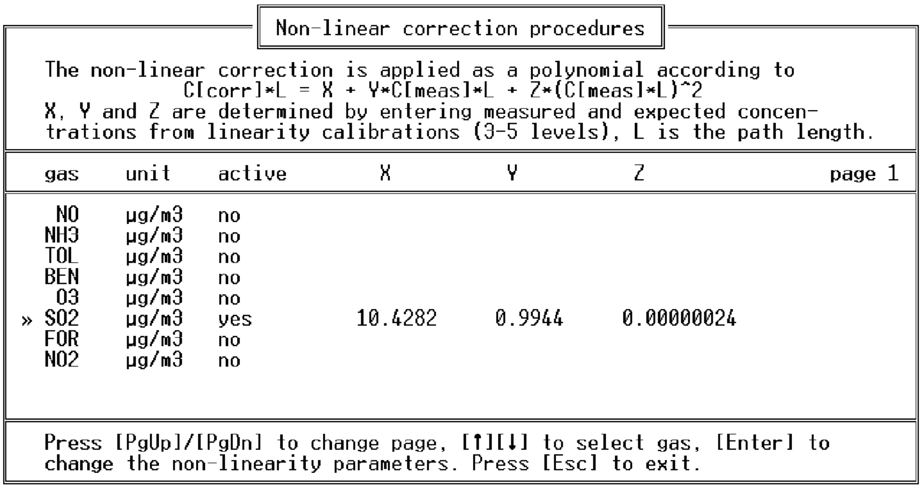
9.7.5.1 Non-linear correction performance

1. Refer to section 4 in the QA/QC Manual in order to make an accurate span calibration consisting of at least three calibration points. Make sure that the full measurement range is covered but not exceeded.
2. Open the Non-linear correction menu, activate the gas in question. Enter the calculated concentration and the analyser response for each one of the calibration points.
3. Repeat the span calibration in order to verify the analyser response.



```
Correction for SO2

No. of calibration points (3..5): 5

pair No. measured    expected (µg/m3)
1       0.000        0.000
2       47.3         47.4
3       94.5         94.7
4       148.4        149.9
5       212.8        216.1
Calibr. path length (m) :420_
```

Figure 9.16. Example of data entry for non-linear correction.



```
                    Non-linear correction procedures

  The non-linear correction is applied as a polynomial according to
            C[corr]*L = X + Y*C[meas]*L + Z*(C[meas]*L)^2
  X, Y and Z are determined by entering measured and expected concen-
  trations from linearity calibrations (3-5 levels), L is the path length.

  gas    unit     active        X          Y          Z              page 1

   NO    µg/m3    no
  NH3    µg/m3    no
  TOL    µg/m3    no
  BEN    µg/m3    no
   O3    µg/m3    no
» SO2    µg/m3    yes        10.4282     0.9944     0.00000024
  FOR    µg/m3    no
  NO2    µg/m3    no

  Press [PgUp]/[PgDn] to change page, [↑][↓] to select gas, [Enter] to
  change the non-linearity parameters. Press [Esc] to exit.
```

Figure 9.17. The resulting correction with polynomial coefficients.

9.7.6 Cross-sensitivities

A cross-sensitivity occurs when the concentration of a certain gas changes the reported concentration of another gas. This may happen for some specific combinations of gases when the Opsis instrument is used beyond the normal operating limits found in the instrument specifications. When a cross-sensitivity does occur, it is however often possible to compensate for it.

9.7.6.1 What gases may show cross-sensitivities?

Continuous Emissions Monitoring and Process Control (CEM): When measuring nitrogen oxide, NO, there is a specified upper limit of allowed SO_2 concentration. If the SO_2 concentration exceeds this limit, the NO measurements will be affected.

Ambient Air Quality Monitoring (AQM): When measuring cyclic hydrocarbons like benzene or toluene on measurement paths with lengths considerably above the maximum recommended 800 m, high ozone concentrations may affect the hydrocarbon concentration readings.

Other situations where cross-sensitivities occur are imaginable, but the two examples above cover almost all reported cases. In the examples below, the two type situations are further discussed.

9.7.6.2 What is the size of the error?

The induced error depends on the path length and the concentration of the gas. In the ambient case, as long as the path length is kept within the limit and the ozone concentration is limited to a few hundreds of $\mu g/m^3$, the cross-sensitivity should be within a few $\mu g/m^3$, i.e. in the range of the normal accuracy of the instrument. However, at installations with path lengths far above one kilometer, there has been reported induced errors of several tenths of µg/m^3. In the CEM case, the error may be relatively of the same size.

The size of the error increases if the reference calibration or the recording of the oxygen background (AQM) was not carried out in the correct manner. If this is the case, there are usually other problems as well.

9.7.6.3 What is the solution?

For the AQM case, ozone has some absorption features in the wavelength window where the cyclic hydrocarbons are measured, giving rise to the cross-sensitivities. However, the ozone concentration is evaluated based on a spectrum obtained at a different wavelength window. By using this ozone concentration, concentrations of hydrocarbons obtained in the other window where cross-sensitivity may occur can be corrected. In the same way, it is possible to correct NO readings based on SO2 in the CEM case.

9.7.6.4 Requirements

A potential cross-sensitivity can be checked by adding known concentrations of the interfering gas to a known concentration of the measured gas. This is done either by using the normal measurement path, adding the interfering gas in a CC110/CC150 calibration cell ("add-on cell"), or by using a calibration bench with cells containing known concentrations of both the interfering and the measured gas.

Hardware requirements and instructions for these measurements can be found in the QA/QC for AQM Manual, section 4.

To check a cross-sensitivity, there are at least three conditions that must be met:

1. Reference calibration, oxygen background recording (AQM), etc. must have been performed in the correct manner according to any of the above manuals.
2. If an add-on cell is used, at the time of the cross-sensitivity check, the interfering gas should be present in as low concentrations as possible.
3. In the add-on cell case (AQM), there must be stable meteorological conditions, with no or only minor fluctuations in the actual concentrations of both ozone and the hydrocarbons.

9.7.6.5 Cross-sensitivity check performance

The software routines makes it possible to perform a true two-dimensional mapping of the relationship between the two gases for varying concentrations of both of them. This is the proper approach, but sometimes it is for practical reasons only possible to vary the concentration of the interfering gas.

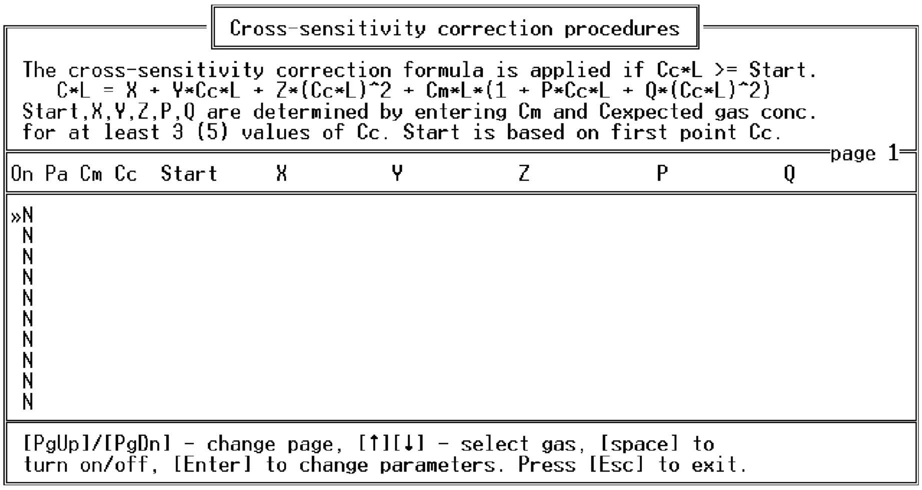
- A two-dimensional mapping is made using a calibration bench with different cells containing separated, but well-known concentrations of the two gases. An example on how this is performed is found in section 9.7.6.7, Example 1: SO_2/NO.

- When an add-on cell is used in the AQM case, the background concentration of the hydrocarbon(s) can not be changed (unless a special arrangement is made using two separated add-on CC110/CC150 cells). The ozon concentration can be increased, however, by adding ozone in the cell. The cross sensitivity test can only be made as an offset adjustment check. This implies a special handling of the measurement data as it is entered in the analyser menu. This case is described in the example in section 9.7.6.8, Example 2: ozone/benzene.

Please read through the two examples further down to see how the tests are performed and how data is entered in the menus.

9.7.6.6 The Cross-sensitivity correction menu

The cross-sensitivity correction menu is accessed by pressing [F6] in the Advanced calibration menu. Doing so, the Cross-sensitivity correction menu is displayed as shown in figure 9.18.



```
                    Cross-sensitivity correction procedures

 The cross-sensitivity correction formula is applied if Cc*L >= Start.
    C*L = X + Y*Cc*L + Z*(Cc*L)^2 + Cm*L*(1 + P*Cc*L + Q*(Cc*L)^2)
 Start,X,Y,Z,P,Q are determined by entering Cm and Cexpected gas conc.
 for at least 3 (5) values of Cc. Start is based on first point Cc.
                                                                  page 1
On Pa Cm Cc  Start     X         Y          Z          P          Q

»N
 N
 N
 N
 N
 N
 N
 N
 N
 N

 [PgUp]/[PgDn] - change page, [↑][↓] - select gas, [space] to
 turn on/off, [Enter] to change parameters. Press [Esc] to exit.
```

Figure 9.18. The Cross-sensitivity correction menu, with no corrections enabled.

Menu basics

Up to 40 cross-sensitivity *relations* can be specified. A relation determines how the measured concentration of a gas, C_m, on one path is influenced by the concentration of another *correcting* gas, C_c, on the same path. There are four pages in the menu, which are selected by pressing the [PgUp] and [PgDn] keys. Within a page, a particular relation is selected by using the up and down arrow keys.

A relation is activated or deactivated by pressing the [Space] bar. However, for memory management reasons, some relation positions cannot always be used. These positions are marked with an "R" (as in "reserved") in the "active" column. If a particular row is reserved, simply select the next non-reserved line instead to specify the cross-sensitivity relation.

A relation is set up by pressing the [Enter] key. First, the path number and the path length (*l*), followed by the number of the measured and the correcting gas is to be entered. The gas numbers are found in the manuals or in the Data presentation menu.

Secondly, the measurement points are to be entered. Specify the number of points, and then, for each point, enter the correcting gas concentration C_c, the reported concentration of the measured gas C_m, and the expected concentration C.

When the data points have been entered, the analyser calculates the best fit of a double second order polynomial, which is used to correct the measured concentration. The following polynomial is used:

$$\begin{aligned}(C \cdot l) &= X + Y \cdot (C_c \cdot l) + Z \cdot (C_c \cdot l)^2 \\ &+ (C_m \cdot l) \cdot [1 + P \cdot (C_c \cdot l) + Q \cdot (C_c \cdot l)^2]\end{aligned} \tag{9.3}$$

Note that the polynomial is applied on absorption level, i.e. the variables are all concentration times length. In this way, the same coefficients can be used even if the path length is changed. The calculation results are displayed on the screen. The residual column shows the remaining error when comparing the concentration after correction with the expected concentration. The polynomial coefficients X, Y, Z, P and Q are shown in the menu. Also note that the X parameter actually is a constant offset, "competing" with the normal offset parameter set in the standard calibration menu!

The lowest correcting concentration C_c being entered will also act as a start point for when the correction is to be used. If the correcting concentration is below this level, no correction will take place even if it is set active in the menu. In order to always get corrections, the lowest correcting concentration should be selected to zero.

Please see the two examples below for a more detailed description of the handling of cross-sensitivity correction data.

Operation

If activated, the cross-sensitivity correction is used as the last step in the evaluation process of the concentration. First, the analyser searches for any relation where the current gas is corrected. Provided that a correcting concentration is available (see below), the concentration is corrected. If there are more than one relation, the gas is corrected in the order the correction appears in the menu.

Secondly, the analyser searches for any relation where the current gas is used to correct another gas. If found, the current concentration, deviation and light level is checked against the filters defined in the analyser installation menu. If the measurement result passes the filter, the concentration values is stored to be used for correction.

Cross-sensitivity correction may be useful, but it may also be a source of confusion and mistakes. When setting up and using the cross-sensitivity corrections, a number of issues should be considered:

1. A filter should be set up for (at least) all correcting gases. If not, the results of the correction can be unpredictable in case of a bad correcting gas measurement, e.g. due to low light levels. If a light level filter is defined, the correcting gas concentration is only accepted if the light level exceeds the filter level. If a deviation filter is set up, but not an S/N filter, the correcting gas concentration is only accepted if the deviation D is below the filter level. If both a deviation level and an S/N level filter is defined, the correcting gas concentration is accepted only if the concentration C fulfils the relation

   $$C > (S_{limit}) \cdot (D - D_{limit}) \qquad (9.4)$$

   S_{limit} = S/N limit, D_{limit} = deviation limit

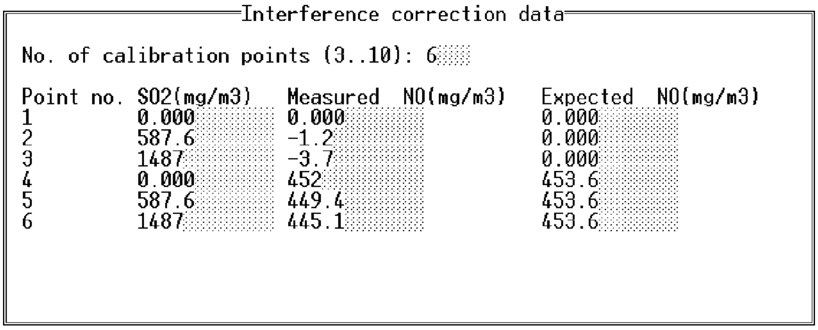
   which corresponds to acceptance of low concentrations at low deviations and high concentrations at slightly higher deviations. See the Data Validation section in the QA/QC Manual for further explanation.
2. The internal buffer storing the most recent (accepted) correcting gas concentrations is reset when (and only when) entering measurement mode in the analyser. This means that results from the first measurement cycle remains non-corrected, providing that the correcting gas is measured after the corrected gas. In that situation, the correcting gas concentration is undefined, and obviously no correction can take place.
3. The correction procedure always uses the most recent *accepted* correcting concentrations. In cases of longer time periods where no correcting concentration values are accepted, there is a potential risk that the correction is based on old and irrelevant measurement result, giving rise to undesired corrections.
4. When leaving measurement mode, the buffer containing the most recent correcting concentrations is *not* reset, but the most recent values are maintained. When span/ offset and other calibrations are to be performed, it may or it may not be desired to keep the most recent correcting concentrations and use them in the evaluation process. It may therefore be necessary to manually deactivate the interference correction prior to performing the calibrations and using the reported concentrations.
5. If a gas is both corrected and used for correction, it is the *corrected* value that is used for correction, *not* the raw value.

9.7.6.7 Example 1: SO_2/NO

In a calibration bench, a true two-dimensional relationship between SO_2 and NO is investigated. By measuring NO, and inserting only calibration cells containing SO_2, the SO_2 influence on NO at zero NO concentration is investigated. Here, three different SO_2 concentrations are generated by using combinations of two cells with different lengths.

Then, a third calibration cell is inserted containing a known concentration of NO. Still measuring NO, the insertion of the different SO_2 cells are repeated, giving the SO_2 influence on NO at an elevated NO concentration. Thereby, three more data points are obtained, and the two-dimensional mapping with different NO and different SO_2 concentrations is completed.

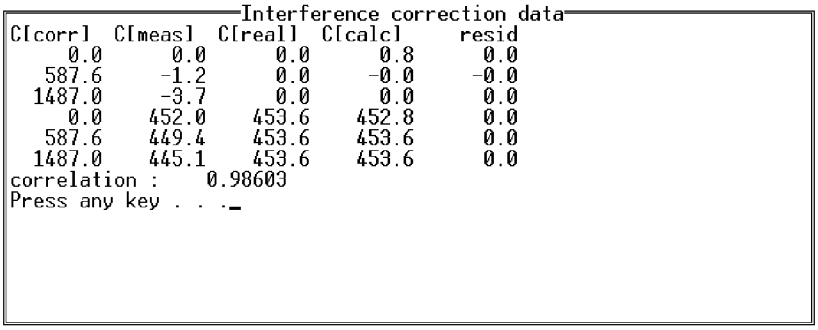
The data is entered according to figure 9.19. Note that since the lowest SO_2 concentration used is 0, the correction will be made for any, also for low, SO_2 concentrations.



```
Interference correction data

No. of calibration points (3..10): 6

Point no. SO2(mg/m3)   Measured  NO(mg/m3)    Expected  NO(mg/m3)
1         0.000        0.000                  0.000
2         587.6        -1.2                   0.000
3         1487         -3.7                   0.000
4         0.000        452                    453.6
5         587.6        449.4                  453.6
6         1487         445.1                  453.6
```

Figure 9.19. Entering SO_2/NO data.

When the data has been entered, the analyser calculates the polynomial coefficients giving the best fit to the data. The result is presented as shown in figure 9.20.

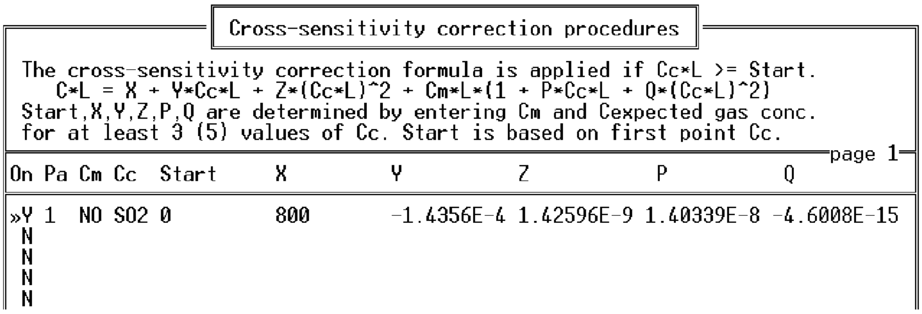


```
Interference correction data
C[corr]  C[meas]  C[real]  C[calc]     resid
    0.0      0.0      0.0      0.8       0.0
  587.6     -1.2      0.0     -0.0      -0.0
 1487.0     -3.7      0.0      0.0       0.0
    0.0    452.0    453.6    452.8       0.0
  587.6    449.4    453.6    453.6       0.0
 1487.0    445.1    453.6    453.6       0.0
correlation :    0.98603
Press any key . . ._
```

Figure 9.20. Showing the result when the best fitting polynomial is applied.

In the menu in figure 9.20, the entered concentrations are repeated. Additionally, the calculated concentrations based on the polynomial, taking the measured C_c and C_m are shown, and the differences between the expected and calculated concentrations C are presented as *residuals*. By looking at the results, it is possible to verify that the entered data is correct, and that the residuals are small. If the polynomial fits badly to the data, the residuals will be larger than shown. This should normally not happen, but if it does, please check that the data is correct. Either the measurement data has been entered wrong, or there may be some measurement error in the raw data.

The resulting polynomial coefficients are shown in figure 9.21.



```
Cross-sensitivity correction procedures

 The cross-sensitivity correction formula is applied if Cc*L >= Start.
    C*L = X + Y*Cc*L + Z*(Cc*L)^2 + Cm*L*(1 + P*Cc*L + Q*(Cc*L)^2)
 Start,X,Y,Z,P,Q are determined by entering Cm and Cexpected gas conc.
 for at least 3 (5) values of Cc. Start is based on first point Cc.
                                                                page 1
On Pa Cm Cc  Start     X         Y          Z          P          Q

»Y 1  NO SO2 0         800       -1.4356E-4 1.42596E-9 1.40339E-8 -4.6008E-15
 N
 N
 N
 N
```

Figure 9.21. SO2/NO polynomial coefficients.

9.7.6.8 Example 2: ozone/benzene

The best way to investigate how ozone influences hydrocarbon (HC) measurements is to introduce ozone in an add-on cell installed in front of the receiver on the normal measurement path. However, the data set will then be limited compared to the SO_2/NO case.

First, it is not possible to do the checking at lower ozone concentrations than presently can be found in the ambient air (background). Secondly, it is only possible to do the check for the present ambient air HC concentration. This means that:

- Both the background ozone and the background HC concentration must be stable during the entire test. This can be checked by regularly filling the calibration cell with clean air during the test, and checking the levels.
- The test should be made at a time when the background ozone concentration is as low as possible. Only then, a fully representative range of ozone concentrations can be checked by introducing additional ozone in the cell. If this requirement is not fulfilled, there will be low ozone data points for which the cross-sensitivity correction relation has never been checked. The mathematical behaviour of the polynomial, i.e. correction result, can then be unpredictable.
- The data entered in the analyser must represent at least two different and well separated HC concentrations. Otherwise, the double polynomial may behave very unstable as soon as the HC concentration starts to deviate from the concentration at which the test was made.

There are three ways to handle the problem in this test situation:

1. Do the test at two different times, with two different background HC concentrations.
2. Use a second add-on cell on the path, where additional HC can be introduced much like the case of SO_2/NO in the calibration bench.
3. If the corrections are small, one can assume that it is mainly an offset correction. A second set of data can then be generated simply by adding a fixed offset to the HC concentrations. This approach is used in this example.

In this example, the background ozone concentration is 53.8 µg/m^3, and the background benzene concentration is 10.3 µg/m^3. At these low concentrations, one can assume that the ozone influence on benzene is negligible. Thus, assuming that the benzene calibration is correct, the expected benzene concentration is also 10.3 µg/m^3. In worst case, the assumption introduces a fixed offset error in the data set, which easily can be corrected by post-processing measurement data.

Since ozone is reactive, it must be generated at the time of the test. This can be done by using either of two devices. An ozone *calibrator* contains measurement an control electronics so it constantly can generate an adjustable and stable ozone concentration. An ozone *generator* also generates different concentrations, but there is no control of the concentration, and an external ozone monitor is therefore required. Both types of devices are available from Opsis.

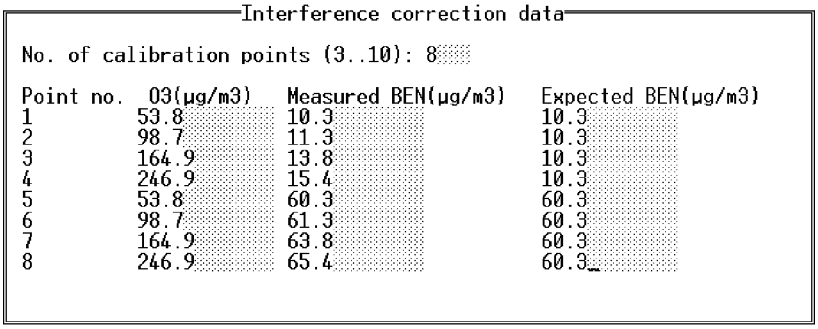
Naturally, since the Opsis analyser does measure ozone, a generator is fully sufficient for checking the current generated ozone concentration. In fact, it is required to monitor both ozone and benzene at the same time, since the background ozone concentration still needs to be established.

So, let the analyser measure both ozone and benzene. Fill the cell with clean air and establish the background concentrations. Then start the ozone generator at a low generation rate and fill the cell with ozone. When the analyser readings stabilise, the first set of data at an elevated ozone concentration can be read. Repeat the test for increasing ozone concentrations. Make sure that the background levels of ozone and benzene do not change during the test by purging the cell with clean air in between each ozone concentration test.

In this example, the tests were carried out for three elevated ozone concentrations: 99, 165 and 247 µg/m^3, corresponding to what ozone concentrations the generator happened to generate. The absolute values are not important as long as they fairly well match the normal measurement range of ozone.

Since only one benzene level was tested, one has to assume that the correction should be an offset adjustment of the benzene concentration. Therefore, a second set of ozone/benzene data is created simply by numerically adding 50 µg/m^3 to the recorded benzene data. Thereby, we assume that the ozone cross-sensitivity at 60.3 µg/m^3 benzene is the same as the cross-sensitivity at 10.3 µg/m^3 benzene. Thus, data is entered as if we had checked two different benzene levels, and the check gave a pure offset cross-sensitivity. The size of the addition, here 50, should be selected to correspond to a "high" value, if the measured concentration is "low", and vice versa. In this way, the polynomial will be forced to cover a large range of the expected benzene concentrations.

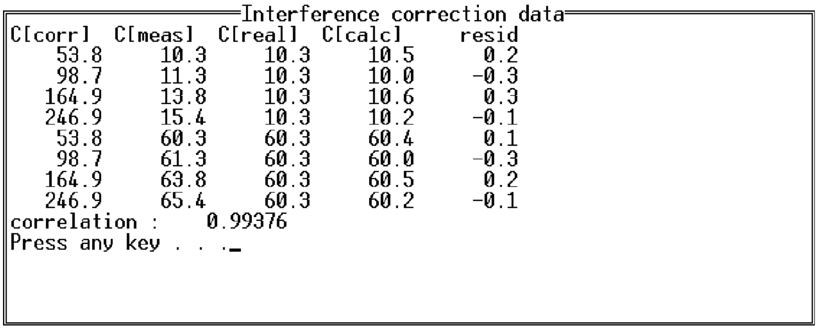
The entered data can be found in figure 9.22. Note that since the lowest ozone concentration is 53.8 µg/m^3, this will also be the start concentration to apply the correction.



```
                    Interference correction data

 No. of calibration points (3..10): 8

 Point no.  O3(µg/m3)   Measured BEN(µg/m3)    Expected BEN(µg/m3)
 1         53.8         10.3                   10.3
 2         98.7         11.3                   10.3
 3         164.9        13.8                   10.3
 4         246.9        15.4                   10.3
 5         53.8         60.3                   60.3
 6         98.7         61.3                   60.3
 7         164.9        63.8                   60.3
 8         246.9        65.4                   60.3_
```

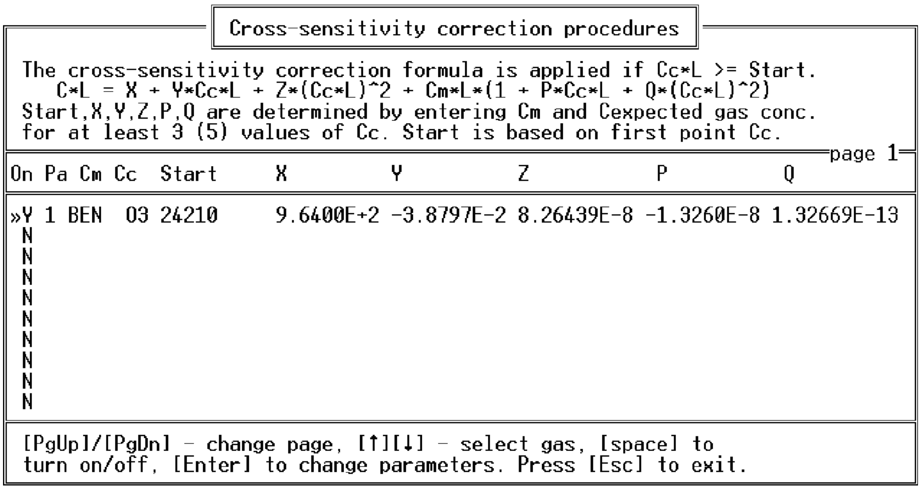
Figure 9.22. Entering ozone/benzene data. The last four data points were created simply by numerically adding 50 µg/m3 benzene to the first four points.

The residuals are shown in figure 9.23 and the final coefficients in figure 9.24.



```
                    Interference correction data
C[corr]  C[meas]  C[real]  C[calc]     resid
    53.8     10.3     10.3     10.5      0.2
    98.7     11.3     10.3     10.0     -0.3
   164.9     13.8     10.3     10.6      0.3
   246.9     15.4     10.3     10.2     -0.1
    53.8     60.3     60.3     60.4      0.1
    98.7     61.3     60.3     60.0     -0.3
   164.9     63.8     60.3     60.5      0.2
   246.9     65.4     60.3     60.2     -0.1
correlation :     0.99376
Press any key . . ._
```

Figure 9.23. The residuals of the ozone/benzene data set.

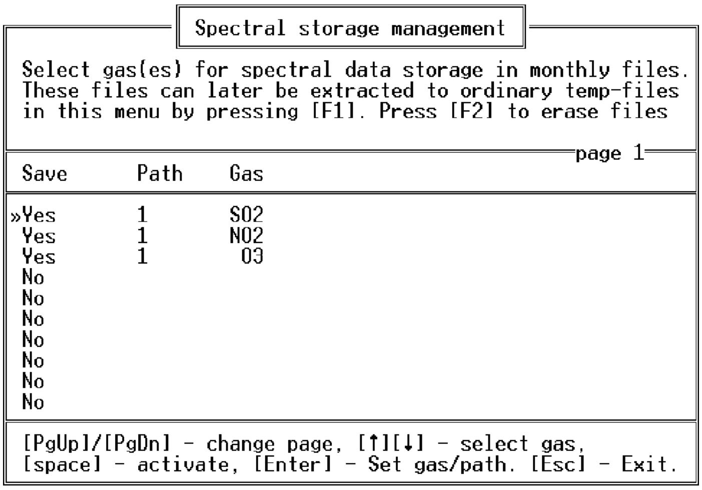


```
                  Cross-sensitivity correction procedures

 The cross-sensitivity correction formula is applied if Cc*L >= Start.
    C*L = X + Y*Cc*L + Z*(Cc*L)^2 + Cm*L*(1 + P*Cc*L + Q*(Cc*L)^2)
 Start,X,Y,Z,P,Q are determined by entering Cm and Cexpected gas conc.
 for at least 3 (5) values of Cc. Start is based on first point Cc.
                                                                page 1
On Pa Cm Cc  Start     X          Y          Z          P          Q

»Y 1 BEN  O3 24210     9.6400E+2 -3.8797E-2 8.26439E-8 -1.3260E-8 1.32669E-13
 N
 N
 N
 N
 N
 N
 N
 N
 N

 [PgUp]/[PgDn] - change page, [↑][↓] - select gas, [space] to
 turn on/off, [Enter] to change parameters. Press [Esc] to exit.
```

Figure 9.24. The ozone/benzene polynomial coefficients.

9.7.7 Spectral management

From the Advanced calibration menu, it is possible to press [F7] to enable permanent storage of all measurement spectra for specified gases and measurement paths. Doing so, a menu as shown in figure 9.25 is displayed.



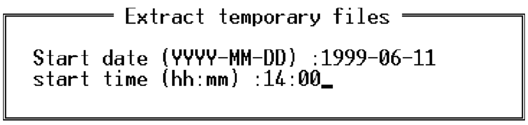
```
Spectral storage management

Select gas(es) for spectral data storage in monthly files.
These files can later be extracted to ordinary temp-files
in this menu by pressing [F1]. Press [F2] to erase files
                                                  page 1
Save       Path    Gas

»Yes        1      SO2
 Yes        1      NO2
 Yes        1       O3
 No
 No
 No
 No
 No
 No
 No

[PgUp]/[PgDn] - change page, [↑][↓] - select gas,
[space] - activate, [Enter] - Set gas/path. [Esc] - Exit.
```

Figure 9.25. The Spectral storage management menu.

On each line, storing spectra of a specified gas at a specified path can be enabled. Use the arrow keys to choose a new line and [PgUp]/[PgDn] to select a new page with additional lines. A line is enabled by pressing the [Space] key. Pressing [Enter] at an enabled line makes it possible to set the gas and path numbers.

When enabled, the spectra will be written to a month file in the special \DATA\LTMP library on the analyser hard disk. The file name will be "yymm_1xx.1yy", with "yymm" being the year and month, "xx" the gas number and "yy" the path number. Additionally, the spectra will also be written to the temporary "TEMP1xx.1yy" files in the standard \DATA directory.

The spectra are not directly accessible in the permanent files. Instead, one must select spectra and move them to the corresponding "TEMP" file. This is done by selecting the desired gas and path and pressing [F1]. The menu in figure 9.26 is shown.



```
Extract temporary files

 Start date (YYYY-MM-DD) :1999-06-11
 start time (hh:mm) :14:00_
```

Figure 9.26. Specifying start data and time for the spectra.

The first ten spectra found in the permanent file, generated after the specified date and time, will then be written to the "TEMP" file. Any spectra already stored in the TEMP file will be overwritten. Once the "TEMP" file has been filled with the desired spectra, it is possible to study them e.g. by using the View residuals function in the Advanced calibration menu.

Once the analyser starts measuring again, the old spectra now found in the "TEMP" file will be overwritten by new spectra. Of course, the new spectra will also be added to the permanent file, if specified.

The monthly permanent file can grow very big, about 100 MB per gas and path, assuming a 2 minute measurement cycle. To avoid unnecessary disk access and to save disk space, it is important to disable all permanent storing of spectra unless the function is specifically required and used.

By selecting a path and gas and pressing [F2], existing permanent files can be deleted from the hard disk. Make sure to use this function frequently if the permanent storage is enabled. If old files are not removed, the hard disk will very quickly become full, and the analyser will not be able to work properly.

For memory management reasons, some rows in the menu may be marked "Reserved". These rows cannot be used for defining a permanent spectral storage. Find another available row, and specify the storage there instead.

System Check 10

The analyser software provides functions for testing the basic performance of the monitoring hardware. These functions are accessed from the root menu by selecting [F5] System check.

Since the hardware differs between the spectrometer based AR500/600 series and the interferometer based AR550/650 series analysers, the functions are different for the two types of analysers.

The system checks verifies the function of the optics and the primary detectors which the gas measurements depend on. Diagnostic messages and numeric test results are presented as an aid for possible fault finding.

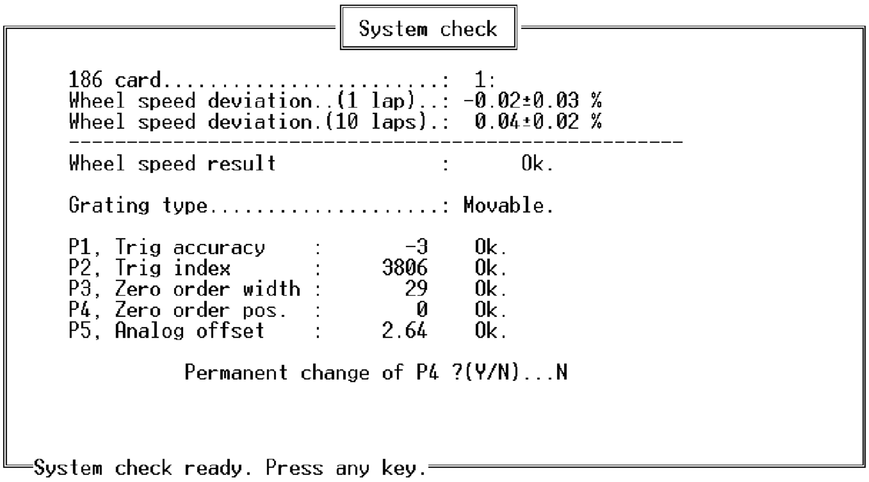
10.1 AR500/600 series analysers

The function of the spectrometer and the electronics of the analyser is of course essential for obtaining measurement results. [F5] System check in the Analyser root menu initialises an internal check of the hardware, which gives important information on how the analyser is performing.

Three hardware related tests are carried out:

- Rotating disk stability
- Grating positioning
- Detection system

The system check starts with testing the stability of the rotating disk. Provided that a light source is available, the test can continue with checking the grating positioning and the detection system. The interpretation of the test results is described on the following pages.



```
                    System check

186 card........................:  1:
Wheel speed deviation..(1 lap)..: -0.02±0.03 %
Wheel speed deviation.(10 laps).:  0.04±0.02 %
-----------------------------------------------------
Wheel speed result              :      Ok.

Grating type....................: Movable.

P1, Trig accuracy    :       -3    Ok.
P2, Trig index       :     3806    Ok.
P3, Zero order width :       29    Ok.
P4, Zero order pos.  :        0    Ok.
P5, Analog offset    :     2.64    Ok.

          Permanent change of P4 ?(Y/N)...N



System check ready. Press any key.
```

Figure 10.1. Information after a completed system check in AR500/600 series analysers.

All test results should be "Ok". If any test result is "Fail", then repeat the system check. This may be necessary depending on the state of the analyser when the system check started. If the check still fails, contact your Opsis supplier, who has trained staff for interpretation and correction of errors.

10.1.1 Rotating disk stability

A rotating disk is mounted in front of the detectors in order to scan the spectra provided by the grating. The time between two slits is measured during one and ten disk revolutions. The result is presented as a relative standard deviation. The deviation should be as close as possible to 0 %.

The Wheel speed result is "Ok" if the standard deviation is below 0.1 %. If more than one 186 cards are installed, the result must be below 0.1 % for all cards. If not, the result will be "Fail". If any of the deviations are greater than 0.1 %, please contact your Opsis representative.

10.1.2 Grating positioning

An analyser is equipped either with a fixed or a moveable grating. A moveable grating must be positioned very accurately. To ensure a proper grating setting, the grating is normally moved to a zero point every tenth or twentieth measurement cycle. It is resetting at a dual light barrier, and the co-ordinate for the grating motor is set to zero.

The grating positioning and the detection system can be checked only when the grating is moveable. A light source must be connected to the analyser through a fibre optic cable. The type of light source is insignificant. The grating positioning and the detection system check will fail if light is not introduced properly into the spectrometer.

The grating positioning check is performed as the analyser rotates the grating. The result of the test is two numbers, P1 and P2.

- P1 is the difference between the actual number of steps between the grating start position and the trigger position, and the pre-calculated number of steps for this movement.
- P2 is the width of the dual light barrier, expressed in number of steps.

The values should be within the following ranges:

Parameter	Allowed range
P1	-150 to 150
P2	3000 to 7000

***Note**: Older versions of the analyser may be equipped with another type of grating motor. These analysers are marked with an X in the serial number. As a consequence the ranges for P1 and P2 are different. P1 should be within -45 and 45, P2 within 300 and 1700.*

10.1.3 Detection system

The three last parameters P3, P4 and P5 provide information concerning the detection system performance. When the check of P1 and P2 is finished the grating moves to a position where the image of the opto-fibre is projected onto the detector. The grating is then used as a common mirror, and no wavelength dispersion occurs.

- P3 refers to the width of the image on the detector. The width will vary a little, dependent on the light intensity. A low light level will result in a lower number.
- P4 is the accuracy of the grating position with respect to the detector. The image should be as centred as possible in the detector. This position is used as the reference point for the grating movement in the next measurement cycle.
- P5, finally, shows the analogue offset in the detection system. See the figure below.

The values should be within the following ranges:

Parameter	Allowed range
P3	20 to 40
P4	-20 to 20
P5	0.1 to 100

***Note**: The permissible range of P3 for AR610-series analysers is 20 - 200, since those analyser detects light only in the infrared region.*

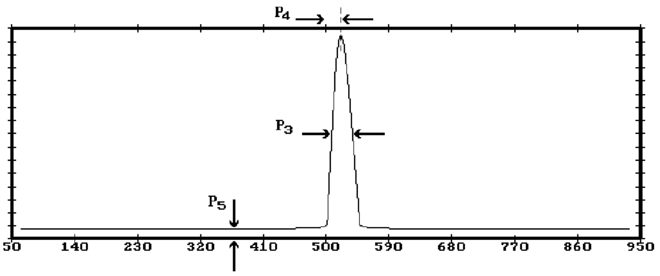


Figure 10.2. Illustration of the system check parameters P3 to P5. The numbers on the x-axis indicate the channel number which is proportional to the wavelength, and the y-axis is the light intensity.

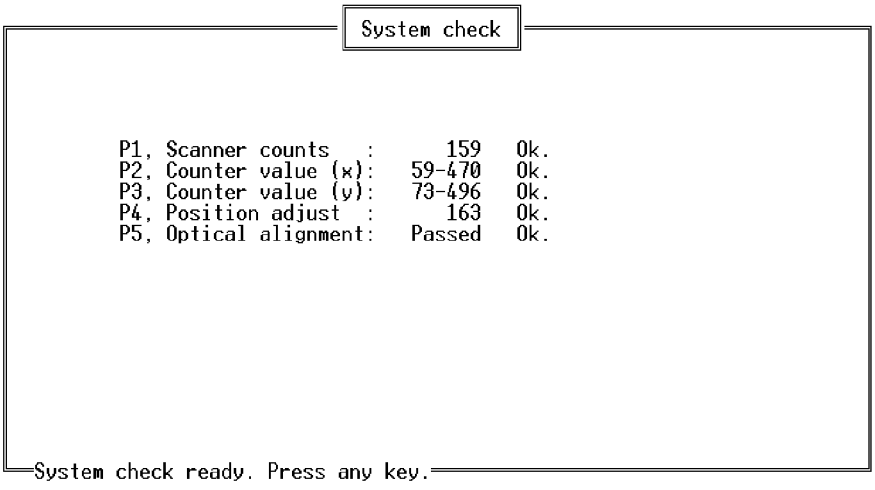
10.2 AR550/650 series analysers

When activating [F5] System check in the AR550 and AR650 analysers the function of the interferometer and the electronics inside the analyser is tested.

Three hardware related tests are carried out:

- Scanner positioning
- Wave-meter control
- Optical alignment

The interpretations of the test results are described below.



```
P1, Scanner counts   :      159   Ok.
P2, Counter value (x):   59-470   Ok.
P3, Counter value (y):   73-496   Ok.
P4, Position adjust  :      163   Ok.
P5, Optical alignment:   Passed   Ok.

System check ready. Press any key.
```

Figure 10.3. Information after a completed system check in AR550/650 series analysers.

10.2.1 Scanner positioning

The scanner inside the analyser moves two mirrors. This movement generates the spectral information for the detector. The System check starts by moving the scanner to a mechanical home position defined by a light barrier. The number of counts for this movement is presented as P1.

In a later step the scanner is moved to an optical home position. This start position is given by an internal light source. The number of steps from the mechanical home position to the optical home position is presented as P4.

***Note**: P1 may fail if the measurements were aborted in an abnormal way, e.g. after a power failure. Repeating the check will remove this warning.*

10.2.2 Wave-meter check

To monitor the movement of the interferometer scanner, a built in HeNe-laser serves as a wave-meter. This device monitors the position of the scanner with an extremely high accuracy, down to less than 50 nm. The system check verifies the output signals from the wave-meter. The wave-meter depends on two laser detectors, each which optimally sees a laser signal varying as a sinus wave, as the scanner moves. The test results are the lowest and highest value of the sinus signal (i.e. the visibility). The results are given as the parameters P2 and P3.

10.2.3 Optical alignment

The optics inside the interferometer has to be realigned on a regular basis in order to compensate for temperature effects. This alignment is performed by adjusting the angle of the beam splitter of the interferometer.

During the alignment procedure, two numbers, D1 and D2 are shown on the screen. These are indicators of the amount of misalignment. The alignment procedure is designed to minimise these numbers. The target is to get the numbers below ±0.2. When this is done, the test result is reported as "passed".

10.2.4 System check results

The system check values should be within the following ranges:

Parameter	Allowed range
P1	-1600 to 1600
P2	X_2-X_1>100, X_2+X_1>250
P3	Y_2-Y_1>100, Y_2+Y_1>250
P4	-1600 to 1600
P5	"passed"

10.3 Automatic system checks

In an AR500/600 series analyser, the system check can be executed automatically at regular time intervals. This is enabled as a part of a calibration sequence, see the section about calibration set-up in section 7, The Installation Menu. The system check can be performed as a stand-alone operation, or an initial check before an automatic span/offset or reference calibration procedure.

In an AR550/650 series analyser, the system check is always carried out automatically at regular time intervals, typically once every 20 measurement cycles. This is required because of the necessary alignment checks of the interferometer. The interval can be adjusted upon request.

The ComView protocol A

This appendix describes routines used for serial communication between Opsis analysers and external computers. Two routines are included: one for collecting results from gas measurements, and one for collecting results from an Opsis datalogger (option).

The last 100 gas measurement results are stored in a buffer memory in the analyser. A second buffer stores the last results from an optional datalogger. The number of stored measurements is dependent on the number of measurement parameters in the datalogger. 100 measurements will be stored using 11 data parameters. If a smaller number of data parameters are used, more measurements will be stored, and vice versa.

Communication routines may at any time read data from these buffers. It is always the oldest values which are returned. If the buffers are filled without being emptied, old data will be overwritten.

A.1 Hardware requirements

The communication is serial, using RS232 interface. The analyser needs only two signals: Send data (SD) and Transmit data (TD), and it does not support handshaking like RTS/CTS etc.

The protocol is available at any serial communication port which has been activated in the communication set-up menu.

A.2 Software settings

In the serial communication 8 data bits, 1 stop bit and no parity is used. Since no handshaking is used, it is important that a high baud rate is used, at least 9600 bps. Otherwise some bytes may be lost.

The communication starts by the acquisition computer, sending a measurement request message to the analyser. An answer message from the analyser is returned, containing measurement information. A password must be passed to the analyser in order to read a measurement value. The password must be the same as specified in the analyser's communication set-up menu. If no password is used, the length of the password (see below) is 0. If the password is incorrect, a buffer empty message will always be returned.

A.3 Messages for gas measurement results

Table A.1: Request message. The password may have length (L) 0.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	49
4	46
5	32 + length of password (L)
6	checksum of byte 1 to byte 5, see below
7	3
8	first character of password
9	second character of password
...	...
8+L-1	last character of password
8+L	checksum of byte 8 to byte 8+L-1
9+L	4

Table A.2: Answer message: measurement value returned.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	49
4	46
5	44
6	216 (= checksum of byte 1 to byte 5)
7	3
8	first character of measurement information, see below
...	...
19	12th character of measurement information
20	checksum of byte 8 to byte 19
21	4

Table A.3: Answer message: buffer empty or wrong password.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	49
4	46
5	32
6	192 (= checksum of byte 1 to byte 5)
7	3
8	0

Table A.3: Answer message: buffer empty or wrong password.

Byte No.	Character(s) (decimal notation)
9	4

A.4 Messages for logger measurement results

Table A.4: Request message. The password may have length (L) 0.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	49
4	47
5	32 + length of password (L)
6	checksum of byte 1 to byte 5
7	3
8	first character of password
9	second character of password
...	...
8+L-1	last character of password
8+L	checksum of byte 8 to byte 8+L-1
9+L	4

Table A.5: Answer message: measurement value returned.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	49
4	47
5	37 + 3* number of data parameters (n)
6	checksum of byte 1 to byte 5
7	3
8	first character of measurement information, see below
...	...
12+3*n	(5+3*n):th character of measurement information
13+3*n	checksum of byte 8 to byte 12+3*n
14+3*n	

Table A.6: Answer message: buffer empty or wrong password.

Byte No.	Character(s) (decimal notation)
1	2
2	32

Table A.6: Answer message: buffer empty or wrong password.

Byte No.	Character(s) (decimal notation)
3	49
4	46
5	32
6	196 (= checksum of byte 1 to byte 5)
7	3
8	0
9	4

The transfer of datalogger information is limited to 24 channels. If the datalogger in the analyser has more than 24 channels, only the first 24 channels will be transferred.

A.5 Synchronisation message

Table A.7: Synchronisation message.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	48
4	49
5	32
6	196
7	3
8	0
9	4

Table A.8: Answer message.

Byte No.	Character(s) (decimal notation)
1	2
2	32
3	48
4	49
5	32
6	196
7	3
8	0
9	4

A synchronisation message may have to be sent if a request message is corrupted on it's way to the analyser. It is recommended to send a synchronisation message before starting the communication session, and then as soon as the analyser does not return an answer to a request message.

The analyser should always return the answer when sending a synchronisation message to it. If not, a hardware error has probably occurred.

A.6 Description of data fields

The length of the password (L) is the number of characters used for the password as it is seen in the analyser's communication menu.

The number of data parameters (n) from the datalogger depends on the set-up of the datalogger, but is at the least 1 and at the most 24.

The checksum byte is calculated according to the following procedure:

```
Sum = 0
For each of the characters do
        Sum = Sum + character ascii code
        Sum = (Sum SHL 1) + (Sum SHR 7)
```

(SHL = shift left, SHR = shift right.)

The result from a gas measurement is transferred in 12 bytes:

Table A.9: Gas data format.

Byte No.	Data type	Description
1 - 2	WORD	Bit 1-5 = day, bit 6-9 = path No., bit 10-16 = gas No
3 - 4	WORD	Time stamp in units of 2 seconds (0 - 43199)
5 - 7	ShortSingle	Concentration in µg/m3
8 - 10	ShortSingle	Deviation in µg/m3
11-12	INTEGER	Light level in %

The result from a datalogger measurement is transferred using a varying number of bytes, depending on the number of parameters (n). The length is (5 + 3n) bytes.

Table A.10: Logger data format.

Byte No.	Data type	Description
1	BYTE	No. of data parameters (1 - 24)
2	BYTE	Day (1 - 31)
3-4	WORD	Time stamp minute (0 - 1439)
5	BYTE	Time stamp second (0 - 59)
6-8	ShortSingle	First measurement value
9-11	ShortSingle	Second measurement value
...	...	...
- 5+3*n	ShortSingle	n:th measurement value

A.7 Description of data types

BYTE	one byte of data ranging 0..255
WORD	two bytes of data ranging 0..65535. The first byte is the least significant byte, the second is the most.
INTEGER	two bytes of data ranging -32768..32767. The first byte is the least significant byte. The most significant bit is the sign flag.
ShortSingle	three bytes of data in the range 1.5E-45..3.4E+38 plus sign and zero value. The type is identical to Intel's SINGLE type (4 bytes), with the least significant byte truncated. The value is stored with the least significant byte first. See description below.

<table>
<tr><td colspan="2">Most significant byte</td><td colspan="2"></td><td>Least significant byte</td></tr>
<tr><td colspan="2">Byte 3</td><td colspan="2">Byte 2</td><td>Byte 1</td></tr>
<tr><td>1 bit</td><td colspan="2">8 bits</td><td colspan="2">15 bits</td></tr>
<tr><td>s</td><td colspan="2">e</td><td colspan="2">f</td></tr>
</table>

If $0 < e < 255$ then	value = $(-1)^s * 2^{(e-127)} * (1.f)$
If $e = 0$ and $f \neq 0$ then	value = $(-1)^s * 2^{-126} * (0.f)$
If $e = 0$ and $f = 0$ then	value = $(-1)^s * 0$
If $e = 255$ and $f = 0$ then	value = $(-1)^s$ * INF
If $e = 255$ and $f \neq 0$ then	value = NAN

(INF = infinity. NAN = not a number.)

A.8 Additional information

A sample program including source code is available from Opsis AB on request. The program is written in Pascal for PC-compatible computers, and illustrates the basics of the communication procedures. Last-minute information on the protocol is also given in the code.

Correcting measurement results B

The analyser can present gas concentrations as weight per standardised volume (e.g. µg/$m^3{}_n$), or as volume fraction (e.g. ppbV).

The analyser measures the pollutant concentrations in the unit µg/m^3 (per definition, the system measures the pollutant concentration as weight per volume gas). This value can then corrected to a weight per standardised volume value (µg/$m^3{}_n$, sometimes written as µg/scm). The correction is done with respect to three parameters:

- temperature T_0
- pressure P_0
- humidity (AR600 and AR650 series only).

The measured concentrations are always stored in the unit µg/m^3 on the hard disk of the analyser. The concentrations are corrected for the current temperature and pressure (and possibly humidity) prior to data storage and presentation of the results on the screen. The values presented on the screen are converted from the mass-per-volume unit µg/$m^3{}_n$ to volume fraction (e.g. ppbV) based on the molar volume at the temperature T_0 and the pressure P_0. T_0 is set to 273 K (0 °C, 32 °F) or 298 K (25 °C), and P_0 to 101.325 kPa (1.01325 bar, 760 mm Hg). (The U.S. EPA convention for T_0 is 298 K.) The molar volume 22.4 m^3/kmol, corresponding to an ideal gas at T_0 = 0 °C and P_0 = 101.325 kPa, is therefore valid for all gases, please see table B.1 for conversion factors.

B.1 Temperature

If the NTP correction is enabled, the analyser is automatically correcting the measured concentration made at the temperature T to the standard temperature T_0. The correction is made according to the following formula:

$$C_0 = C\frac{T}{T_0} \tag{B.1}$$

where

T = actual temperature in K
T_0 = reference temperature, 273.15 K or 298.15 K
C = measured concentration
C_0 = corrected concentration.

The actual temperature T can either be set as a constant by the operator, or be measured and logged by the analyser. In the latter case the pollutant concentrations are corrected for the instantaneous temperature at the measurement path.

B.2 Pressure

The measured concentration is corrected for the current pressure P to the standard pressure P_0. The following formula is used by the analyser:

$$C_0 = C\frac{P_0}{P} \tag{B.2}$$

where

P = actual pressure at the measurement path in kPa
P_0 = reference pressure, 101.325 kPa
C = measured concentration
C_0 = corrected concentration.

Similar with the temperature, the pressure P can either be set as a constant by the operator, or be measured and logged by the analyser.

The two corrections can be combined into one formula, using the same denotations as above:

$$C_0 = \frac{T}{T_0} \cdot \frac{P_0}{P} \tag{B.3}$$

Example 1: A certain measurement of SO_2 gives the result 62.8 µg/m^3. The temperature is 33.0 °C and the pressure is 777 mm Hg. The analyser is logging the temperature and pressure readings, and prior to data storage the result is corrected to 0 °C according to the following equation:

$$C_0 = 62,8 \cdot \frac{273,15 + 33,0}{273,15} \cdot \frac{760}{777}\ \mu\text{g/m}^3 = 68.8\ \mu\text{g/m}^3{}_\text{n} \tag{B.4}$$

Example 2: The analyser above is set to present the results in the unit ppbV (see section 7.3.4, Measurement time). The conversion factor for SO_2 from µg/m^3 to ppbV is

0.3497, see table B.1. The result C_0 = 68.8 µg/m^3 is thus presented as 24.1 ppb on the screen.

Note*: The conversion from the mass-per-volume unit µg/m^3 to the volume fraction ppbV is not performed until after the measurement value has been calculated and corrected for temperature and pressure, and the results have been stored on the hard disk. As a consequence, it is important that accurate temperature and pressure values are used in the evaluation, see section 7.3.3, Path specifications. It is equally important that these values are changed when the instrument is span calibrated, so that the input values are set in accordance with the current conditions.*

B.3 Humidity

The humidity correction gives the concentration as if it had been measured in dry gas, and not in wet gas. The following formula is used by the analyser:

$$C_0 = C\frac{1}{1-\frac{W_n}{804,0}} \qquad \text{(B.5)}$$

where

W_n = humidity in the wet gas, expressed in g/m^3
C = measured concentration in wet gas
C_0 = corrected concentration as dry gas.

Example 3: The NO concentration in wet gas is 298.0 mg/m^3. The humidity is 118.5 g/m^3. The corrected dry NO concentration is then calculated as

$$C_0 = 298,0\frac{1}{1-\frac{118,5}{804,0}}\ \text{mg/m}^3 = 349.5\ \text{mg/m}^3 \qquad \text{(B.6)}$$

The temperature and pressure corrections are calculated prior to the humidity correction.

Once the weight per standardised volume has been calculated (as wet or dry gas), the concentration can be converted to the volume fraction, e.g. ppm or %. The conversion factor is individual for each gas since it is dependent on both the molar weight and the molar volume. The molar volume 22.40 m^3/kmol, corresponding to an ideal gas at 0 °C and 101.32 kPa, is used for all gases.

The conversion factors are found on the next page.

B.4 Conversion factors

Table B.1: Conversion factors at T_0 *= 273.15 K and* P_0 *= 101.32 kPa. The molar volume is 22.40* m^3*/kmol. Please contact Opsis AB for information about other gases.*

Gas No.	**Formula**	**Gas name**	**Opsis label**	**1 µg/m3 ⇔ n ppbV, n =**	**1 ppbV ⇔ n µg/m3, n =**
1	SO_2	sulphur dioxide	SO2	0.3497	2.860
2	NO	nitric oxide	NO	0.7465	1.340
3	NO_2	nitrogen dioxide	NO2	0.4869	2.054
4	CO	carbon monoxide	CO	0.7997	1.250
5	H_2S	hydrogen disulphide	H2S	0.6573	1.521
6	HF	hydrogen fluoride	HF	1.1196	0.893
7	HCl	hydrogen chloride	HCL	0.6144	1.628
8	O_3	ozone	O3	0.4667	2.143
11	NO_3	nitrogen trioxide	NO3	0.3613	2.768
12	N_2O	nitrous oxide	N2O	0.5089	1.965
14	HNO_2	nitrous acid	HNO	0.4765	2.099
16	H_2O	water vapour	H2O	1.2434	0.804
17	NH_3	ammonia	NH3	1.3153	0.760
18	Hg^0	metallic mercury	HG	0.1117	8.955
19	O_2	oxygen	O2	0.7000	1.429
21	C_6H_6	benzene	BEN	0.2868	3.487
22	C_7H_8	toluene	TOL	0.2431	4.113
23	C_8H_{10}	p-xylene	PXY	0.2110	4.740
24	C_8H_{10}	m-xylene	MXY	0.2110	4.740
25	C_8H_{10}	o-xylene	OXY	0.2110	4.740
26	C_8H_8	styrene	STY	0.2151	4.650
27	CH_2O	formaldehyde	FOR	0.7460	1.340
28	C_6H_5OH	phenol	FEN	0.2380	4.202
29	C_8H_{10}	ethyl benzene	ETB	0.2110	4.740
30	C_6H_5Cl	monochl. benzene	MCB	0.1992	5.020
31	$C_6H_4Cl_2$	dichloride benzene	DCB	0.1525	6.558
32	C_9H_{12}	124 trimet. benzene	124	0.1864	5.366
33	C_9H_{12}	135 trimet. benzene	135	0.1864	5.366
34	C_9H_{12}	123 trimet. benzene	123	0.1864	5.366
35	C_2H_4O	acetaldehyde	ACE	0.5091	1.964
40	Cl_2	chlorine	CL2	0.3159	3.165
41	ClO_2	chlorine dioxide	CLO	0.3321	3.011
42	CO_2	carbon dioxide	CO2	0.5090	1.965
43	CS_2	carbon disulphide	CS2	0.2942	3.399
60	CH_4	methane	CH4	1.3963	0.716