

Manual

ISA Spectrometer

Operation at Work



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When installing the system, it is necessary to ensure correct electrical connection, protection against moisture and foreign bodies and excessive condensation, and system heating which can arise from both correct and incorrect use. It is the responsibility of the installer to ensure that the correct installation conditions are provided.

Notes on the Compatibility of Older and Newer Spectrometers

There are three generations of ISA Spectrometers.

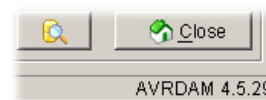
- **First generation**

The CAN ID begins with isa in small letters, e.g. isa00001. Hardware: BlueBox TS and external Spectrometer Module with Article-No. 486 6002 or 486 6004.

- **Second generation**

The CAN ID begins with ISA in capital letters, e.g. ISA00001, and the firmware version of the spectrometer electronics is < 5.00.

The firmware version of the spectrometer electronics is displayed as **AVRDAM** at the bottom right of the spectrometer's sensor setup window.

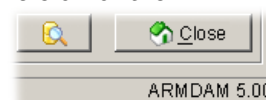


Hardware: BlueBox TS and external Spectrometer Module with Article-No. 486 6002 or 486 6004

- **Third and current generation**

The CAN ID begins with ISA in capital letters, e.g. ISA00001, and the firmware version of the spectrometer electronics is ≥ 5.00.¹

The firmware version of the spectrometer electronics is displayed as **ARMDAM** at the bottom right of the spectrometer's sensor setup window.



Hardware: BlueBox RS and external spectrometer module with Article-No. 486 6000.

Spectrometers of the second and third generation are largely compatible.

⇒ Third generation spectrometers on BlueBox T4/TS are compatible with BlueBox firmware version ≥ 4.05.29 with minor restrictions² in menu operation.

BlueBox PC Software

⇒ The BlueBox PC Software is compatible with older hardware

⇒ Utilisation of the full functionality of third generation spectrometers on BlueBox R1, RP and RS with the BlueBox PC Software with software version ≥ 5.0.

For more information, please contact GO Systemelektronik.

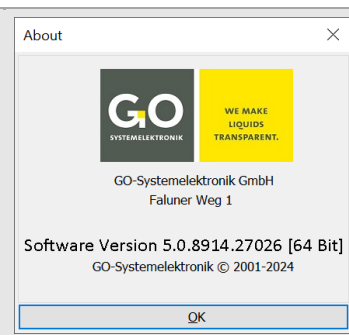
Software version of the BlueBox PC Software: The lead version of the BlueBox PC Software is the version of the AMS program. The AMS program is part of the BlueBox PC Software.

Query the software version of your BlueBox PC Software in AMS:

Call up in the AMS start window under Help>About

The software version of the BlueBox PC Software in this example is 5.0.

The information after the second full stop is for internal purposes.



¹ in addition, the serial number on the label on the spectrometer board is ≥ 1800

² In the T4/TS menu operation, the light power setting of the flash lamp and the entry of a validity limit for the SQL are missing.

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1 Introduction

This manual describes the **operation at work** of the ISA* Spectrometer System of GO Systemelektronik. The operation performs at the display of the BlueBox and with the BlueBox PC Software, here especially with the program AMS and the program Spectrum Visual.

- Described firmware version BlueBox R1/RS and BlueBox Panel: ≥ 5.00
- Described firmware version spectrometer electronic: ≥ 5.00
- Described software version AMS: ≥ 5.00 and Spectrum Visual: 4.6

This manual describes **only the spectral analyser specific operation**.

The general operation of the BlueBox and the BlueBox PC Software is described in the manuals:

- *Manual BlueBox R1 and Panel*
- *Manual BlueBox PC Software*

i A comprehensive documentation of the BlueBox system can be found on www.go-sys.de/downloads.

This manual **does not describe the commissioning, maintenance and service**. This is described in the *Manual ISA and Process Spectrometer Commissioning – Maintenance – Service*.

The symbol **i** indicates useful additional information.

The symbol **!** indicates a note to avoid an operating error.

The symbol **!** indicates an instruction, the non-fulfilment of which may affect the measuring operation.






Note on Text References

References to passages in this document or to passages in other documents are marked in italics.

- *5.1 Overview* e.g. refers to the section 5.1 in this document. The short form is *5.1*.
- *Manual BlueBox PC Software* there *5 AMS – Advanced Managing Software* e.g. refers to the chapter 5 in the Manual BlueBox PC Software

The products of GO Systemelektronik are constantly being developed, therefore deviations between this manual and the delivered product can result. Please understand that no legal claims can be derived from the contents of this manual.

1.1 Meaning of the Safety Instructions

	Danger: Used if non-observance threatens serious injury or death.
	Warning: Used if non-observance threatens slight injuries or serious property damage.
	Caution: Used if non-observance threatens minor property damage.
	Symbol of safety instruction relating to the use of electricity.
	Symbol of safety instruction relating to the ATEX directive.

* Intelligent Spectral Analyser

2 Scope of Delivery

The ISA Spectrometer is available in two versions:

- **ISA BlueBox RS** BlueBox RS with integrated spectrometer sensor unit*
- **ISA BlueBox R1 and Panel** BlueBoxR1 or Panel with one or more external spectrometer modules

1. BlueBox

If the spectrometer will not be integrated into an existing BlueBox system, the BlueBox is part of the delivery scope. Measured values are recorded and forwarded in the BlueBox, the values for the desired parameters are calculated and calibration values are saved. All data and settings can also be read out and changed remotely via the interface to a PC.

For information on the features, installation and general operation, please refer to the *Manual BlueBox R1 and Panel*.

i A comprehensive documentation of the BlueBox system can be found on www.go-sys.de/downloads.

2. Sensor head

The sensor head is available in two versions:

- **Sensor head ISA** Article-No. 410 6012 The measurement path is stepless adjustable from 0.5 to 20 mm with a screw thread. The sensor head has an integrated compressed air cleaning.
- **Sensor head ISA-SDU** Article-No. 461 6010 The measurement path is stepless adjustable from 0.5 to 20 mm with a screw thread. The sensor head is mounted in a flow-through housing with integrated cleaning wiper and has no compressed air cleaning.
see 6 *Technical Data* there *Specifics Sensor Head ISA-SDU*

The sensor head of the ISA is made of high-quality steel (optional titanium). Only the optics and the compressed air cleaning (exception ISA-SDU) are integrated in the sensor head. The sensor head can thereby be deployed in high temperature ranges (up to +110 °C).

3. Sensor head cable (does not affect ISA-SDU)

The sensor head is connected with the spectrometer sensor unit via the special covered sensor head cable. The spectrometer sensor unit contains all the electronics. In the sensor head cables, there are two fibre optic cables and a compressed air line. The sensor head cable must not be bent or kinked in a tighter radius than 40 mm. At installation the sensor head shall not be hung up at the measuring head cable; therefore use the appropriate eyebolts.

4. Spectrometer sensor unit with compressed air connection and cleaning wiper connection

Either integrated (BlueBox RS) or in an external spectrometer module.

The entire control and analysis electronics of the ISA are located in the spectrometer sensor unit.

5. Software (optional)

USB stick with the system software

6. USB Dongle (optional)

Protection against unauthorized access

7. CAN-bus cable (only spectrometer module)

8. Spectrometer data sheet of Zeiss

9. Configuration data sheets and test protocols

* Additional sensor units can be connected with external sensor modules via the CAN-bus interface.

3 Commissioning

The commissioning of the ISA spectrometer is described in detail in the *Manual ISA and Process Spectrometer Commissioning - Maintenance - Service.*

4 Notes on Operation

4.1 Safety Instructions and Warnings



Never deliver the BlueMon to other persons without this manual. The manufacturer is not liable for improper or unintended usage.

The instrument is constructed according to the low voltage code and to the safety regulations for electronic measuring devices.

Correct function and safety can only be ensured when both general and system-specific safety measures are followed.

Before connecting the power supply, make sure that the power supply voltage is suitable.

The proper functioning and operational safety of the devices can only be maintained under the ambient conditions specified in chapter 6 Technical Data in this manual.

If the instrument is moved from a cold to a warm environment, condensation might form which could influence its function. In this case, wait for the instrument to reach equilibrium with the new surroundings before use.

Maintenance and repairs may only be carried out by GO-authorized technicians.

If it can be assumed that the devices can no longer be operated safely, they must be taken out of service and secured against further use by labelling.

The user's safety might be affected if the instrument shows signs of damage, does not function properly, has undergone long storage under unsuitable conditions or was subject to extreme transport conditions.

If in doubt, contact the manufacturer GO Systemelektronik GmbH and send the instrument for repair or maintenance if necessary.



Caution: The sensor head must not be exposed to negative pressure or pressure shocks.



Caution: The sensor head cable must not be bent or even kinked in a tighter radius than 40 mm.





Caution: The sensor head must not be hung on the sensor head cable, use the eyebolts for installation of the sensor head.

4.2 ATEX Notes

These ATEX notes only apply to the ISA R1 version with the sensor head ISA at a Spectrometer Module.

Guideline 2014/34/EU, known as the ATEX directive of the European Union, requires in Annex II to the fulfilment of basic safety requirements for devices that are provided within the EU for use in potentially explosive atmospheres.




The sensor head of the spectrometer has the following ATEX-characterisation:
 II 3/- G Ex op is IIA T4 Gc/-


A version with ATEX category 2 is available on request; further details on request from GO Systemelektronik.




When using the GO cleaning wiper (Article-No. 462 SW00) on the sensor head ISA the ATEX directive is no longer fulfilled



Danger: The spectrometer module must absolutely be located outside the explosion-endangered area.



Warning: The supply voltage must not be applied to the housing of the spectrometer module; the housing of the spectrometer module must always be earthed.



Danger: The electrical resistance between the lower eyebolt of the sensor head and the earthing screw of the spectrometer module must be less than 50 Ω.

Parameter:

Electrical data:	maximal input voltage of the sensor module:	28 VDC
Range of ambient temperature:	Sensor head:	0 °C to +110 °C
	Sensor module:	0 °C to +40 °C

Special conditions for safe use:

- The ambient temperature of the sensor is 0 °C to +110 °C.
- The sensor module must be installed outside of explosion-endangered areas.
- The ambient temperature of the sensor module is 0 °C to +40 °C.

The basic safety and health requirements are fulfilled by compliance with:

- DIN EN 60079-0:2014-06 General requirements
- DIN EN 60079-28:2016-04 Optical Radiation 'op is'



Identification of the sensor head:
Laser engraving



Identification of the spectrometer module:
abrasion resistant label on the outside right



5 Description of the ISA Spectrometer

5.1 Overview

The ISA Spectrometer is available in two versions:

- **ISA BlueBox RS** BlueBox RS with integrated spectrometer sensor unit¹
- **ISA BlueBox R1 and Panel** BlueBoxR1 or Panel with one or more external spectrometer modules

The ISA measures the absorbance² in the wavelength range from 200 to 708 nm (UV/VIS). The result of a single measurement is each a raw spectrum and an absorbance spectrum calculated there from over the entire wavelength range.

A spectrometer is a very multi-purpose measuring instrument because it can be implemented in very diverse applications through a relevant calibration. In contrast to electrochemical sensors, multi-parameter measurements are also possible. Moreover, the ISA offers an adjustable measurement path length whereby the number of potential applications is increased even more.

A great advantage of the ISA is the special coating of the glass panes in the optical measurement path and the possibility to clean the measurement path automatically with compressed air (exception ISA-SDU, here cleaning is done with a wiper), thus very long service lives and service intervals can be achieved.

Only the optics and the compressed air cleaning system are integrated in the in situ submersible measuring head made of stainless steel (material number 1.4404) or titanium. The entire control- and analysis-electronics are mounted in a BlueBox RS with integrated spectrometer sensor unit or in an external spectrometer module. The ISA is thereby usable in a high temperature range (up to 110 °C). ISA is thus suitable for use in medicine or in the food industry, since the measuring head can be sterilized at high temperatures.

All necessary settings are stored in the spectrometer electronic, so the external spectrometer modules can be connected to another BlueBox without changing the BlueBox settings.³

The ISA R1 can be used in potentially explosive areas, for details see 4.2 ATEX Notes.

The properties of the ISA in summary:

- Connection of the only optical sensor head with the analysis unit via the sensor head cable (integrates two fibre optic cables and a compressed air line).
- Measurement path length freely adjustable from 0.5 – 20 mm
- Automatic cleaning of the measurement path with compressed air or wiper
- Suitable for a wide temperature range (0 °C to +110 °C)
- Recording of absorbance spectra and raw spectra in the range 200 – 708 nm
- Saving of raw data and calibrated data
- Calibration and service software
- Calculation of the statistical reliability of measured values (SQI)
- Adjustment of calibration by remote maintenance
- Multi-parameter calculation
- Simple installation
- High cost-efficiency

¹ Additional sensor units can be connected with external sensor modules via the CAN-bus interface.

² In absorption, radiation is absorbed by a substance. Further attenuating effects due to scattering or reflection are summarized in the optics together with the absorption under the term **absorbance**, also called **extinction**.

³ Applies only to spectrometers of the second and third generation.
see *Notes on the Compatibility of Older and Newer Spectrometers on page 3*

Applications:

- Sewage treatment plants (inflow, outflow, process control)
- Industrial waste water (process water, waste water treatment)
- Waste water collection systems (load monitoring, corrosion protection)
- Water treatment, reuse and irrigation
- Environmental monitoring (monitoring of surface water)
- Aquacultures and fish farms
- Monitoring of landfill leachate
- Drinking water (source monitoring, process control, early warning of contamination)
- Groundwater management
- and other

Parameter examples:

- **Nitrate:** for NO₃/NO₃-N measurements
Measurement range 0.1 - 100 mg/l NO_x_eq in water bodies (other measurement ranges are possible)
- **Carbon compounds TOC/COD:** Calibration by comparison analysis. Resolution and accuracy depend on the stability of the water-matrix and its ability to be analysed.

5.2 Notes on Compressed Air Cleaning
does not affect ISA-SDU

In most applications, it is useful to use the compressed air cleaning of the spectrometer. The compressed air line must be connected to the provided plug-in connection of the BlueBox RS or the external spectrometer sensor module.

! Use only oil-free compressors.

The air consumption of the compressed air cleaning depends on the connection pressure (4 - 6 bar) and the back pressure in the medium and is at 6 bar at a maximum of 1 litre per second.

Example: At an interval of 60 seconds and a cleaning time of 5 seconds, the maximum consumption is 300 litres per hour.

5.3 Notes on the Cleaning Wipers

The ISA sensor head can be equipped with a cleaning wiper. Precondition is, that the spectrometer board is equipped with a wiper module. *see Appendix B – The Spectrometer Board*

The sensor head ISA-SDU is supplied from the factory with a cleaning wiper. This wiper is controlled by a PLC* program in the BlueBox.

5.4 Notes on the SQI (Spectral Quality Index)

The SQI is a degree of the statistical reliability of measurement values of an application-specific parameter (see 9.3 *The Sensor Setup Window of an Application-Specific Parameter*). Precondition is the creation of a corresponding calibration file in the xml format.

see Manual ISA and Process Spectrometer Commissioning - Maintenance - Service

see Appendix B – SQI (Spectral Quality Index)

* Programmable Logic Controller

6 Technical Data

The ISA Spectral Analyser with its in situ submersible sensor head is either integrated into a BlueBox (BlueBox RS) or into an external sensor module that is connected to a BlueBox system with CAN-bus.

ATEX notes see 4.2

Spectrometer unit	
Wavelength range	200 nm to 708 nm, resolution 2 nm
Measurand	UV/VIS spectra in the range 200 to 708 nm
Measurement principle	Spectral analysis
Measurement interval	Adjustable, min. 30 s
Light source	Xenon flash lamp

BlueBox RS	Article-No. 486 00RS
-------------------	-----------------------------

The technical data of the BlueBox RS are those of a BlueBox R1 with integrated spectrometer board.
see *Manual BlueBox R1 and Panel* see also *Appendix C – Housing Connections at the BlueBox RS*

Spectrometer sensor module (external)	Article-No. 486 6000
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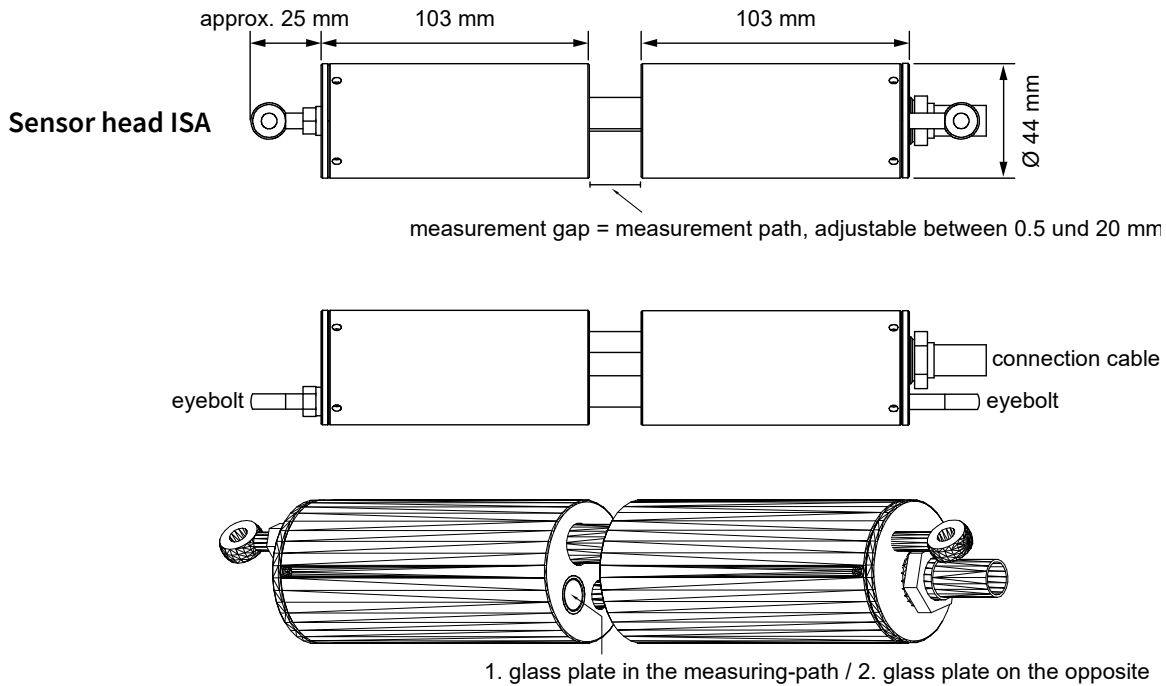
see also 17 *The External Spectrometer Sensor Module*

Power supply	24 VDC (18 – 28 VDC) via CAN-bus cable
Power consumption	typical 3 W
Pulse input	Frequency (rising edge) or static The pulse input is galvanically isolated from the system.
Compressed air connector	Quick connector for 4 mm PU-tube, 4 – 6 bar
Temperature range	0 °C to +40 °C
Weight	2.6 kg
Housing material	Die-cast aluminium, powder coated
Dimensions	303 x 200 x 93 mm (L x W x H)
IP protection code	IP65

Sensor head ISA	Article-No. 410 6012
------------------------	-----------------------------

Material	see also Appendix C High grade steel (material number 1.4404) – Titanium optional
Cable length	2.5 m 6 m 10 m other cable lengths on request
Temperature range	0 °C to +110 °C
Measurement gap	0.5 – 20 mm stepless adjustable Measurement gap = Measurement path
Weight (High grade steel)	1.5 kg
Ambient pressure	max. 6 bar ⚠*
IP protection code	IP68

* ⚠ **Caution:** The sensor head is not suitable for environments with negative pressure or pressure shocks!



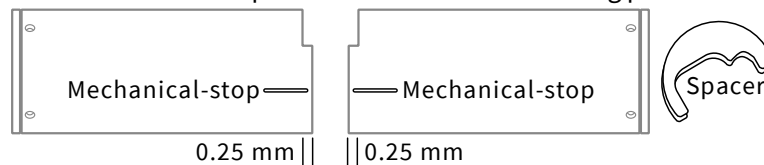
Specifics Sensor Head ISA-SDU

Article-No. 461 6010

- The sensor head has no compressed air cleaning; the sensor head cable has no compressed air line and is therefore more flexible



- The sensor head cable has a length of 1 m, others on request.
- The sensor head is mounted in a flow through fitting with integrated cleaning wiper.
- The sensor head is designed for operation with a cleaning wiper. The wiper is controlled by a PLC* program in the BlueBox.
For more information, please contact GO Systemechnik.
- The measuring path is continuously adjustable from 0.5 to 20 mm with a screw thread.
- The sensor head has a mechanical-stop on each side of the measuring path.



The minimum measuring path length is therefore 0.5 mm.

! The wiper thickness must match the gap of the measuring path.

The standard range of the gap width is 0.5 to 5 mm.

Available spacers in thickness | 0.5 mm | 1 mm | 5 mm | 10 mm | 20 mm |

* Programmable Logic Controller

6.1 Sensor Head ISA – Notes on the Glass Panes in the Measurement Path



Older ISA sensor heads have glass plates made of quartz glass. New ISA sensor heads have glass plates made of sapphire glass: Sapphire glass is more resistant than quartz glass.

Year of manufacture ≤ 2018 ⇒ Quartz glass Year of manufacture ≥ 2019 ⇒ Sapphire glass

Year of Revision ≥ 2019 ⇒ Sapphire glass

In case of doubt please contact GO Systemelektronik.



Caution: Quartz glass plates are not suitable for contact with strong organic solvents (e.g. acetone), strong acids and strong bases.

6.2 Sensor Head ISA – Materials in the Measured Medium

	Component	Material
	Sensor head housing with two cylinders, 4 covers and push rod and guide rod for setting the measurement path	Stainless steel*; optional Titanium**
ISA	Sheathing for sensor cable Press sleeve sensor cable	PU (Polyurethan) Stainless steel *; optional Titanium**
ISA-SDU	Sheathing of sensor cable Cable gland with bend protection	PVC (Polyvinylchloride) PA (Polyamide)
ISA	Potting compound ISA sensor cable	Epoxy resin EA3421 Loctite 3421
	Fibre holder	Stainless steel*; optional Titanium**
	Fibre holder	Stainless steel*; optional Titan**
	Glass discs in the measurement path	Sapphire glass
optional	Spacer	POM (Polyoxymethylene)
	Adjusting screw Inspection screw Headless screws	Stainless steel*; optional Titanium**
	O-rings	FKM (Fluorine rubber) and NBR (Nitrile Butadiene Rubber)
	Eyebolts	Stainless steel ***
	Screw lock	Loctite 3421 Weiconlock AN301-70

* V4A 1.4404 (X2CrNiMo17-12-2)

** Grade 2

*** V4A 1.4571 (X6CrNiMo17-12-2)

7 Measurement Cycle

The settings are made on the BlueBox Display and with the AMS PC software.¹

1. Cleaning (only if automatic cleaning is activated)

Cleaning the sensor head optics with compressed air or wiper

Setting at the display – Duration of a cleaning process ⇒ Cleaning runtime
 – Cleaning interval ⇒ Cleaning interval

Setting with AMS – Duration of a cleaning process ⇒ Cleaning time
 – Cleaning interval ⇒ Cleaning interval

2. Wait (only if automatic cleaning is activated)

The waiting time (Setting Waiting time or Wait time) is the time between the end of the compressed air flushing/wiping activity and the start of the following heating. The purpose of the waiting time after cleaning is to ensure that any remaining air bubbles or swirling dirt do not interfere with the subsequent measurement.

3. Heating

The xenon lamp is heated up by a few light flashes. Number of light flashes: Setting Heating

4. Spectral measurements

A spectral measurement consists of a **single measurement**. A single measurement is made with **light flashes** (number of light flashes per single measurement: Setting Intensity) and a preceding sequence of **dark measurements** of the same number. This single measurement is carried out several times (number of executions: Setting Average).

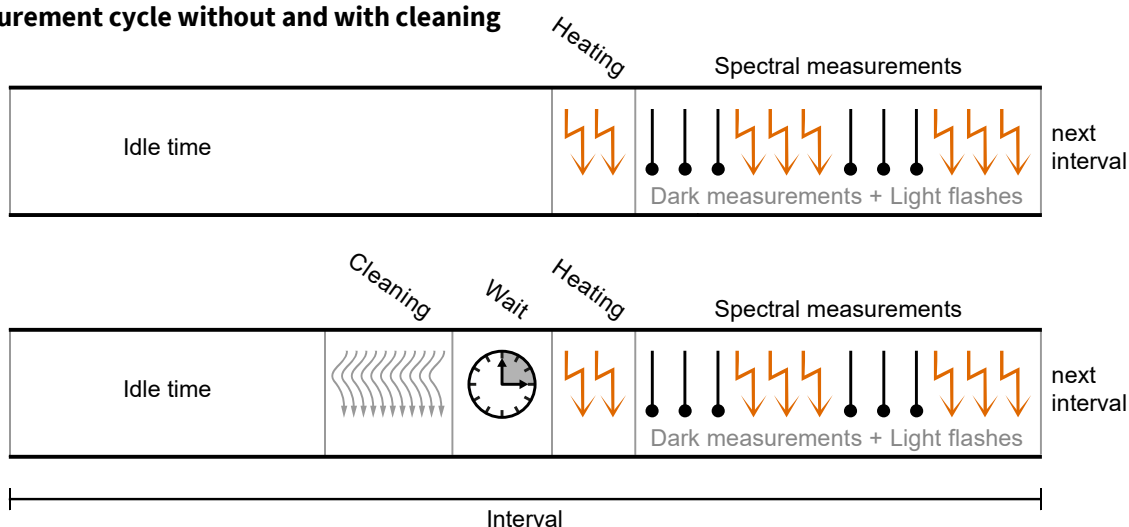
The arithmetic means of the spectral values of the single measurements result in the measured spectrum.

A **dark measurement** is a measurement without a light flash and is used to compensate individual system properties.

5. Interval

The Interval is the duration between the end of a measurement and the end of the next measurement.²
 Setting Interval

Measurement cycle without and with cleaning



It is not possible to change spectrometer settings during the spectral measurements.³

¹ see 8.2 8.2 The Spectrometer Configuration Selection Display and 9.2 The Sensor Setup Window of the Spectrometer and following

² The measurement interval is calculated in advance from the set interval time and the configuration parameters. This results in a low time drift of the recording times of the measured values.

³ Except in extreme cases, there is enough time before and after the spectral measurements for inputs.





Number of light flashes: Intensity x Average 25 light flashes with dark measurements have a duration of approx. 1 second.

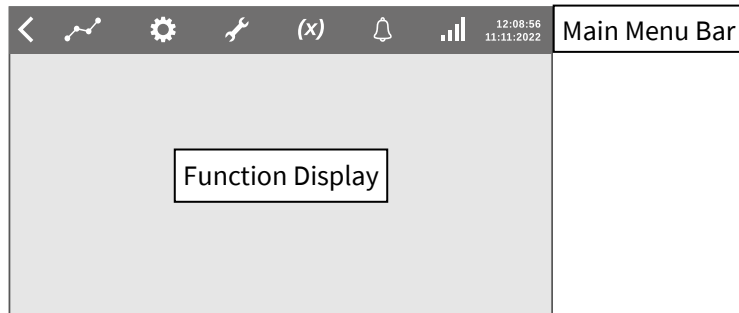
8 Display Operation

BlueBox firmware version: from 5.0

The touch screen is divided in two sections, the Main Menu Bar and the Function Display.









Operating the display

-  tapping
-  swiping horizontal
-  swiping vertical
-  spreading and pinching



Main Menu Bar

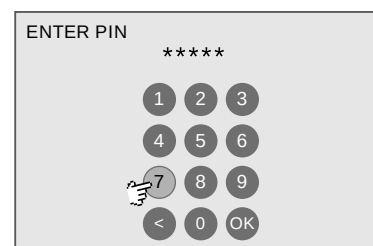


-  Switches back to the previous display.
-  Switches to the Parameter Display.
-  Switches to the System Display.
-  Switches to the Service Display.
-  Switches to the User Variables Display.
-  Switches to the Notifications Display.
-  Bar chart for the intensity of an optional LTE and GPS connection
-  Time and date display







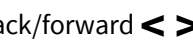
Standard BlueBox Password (PIN) input display

- Tap in the PIN.
- Tap (<) to delete the last entered digit.
- Tap (OK) to enter the PIN.


You will find the PIN in the enclosed Configuration Data Sheet.



Standard alphanumeric input display

- Tapping ABC ⇔ &123 switches back and forth between letter view and digit view with special characters.
-  is off  yellow dot is on
Letter view - Tap  to switch between small and capital letters as well as ;:- and ,_
- Digit view - Tap  to change the special character assignment
- Deletes the last entered character. 
- Saves the entry. 
- One character back/forward 

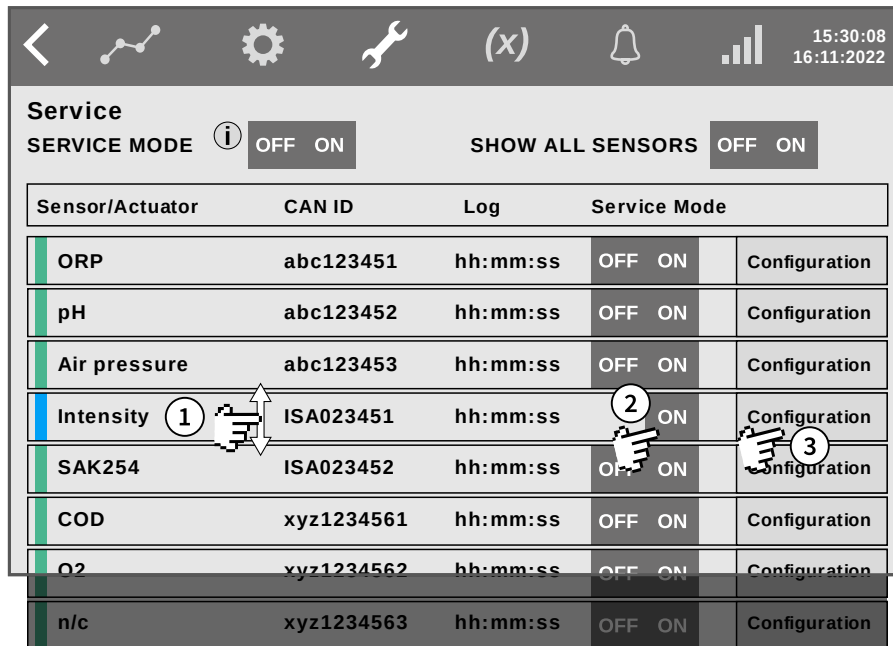


- Tap the keyboard-symbol to return to the previous display without saving an entry. 

8.1 The Service Display



Open the Service Display



Sensor/Actuator	CAN ID	Log	Service Mode	
ORP	abc123451	hh:mm:ss	OFF ON	Configuration
pH	abc123452	hh:mm:ss	OFF ON	Configuration
Air pressure	abc123453	hh:mm:ss	OFF ON	Configuration
Intensity ^①	ISA023451	hh:mm:ss	OFF ON ^②	Configuration ^③
SAK254	ISA023452	hh:mm:ss	OFF ON	Configuration
COD	xyz1234561	hh:mm:ss	OFF ON	Configuration
O2	xyz1234562	hh:mm:ss	OFF ON	Configuration
n/c	xyz1234563	hh:mm:ss	OFF ON	Configuration

The Service Display lists the connected sensors in order of the CAN ID.

In the Service Display, you can switch on the service mode (SERVICE MODE). The service mode deactivates automatic cleaning and data recording and suppresses certain messages.

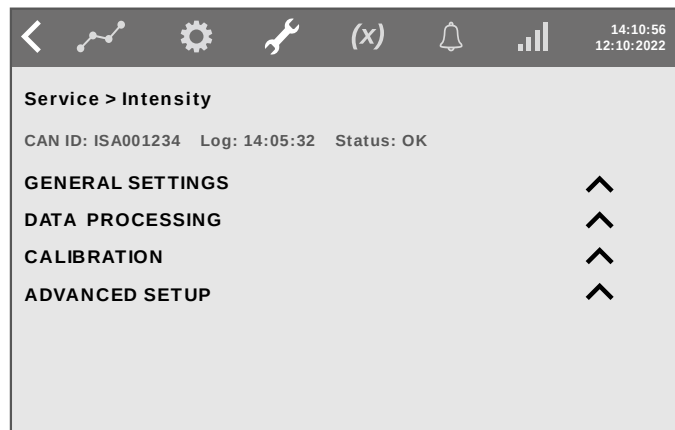
Ensure that the necessary precautions have been taken and that the responsible personnel have been informed.

- ① If necessary, swipe vertical to the Intensity line.
- ② Activate the Service Mode. After the next measurement Intensity is highlighted in blue in the marker bar to the left of it.
- ③ Tap on **Configuration** to open the Spectrometer Configuration Selection Display.

8.2 The Spectrometer Configuration Selection Display

Configuration 8.1 The Service Display > Intensity

Switches back to the Service Display.



Service > Intensity	
CAN ID: ISA001234	Log: 14:05:32 Status: OK
GENERAL SETTINGS	^
DATA PROCESSING	^
CALIBRATION	^
ADVANCED SETUP	^

Switches to the respective Display.


CAN ID: CAN ID of the sensor | **Log:** Time of the last measurement | **Status:** Sensor status

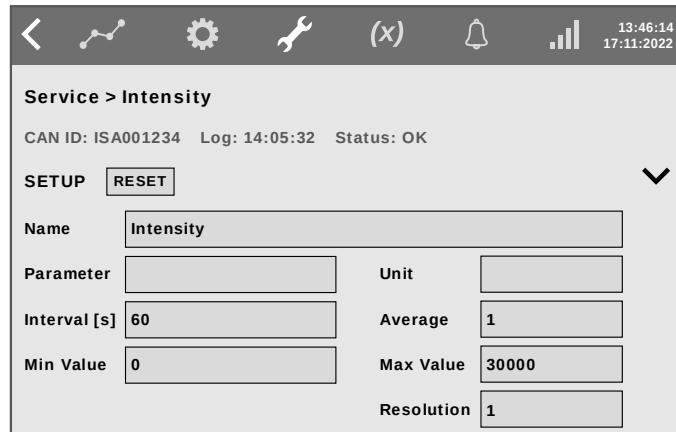
DATA PROCESSING is rarely needed with spectrometers.


When required see *Manual BlueBox R1 and Panel* there 6.2.2 Data Processing


8.2.1 General Settings

GENERAL SETTINGS 8.2 The Spectrometer Configuration Selection Display

 Switches back to the Selection Display.



 Switches back to the Selection Display.

 Tap on a rectangle.

The entries shown here are the factory default settings.

Wait until the end of a spectral measurement before making an input.

RESET Resets the general settings of the spectrometer to the factory settings.

Name Switches to the input of a spectrometer name. max. 20 characters

Parameter Switches to the input of the name of the measured parameter. max. 20 characters

Unit Switches to the input of the unit of the measurement value.

Interval [s] Switches to the input of the measurement interval. see 7 *Measurement Cycle*
Measurement interval = time period between the end of a measurement and the end of the next measurement¹, lowest value is 30.
The higher the interval is set, the fewer spectra are stored, which shortens the download times and saves storage space. One absorbance spectrum needs 1540 Byte (1548 with GPS data). GO Systemelektronik recommends a minimum interval of 60, otherwise the lifetime of the xenon flash lamp will be shortened.

Average The number of single measurements from which the arithmetic mean is derived. The arithmetic mean values of the respective spectral values of the single measurements result the measured spectrum.

Min Value Switches to the input of a Measuring range lower limit/Measuring range upper limit of the
Max Value MVR¹. At underrun and overrun the Sensor Status² is set to 50 or 51. So it is marked by a < or > at List Views and in orange. The entered Min Value or Max Value is the measurement value.

Resolution Switches to the input of the measurement resolution of the MVR³.
Input 1 corresponds to decimal place = 0 in the Sensor setup of AMS⁴.
Input 0.1 corresponds to decimal place = 1 in the Sensor setup of AMS⁴, etc.

¹ The measurement interval is calculated in advance from the set interval time and the configuration parameters. This results in a low time drift of the recording times of the measured values.

² see *Manual BlueBox R1 and Panel* there *Appendix B – Status Messages*

³ MVR = Maximum digital Value of a Raw spectrum

⁴ The program AMS is part of the BlueBox PC Software.

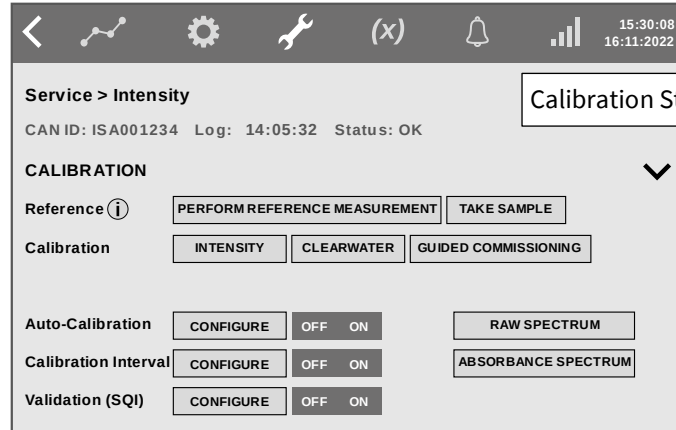
8.2.2 Calibration

i When calibrating a spectrometer, many circumstances must be taken into account. A detailed description of calibration can be found in the *Manual ISA and Process Spectrometer Commissioning – Maintenance – Service there 4 Commissioning*.

CALIBRATION ^

8.2 The Spectrometer Configuration Selection Display


◀ Switches back to the Selection Display.



✓ Switches back to the Selection Display.


☞ Tap on a rectangle.




Reference  Opens the Sample Table.


 Opens the sampling with the last recorded spectrum.

Calibration Leads to intensity calibration, clear water calibration and guided base calibration.

Auto-Calibration functionless

Calibration Interval  Switches to the Input of a calibration interval in days. When this interval is exceeded, the Sensor Status¹ is set to 57 and an entry is set in the List of new Notifications².

Validation (SQI)  Switches to the entry of a validity limit for the SQI³. Above this limit (typically 5), the measurement is no longer reliable. Disables and enables Calibration Interval and Validation (SQI).  The button is also a status indicator. 

 Displays the last recorded spectrum raw spectrum.

 Displays the last recorded spectrum absorbance spectrum.


¹ see *Manual BlueBox R1 and Panel there Appendix B – Status Messages*

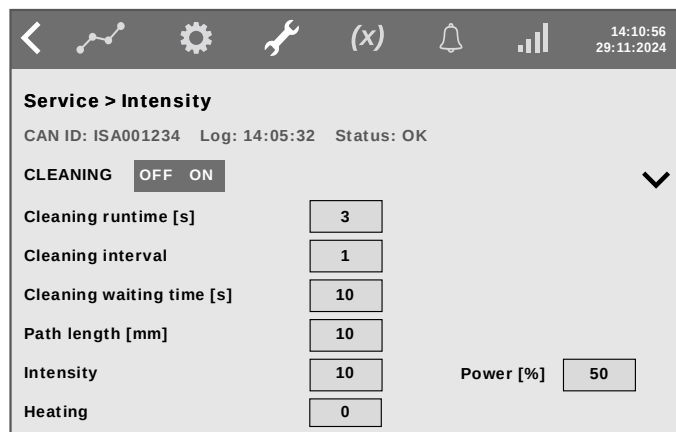
² see *Manual BlueBox R1 and Panel there 10 Notifications*


³ see *Appendix B – SQI (Spectral Quality Index)*


8.2.3 Advanced Setup

ADVANCED SETUP 8.2 The Spectrometer Configuration Selection Display

 Switches back to the Selection Display.



 Switches back to the Selection Display.

 Tap on a rectangle.

The entries shown here are the factory default settings.

Wait until the end of a spectral measurement before making an input.

CLEANING 

Deactivates/activates automatic cleaning with compressed air or wiper. The button is also a status indicator.

Cleaning runtime [s] **Compressed air cleaning** Duration of a cleaning process in seconds

Wiper*

⇒ With a set time of ≤ 8 s, the wiper performs one wipe.

⇒ With a set time of > 8 s and ≤ 16 s, the wiper performs two wipes without interruption.

⇒ corresponding to 24 s, 32 s and so on

Cleaning interval Switches to the input of the Interval of the compressed air flushing/wiper action:

1 ⇒ before every measurement,

2 ⇒ before every second measurement and so on.

Cleaning waiting time [s] To ensure, that air bubbles or swirled-up dirt do not interfere with the following measurement, a waiting time in seconds can be set here. This is the time that elapses between the end of the compressed air flushing/wiper activity and the following measurement.

Path length [mm] Switches to the input menu of the measurement path length of the sensor head in mm. Only visible if the path length is used in an AMS formula. (query command **ISA.PathLength**)

The initial input is performed in the AMS configuration window, see 9.2.1 *The Configuration Window of the Spectrometer*.

Intensity Number of light flashes per single measurement

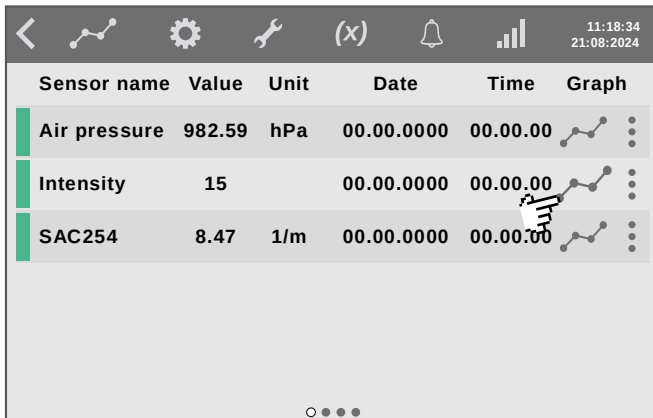
Heating Number of light flashes to heat up the xenon flash lamp before each measurement

Power [%] Light power of the xenon flash lamp
Entry 100 \triangleq Maximum power Entry 0 \triangleq Minimum power


* If not documented separately, the cleaning wiper is set at the factory as follows:
A wiping process has a wiping angle of 70° (once 70° forwards and 70° backwards) with a wiping time of 8 seconds.

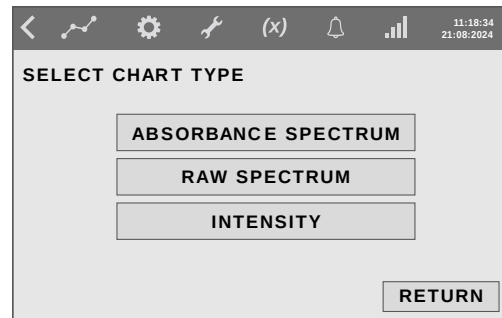
8.2.4 Spectrum View


The spectrum view on the BlueBox Display is called up in the Sensor List View of the Sensor Display.



Sensor name	Value	Unit	Date	Time	Graph
Air pressure	982.59	hPa	00.00.0000	00.00.00	
Intensity	15		00.00.0000	00.00.00	
SAC254	8.47	1/m	00.00.0000	00.00.00	

Tap on  opens a selection display.



 switches back to the Sensor List View.

Use the selection display to open a chart view of the last recorded absorbance spectrum or the last recorded raw spectrum; or the MVR* of the last 24 hours, scaled to min/max of all values. A diagram section is enlarged and reduced by spreading and pinching.

Horizontal swiping in the chart view of the MVR* shifts the X-axis.

Tap the chart view to switch back to the Sensor List View.

* **MVR** = höchster Digitalwert eines Rohspektrums / Maximum digital Value of a Raw spectrum

9 Operation with AMS

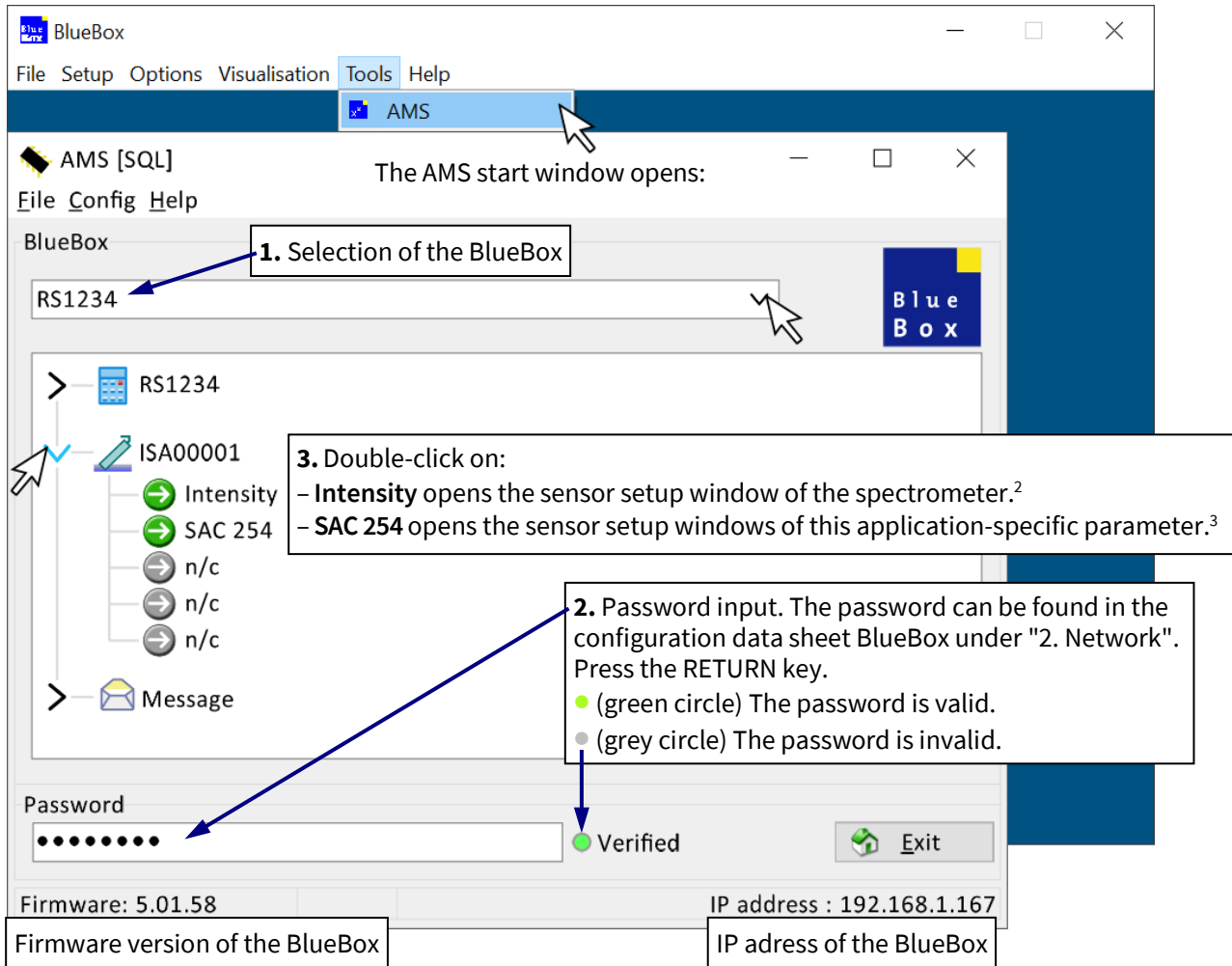
Software version AMS: from 5.0

9.1 The AMS Start Window

If settings are changed at the BlueBox Display, the changes are only transferred to AMS when a connection is established after a program start or with the reconnect function (keyboard key F1 of the computer while the AMS start window is active).

Start the program AMS¹, e.g. via the program BlueBoxSoft like here.

Example: Configuration with only one connected spectrometer and the application-specific parameter SAC254 (set up by default).



The AMS start window opens:

1. Selection of the BlueBox

2. Password input. The password can be found in the configuration data sheet BlueBox under "2. Network". Press the RETURN key.





- (green circle) The password is valid.
- (grey circle) The password is invalid.

3. Double-click on:

- **Intensity** opens the sensor setup window of the spectrometer.²
- **SAC 254** opens the sensor setup windows of this application-specific parameter.³

Firmware: 5.01.58 IP address : 192.168.1.167

Firmware version of the BlueBox IP adress of the BlueBox

 Symbol of a virtual sensor
 Symbol of a spectrometer
 External spectrometer modules connected via CAN bus can have their own symbols. If several spectrometers are connected, these are displayed accordingly.
 Symbol of the messages (SMS and e-mail)
 Sensor status symbols, see next page
 Greyed-out sensor status icons with the name designation n/c are placeholders for further application-specific parameters and the pulse input of the spectrometer unit.

There are three generations of spectrometers.








see *Notes on the Compatibility of Older and Newer Spectrometers* on Page 3

¹ A comprehensive description of the AMS software can be found in the *Manual BlueBox PC Software*, there 5 AMS - Advanced Managing Software.

² see 9.2 *The Sensor Setup Window of the Spectrometer*

³ see 9.3 *The Sensor Setup Window of an Application-Specific Parameter*

There are 6 different sensor status symbols with the following meanings:

-  green The sensor works.
-  grey The sensor name of the spectrometer has been set to "n/c" (not connected), therefore the sensor is not active
-  red Sensor error
-  blue with magnifying glass Waiting for the first measurement value
-  rotating arrows The service mode is switched on. see 8.1 The Service Display
-  Warning sign The measurement value is outside the measurement range limits¹ or the limit value of the SQI value of an application-specific parameter² is exceeded.
-  Scale The maximum calibration interval³ of the clearwater calibration is exceeded.

Double-click opens the corresponding sensor setup window.

Calling up the general configuration window

➡ **n/c** Double-click in the AMS start window to open the general sensor setup window.

Clicking on the Config button opens the general configuration window.

Sensor Setup [ISA000014]

Sensor

Name:

Comment:

Parameter:

Unit:

Digits before: Min. Value:

Digits after: Max. Value:

Interval: Average:

Store mode:

Close

ISA Sensor

Calibration

Name:

Modified:

Options

Normalized 1/m ①

First derivative

Value < 0 = 0

Pressure Sensor ②

Temperature Sensor

Digital Input

Counter (max. 450 Hz) ③

Counter debounced (max. 100 Hz)

SQL settings

Absorbance[Wavelength] x Factor

Bias

x

x

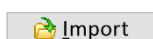
x

x

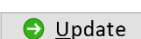
Section ① is used to set up application-specific parameters, see 9.3 and following.

Section ② is used at BlueScan Plus spectrometers to set up internal pressure and temperature sensors.

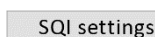
Section ③ is used to set up the internal pulse input of the spectrometer board, see 9.4 and following.



Imports calibration data.



Transfers the settings to the spectrometer board.



Opens the SQI settings window, see 9.3 and following.

¹ see 9.2 The Sensor Setup Window of the Spectrometers there Min. Value and Max. Value

² see 8.2.2 Calibration there Validation (SQI)

and 9.3.1 The Configuration Window of an Application-Specific Parameter there SQI settings/ISA Quality settings

³ see 8.2.2 Calibration there Calibration Interval

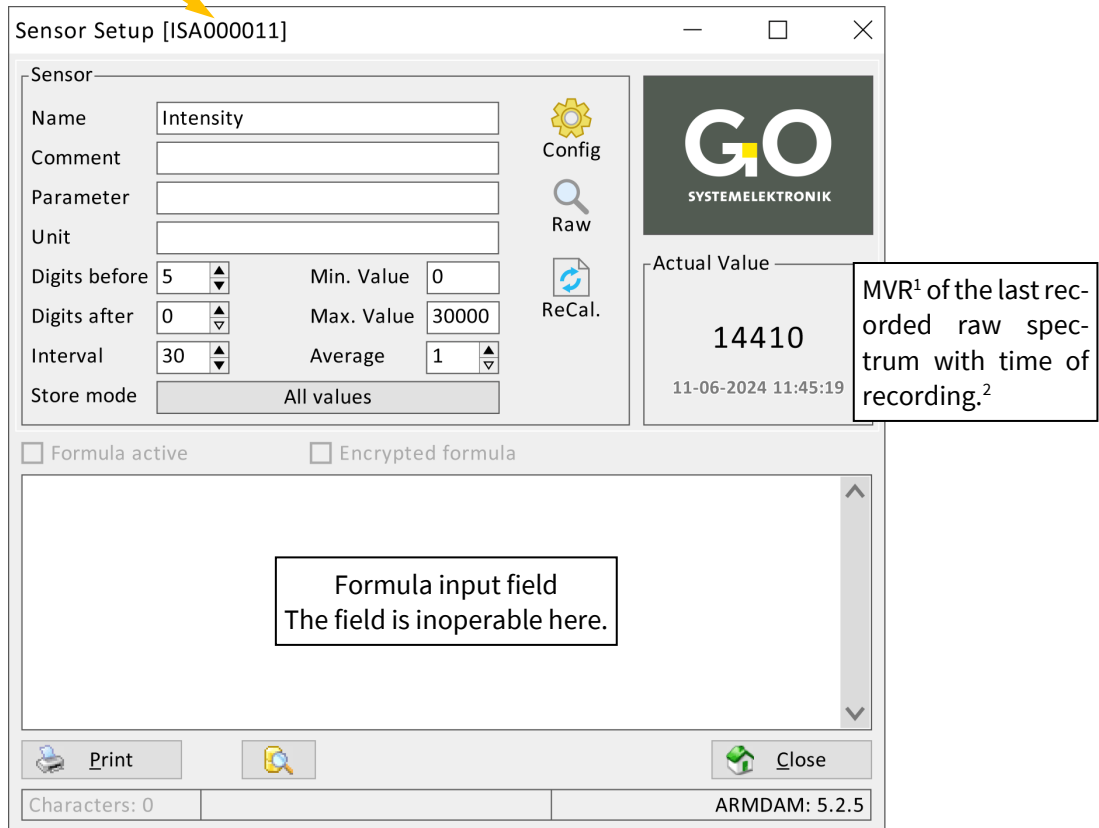
and 9.2.1 The Configuration Window of the Spectrometer there Max. calibration interval [days]

9.2 The Sensor Setup Window of the Spectrometer

➔ **Intensity** Double-click in the AMS start window

The sensor setup window of the spectrometer opens. The default values for the spectrometer are set at the factory. Usually, the user can only change the interval and the average.

Sensor-ID of the spectrometer = CAN-ID + sensor number (uniquely defined for each sensor, set at the factory)



Name, Comment, Parameter and Unit:

Entries take effect after the Enter key has been pressed or an active window element (not — □ ×) has been clicked.



Opens the configuration window of the spectrometer. see 9.2.1 *The Configuration Window of the Spectrometer*



Opens the spectra window.



Opens the spectra window. see 9.2.2 *The Spectra Window*

Name	Name of the sensor, is queried by other BlueBox programs.	max. 20 characters
Comment³	Any comment text	max. 20 characters
Parameter	Designation of the measured parameter	max. 20 characters

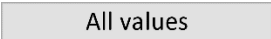


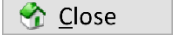
¹ **MVR** = Maximum digital Value of a Raw spectrum

² If the calibration interval of the clear water calibration is exceeded, the scale symbol additionally appears here. ⚖️

³ In older software versions, here it was also possible to determine how a measurement value is saved in the database. Now the setting is made via the button <All values>.

Unit	Unit of the output value More than 5 characters can't be displayed at the BlueBox Display.
Digits before	Factory default setting, 5 pre-decimal places are displayed.
Digits after	Factory preset, 0 decimal places are displayed. Because integer counts are measured here, there are no decimal places.
Interval	Measurement interval = time period between the end of a measurement and the end of the next measurement ¹ , lowest value is 30. The higher the interval is set, the fewer spectra are stored, which shortens the download times and saves storage space. One absorbance spectrum needs 1540 Byte (1548 with GPS data). GO Systemelektronik recommends a minimum interval of 60, otherwise the lifetime of the xenon flash lamp will be shortened.
Min. Value²	Measuring range lower limit, factory setting 0
Max. Value¹	Measuring range upper limit, factory setting 30000
Average	The number of single calculations for averaging. The arithmetic mean values of the respective spectral values of the single measurements result the measured spectrum.

Wait until the end of a spectral measurement before making an input.

	Opens a menu that allows you to specify how measurement values and actuator states are saved in the database. The specification has no effect on spectra themselves and only affects the MVR ³ of the spectra, therefore the default setting <All values> is used in practice.
	Opens a window for printing the sensor setup settings.
	Opens a list of the current variables with their current values.
	Closes the sensor setup window.

¹ The measurement interval is calculated in advance from the set interval time and the configuration parameters. This results in a low time drift of the recording times of the measured values.

² If there is an overrun or underrun of the range, the measurement value is displayed and stored for real sensors. In the case of virtual sensors, the overrun or underrun is marked by a "<" or ">", then the entered minimum or the entered maximum measurement value is stored. In addition, the sensor icon is displayed as a warning sign in the AMS start window.

³ **MVR** = Maximum digital Value of a Raw spectrum

9.2.1 The Configuration Window of the Spectrometer



Sensor setup window

ISA Config ✕

Zeiss serial number

Zeiss-Coefficients 3/4. order fit

C0 <input type="text" value="183.932"/>	Cleaning time [s] <input type="text" value="8"/>
C1 <input type="text" value="2.15482"/>	Cleaning interval <input type="text" value="1"/>
C2 <input type="text" value="1.21551E-05"/>	Wait time [s] <input type="text" value="1"/>
C3 <input type="text" value="-6.77102E-07"/>	Intensity <input type="text" value="15"/>
C4 <input type="text" value="0.0E-01"/>	Path length [mm] <input type="text" value="10"/>
Checksum <input type="text" value="102774"/>	Heating <input type="text" value="0"/>
	Flash lamp power [%] <input type="text" value="50"/>

Options

Enable cleaning Air Wiper

Send Absorbance spectrum Manual start

Send normalized abs. spectrum Send Raw spectrum

Precision mode Ignore dark spectrum

Max. calibration interval [days]

➔ Update

Zeiss serial number

Serial number of the Zeiss spectrometer

Zeiss-Coefficients C0, C1, C2, C3, C4


Zeiss coefficients – Entry according to Zeiss data sheet

Checksum

Checksum of the Zeiss coefficients
The Zeiss coefficients and the corresponding checksum can be found on the Zeiss data sheet supplied. If the checksum displayed does not match that of the data sheet, the input of the coefficients is incorrect.

for pixel	0 to 255
C ₀ / nm	183.932
C ₁ / nm	2.15482
C ₂ / nm	1.21551E-05
C ₃ / nm	-6.77102E-07
Checksum	CS 102 774

Test and Calibration Protocol (page 1 of 3)



Producer	Carl Zeiss Spectroscopy GmbH	Article number	1410-170
Spectrometer	MMS UV-VIS C	Nominal spectral range / nm	190.00 to 720.00
Serial number		Actual spectral range / nm	183.93 to 722.97
Module	102 068		
Grating	1 511 095	Cross section converter	CERAMS2747
Detector	1 206 0571	Total number of pixels	256

Calibration equipment: Hg-Ar-lamp (LOT-01st # LSP030) or Ar-lamp (LOT-01st # LSP030), wavelengths of Hg and Ar-lines ref. NIST (physics.nist.gov/cgi-bin/ASD/main_asd)

Calibration procedure: PA 1134-442 002

Calibration conditions: Illumination with full numeric aperture
all wavelengths in dry air @ 10°C, 1013.25 hPa

Environmental conditions: temperature 23°C ±3 K, rel. humidity 45% ±15%

Coefficients for wavelength calibration - see 102068_Ceram52747_1011095_P2_Coeff_20151008-110939.uni

for pixel	0 to 255	for pixel	1 to 255	for λ / nm =	183.93	to	722.97
C ₀ / nm	183.932	C ₁ / nm	181.777	B ₀	-85.7819	B ₁	-84.7819
C ₁ / nm	2.15482	C ₂ / nm	2.1548	B ₂ / nm	0.469821	B ₃ / nm	0.469821
C ₂ / nm	1.21551E-05	C ₃ / nm	-6.77102E-07	B ₄ / nm ²	-2.40031E-05	B ₅ / nm ²	-2.40031E-05
C ₃ / nm	-6.77102E-07	C ₄ / nm	-6.77102E-07	B ₆ / nm ³	3.67694E-08	B ₇ / nm ³	3.67694E-08
CS	102 774	CS	102 959	CS	103 337	CS	103 333

$p(\lambda) = C_0 + C_1 \cdot p + C_2 \cdot p^2 + C_3 \cdot p^3$
Mean spectral pixel pitch: 2.11 nm

Wavelength verification by Holmium oxide 40 g/l 1 cm

λ_{nom} / nm	λ_{meas} / nm	$\Delta \lambda$ / nm	$\Delta \lambda_{max}$ / nm	as half width at 1/2 λ_{max}
288.38	289.20	-0.18	± 0.50	253.05
361.11	361.04	-0.07	± 0.50	312.95
486.01*	485.98	-0.03	± 0.50	365.25
538.50	538.53	0.03	± 0.50	435.83
656.11*	656.11	0.00	± 0.50	546.07
(nominal wavelengths adapted for spectrometer resolution)				578.05
* emission peak of deuterium				7.30

Zeiss Data Sheet

Final test: PASSED Remarks:

Calibrated by: nm responsible person: quality assurance 2016-05-08 11:09

Cleaning time

Duration of a cleaning process

Compressed air cleaning ⇒ Duration in seconds as set

Wiper* ⇒ With a set time of ≤ 8 s, the wiper performs one wipe.

⇒ With a set time of > 8 s and ≤ 16 s, the wiper performs two wipes without interruption.

⇒ corresponding to 24 s, 32 s and so on

Cleaning interval

Interval of the compressed air flushing/wiper activity:

1 ⇒ before every measurement,

2 ⇒ before every second measurement

and so on

* If not documented separately, the cleaning wiper is set at the factory as follows:

A wiping process has a wiping angle of 70° (once 70° forwards and 70° backwards) with a wiping time of 8 seconds.


- Wait time** To ensure, that air bubbles or swirled-up dirt do not interfere with the following measurement, the waiting time in seconds can be set here. This is the time that elapses between the end of the compressed air flushing/wiper activity and the following measurement.
- Intensity** Number of light flashes per single measurement
Can also be set in the spectra window (see 9.2.2 *The Spectra Window* there *Functions of the button bar*).
- Path length¹** Input of the measurement path length of the sensor head in mm. The path length is measured e.g. with a calliper; take care not to damage the optics.
If the path length is used in an AMS formula (query command **ISA.Pathlength**), you must enter the path length mandatory here. Otherwise, the software uses a default value (10 mm).
- Heating** Number of light flashes to heat up the flash lamp
- Flash lamp power¹** Light power of the xenon flash lamp
Entry 100 $\hat{=}$ Maximum power Entry 0 $\hat{=}$ Minimum power

Wait until the end of a spectral measurement before making an input.

Options

- Enable cleaning** Deactivates/activates automatic cleaning with compressed air or mechanical wiper. Choice between the air cleaning (☉ Air) and the wiper (☉ Wiper)
- Send Absorbance spectrum** Absorbance spectra are stored on the BlueBox.²
- Send normalized abs. spectrum** Absorbance spectra are stored on the BlueBox normalized on 1/m. These normalized spectra have intensity values related to a standardized measurement path of one meter length.
- Precision mode** Switches the flash frequency of BlueScan Plus spectrometers from 50 Hz to 30 Hz.
- Manual start** The spectrometer can be time-controlled with the AMS software.
AMS formula entry **ISA.MEASURE()**
- Send Raw spectrum** Raw spectra are stored on the BlueBox.
- Ignore dark spectrum** The dark spectrum of the dark measurement (see 7 *Measurement Cycle*) is not used.

Max. calibration interval Input of a clearwater calibration interval in days, after this interval, the sensor icon changes to a scale image in the AMS start window. The resetting is carried out after a clearwater calibration.

 **Update** Transmits the settings to the spectrometer unit.

¹ Setting not possible with all spectrometers.

² Only applies to first and second generation spectrometers.

see also *Notes on the Compatibility of Older and Newer Spectrometers* on Page 3

9.2.2 The Spectra Window

The spectrometer measures raw spectra, from the raw spectra the spectrometer unit calculates the absorbance spectra.

In an absorbance spectrum, the **absorbance/attenuation of the single wavelengths** is displayed with a logarithmic scaling. The maximum value is 4.51.

$$Value_i \text{ of the absorbance spectrum} = -\log_{10} \left(\frac{Value_i \text{ of the raw spectrum}}{Value_i \text{ of the clearwater spectrum}} \right)$$

i = 0 to 254¹

For each spectral measurement, 255 raw values are recorded over the range of 200 – 708 nm. For each of these 255 raw values, an absorbance value is calculated for an even wavelength² of 200 – 708 nm.

Main functions of the spectra window

- Display of the currently recorded absorbance and raw spectra and the current clearwater spectrum
- Saving and displaying of fingerprints
- Performance of clearwater calibrations and intensity calibrations in clearwater

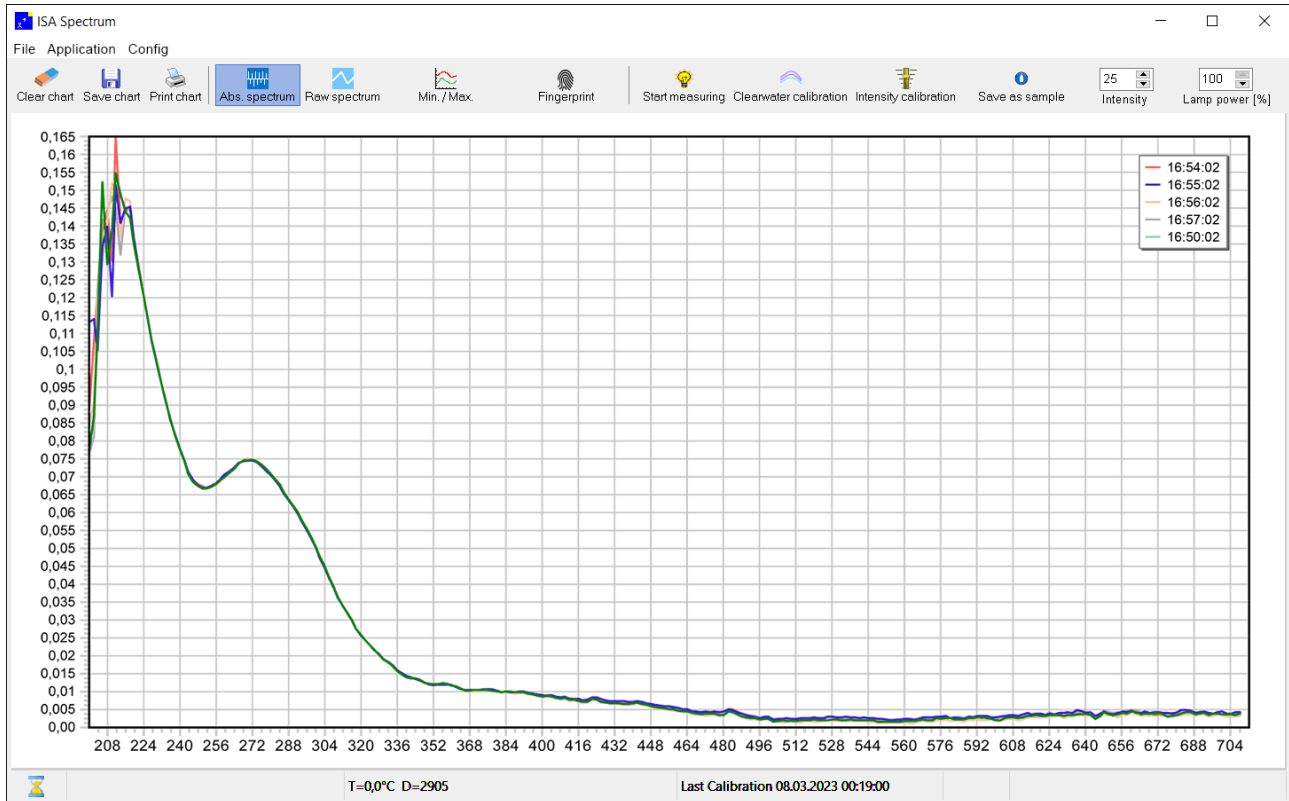
Call up with  or  in the Sensor setup window of the spectrometer

The spectra window with the display of the absorbance spectra appears. see next page

¹ This corresponds to 255 values.

² When querying the absorbance values with AMS formula (see *Manual BlueBox PC Software* there *Appendix H – List of the AMS Formula Elements* there 20. ISA), the absorbance value of the preceding even wavelength is output when entering odd wavelengths from 201 to 709.

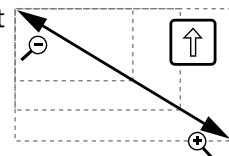
9.2.2.1 The Absorbance Spectra View



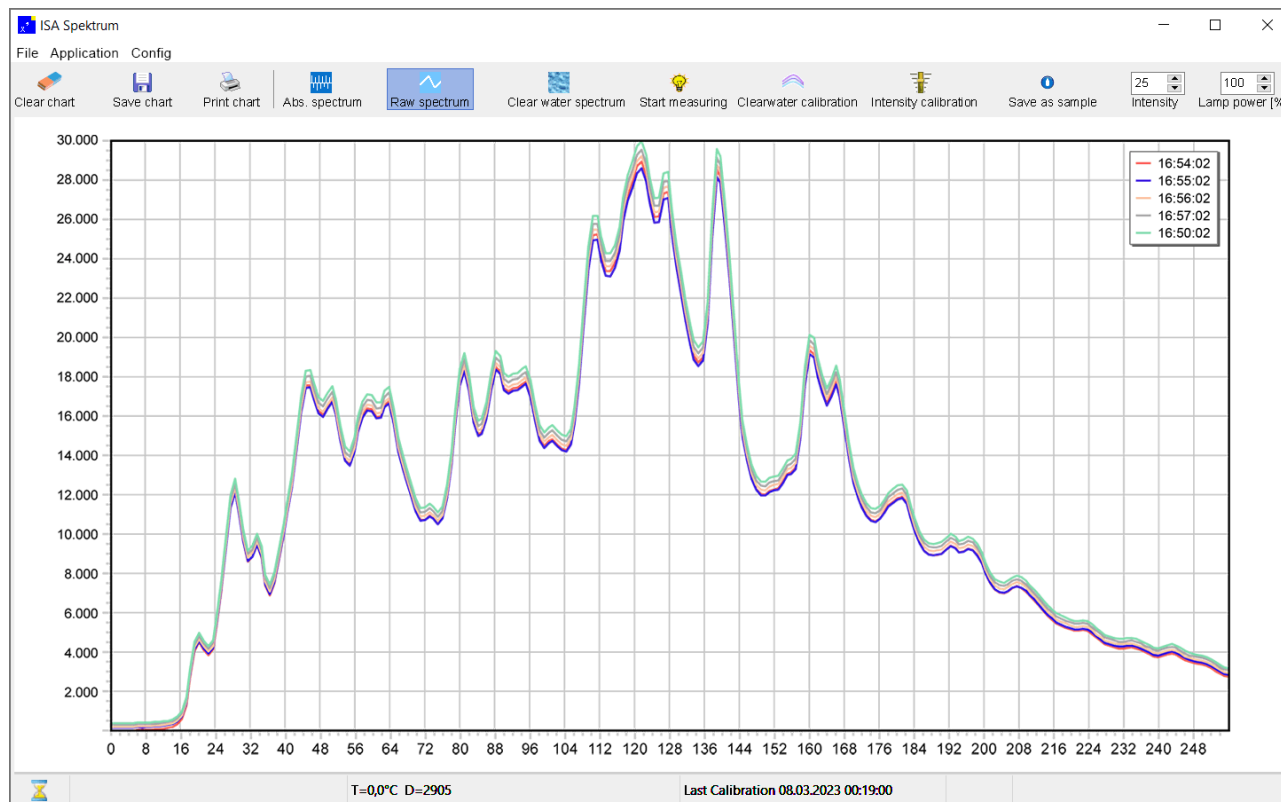
After each measurement an absorbance spectrum is displayed as a line diagram. The most recent 20 absorbance spectra are displayed in different colours. Colour and recording time of the spectra are listed in the upper right. The values of the x-axis are the light wavelengths of 200 nm to 708 nm, the values of the y-axis the absorbance factor.

The spectra shown here are typical clear water absorbance spectra, the corresponding raw spectra are shown on the next page.

You can zoom the spectra view in and out by drawing a rectangle to the right or to the left with the mouse while pushing the left mouse button. Zooms are reset with the next spectrum capture.



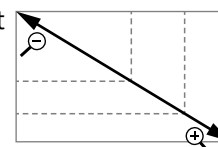
9.2.2.2 The Raw Spectra View



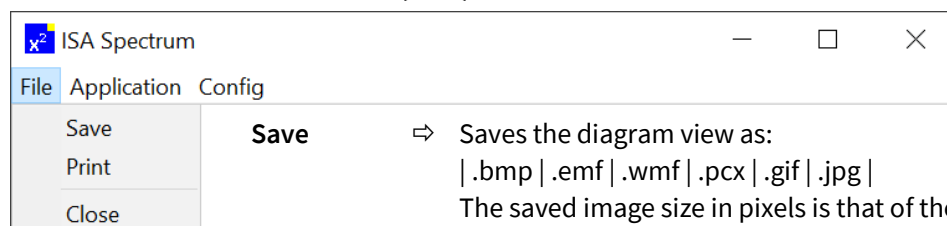
After each measurement a raw spectrum is displayed as a line diagram. The most recent 20 raw spectra are displayed in different colours. Colour and recording time of the spectra are listed in the upper right. The values of the x-axis are the steps of the spectral resolution of the spectrometer (0 – 254), the values of the y-axis the counts of the AD converter (0 – 30000).

The spectra shown here are typical clear water raw spectra, the corresponding absorbance spectra are shown on the previous page.

You can zoom the spectra view in and out by drawing a rectangle to the right or to the left with the mouse while pushing the left mouse button. Zooms are reset with the next spectrum capture.














9.2.2.3 Menu Bar Functions (File)



- Save** ⇒ Saves the diagram view as:
|.bmp | .emf | .wmf | .pcx | .gif | .jpg |
The saved image size in pixels is that of the monitor display.
- Print** ⇒ Prints the diagram view.
- Close** ⇒ Closes the window.

9.2.2.4 Button Bar Functions

 Clear chart	Deletes the spectra view.
 Save chart	Saves the spectra view as a pixel image in jpg format, the size of the saved image is that of the monitor display
 Print chart	Prints the spectra view.
 Abs. spectrum	Displays the absorbance spectra.
 Raw spectrum	Displays the raw spectra.
 Min. / Max.	Opens and closes the Min-Max spectral values view. see 9.2.2.6 <i>Fingerprint</i>
 Fingerprint	Displays the deviation in percent of the last recorded absorbance spectrum from the enveloped area of the fingerprint with the identification number 0. see 9.2.2.6 <i>Fingerprint</i> there <i>Save fingerprint</i> and <i>Applying a fingerprint to an extinction spectrum</i>
 Clearwater spectrum	Only visible in the raw spectra view and when the spectrum window is opened for the first time after a restart. Displays the current clearwater spectrum (raw spectrum of the last clearwater calibration). This clearwater spectrum is used as a reference, the spectra are calculated from the deviation from this reference. The date and time of the current clearwater calibration are displayed above the line diagram.
 Start measuring	Starts a measurement, the measurement interval then starts again.
 Clearwater calibration	Performs a clearwater calibration. see <i>Manual ISA and Process Spectrometer Commissioning - Maintenance - Service</i> there 4.2.6.2 <i>Clear Water Calibration with the program AMS</i>
 Intensity calibration	Performs an intensity calibration. The intensity calibration in DI-water is part of the intensity adaptation, which in turn is part of the base calibration. see <i>Manual ISA and Process Spectrometer Commissioning - Maintenance - Service</i> there 4.2.5 <i>Intensity Calibration (Light Intensity) with the program AMS</i>



Opens an input window for a sample number¹, entered commas are stored as a point. This sample number is assigned to the last spectrum captured.

Definition: A spectrum with an assigned sample number is a reference spectrum. Already assigned sample numbers can be assigned to another spectrum with AMS, but cannot be deleted.

Sample numbers are only deleted in the database with the Spectrum Visual program (see 11 Spectrum Visual there 11.2 Enter and Delete Sample Numbers).




Display and setting of the number of light flashes per single measurement as in 9.2.1 The Configuration Window of the Spectrometer



Light power of the xenon flash lamp
Entry 100 $\hat{=}$ Maximum power Entry 0 $\hat{=}$ Minimum power

9.2.2.5 Base Bar Functions

	Calibration at next measurement	T=0,0°C D=541	Last Calibration 25-06-2024 13:38	65
①	②	③	④	⑤

① Status symbols



Compressed air cleaning is running.



Cleaning wiper is running.



Measurement or intensity calibration in clearwater is running.



Clearwater calibration is running.



Transmission of spectra data to the spectrometer unit is running.

② Field for status messages

③ T= nn,n °C Temperature of the spectrometer electronic

D=nnn MVR² of the dark measuring, see 7 Measurement Cycle

④ Date and time of the last clear water calibration

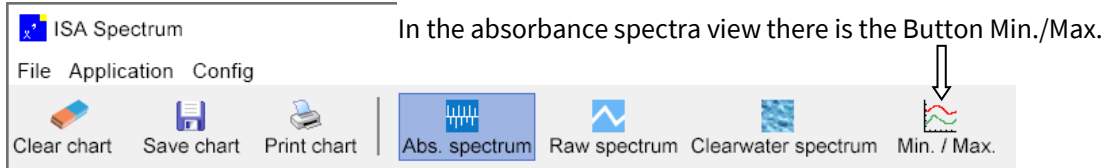
⑤ Number of absorbance spectra recorded after opening the spectrum window, only in the Min-Max spectral values view – see 9.2.2.6 Fingerprint

¹ Also called probe number or probe name. Character set: ASCII standard
This sample number is required in the application-specific calibration in connection with a multi-parameter calibration, and is stored together with the spectra data at an export in the JCAMP-DX format.
see Manual ISA and Process Spectrometer Commissioning - Maintenance - Service there 4.3 Application-Specific Calibration

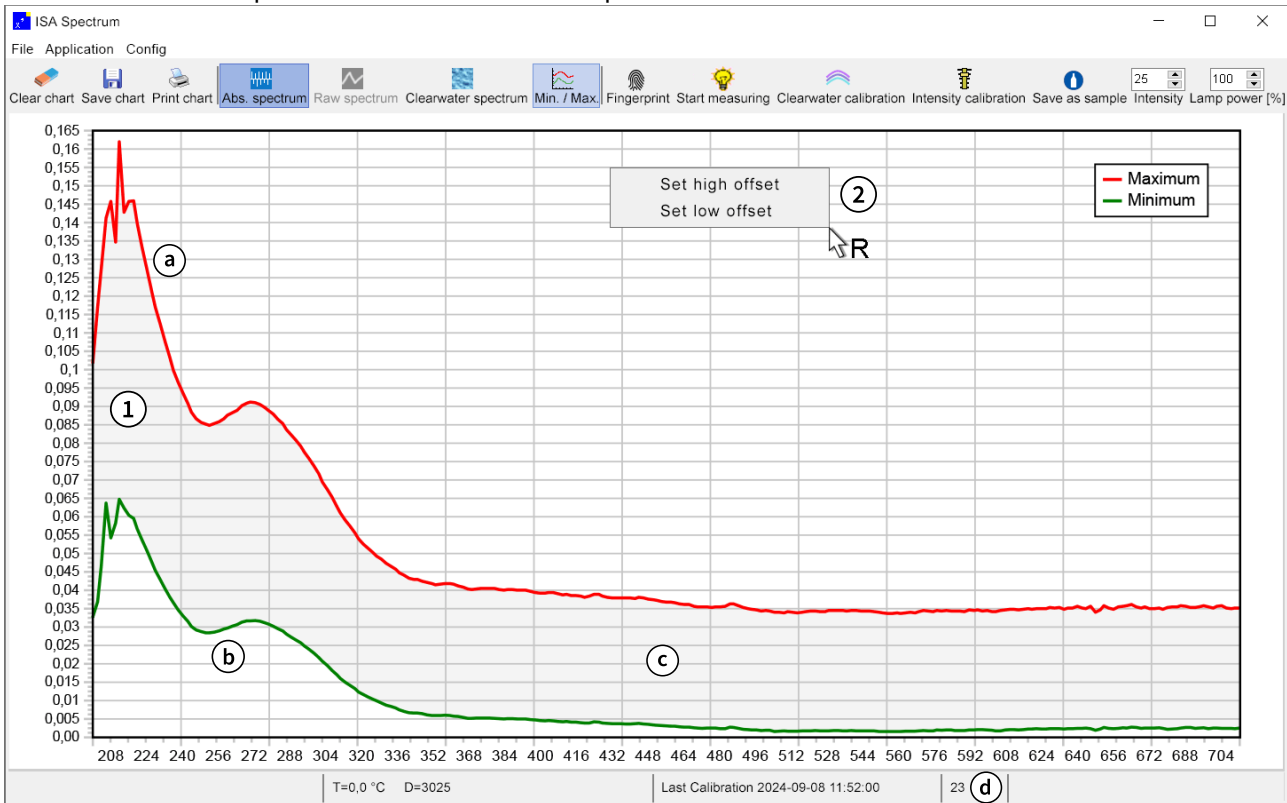
² **MVR** = Maximum digital Value of a Raw spectrum

9.2.2.6 Fingerprint

The fingerprint is the enveloped area between the curves of the maximum values and the minimum values of the extinction spectra recorded after opening the spectra window.

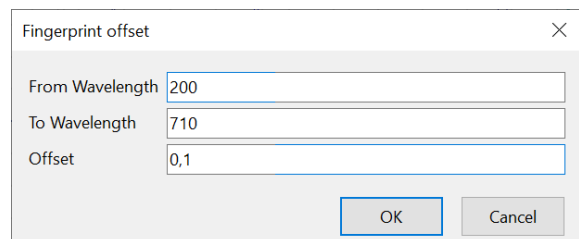


Click on this Button opens and closes the Min-Max spectral values view.

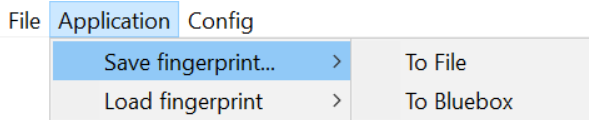


- ① The minimum and maximum values of the single wavelengths of the absorbance spectra recorded after opening the spectra window are displayed.
 - Ⓐ Red line: maximum values curve
 - Ⓑ Green line: minimum values curve
 - Ⓒ Enveloped area (marked grey here)
 - Ⓓ Number of absorbance spectra recorded after opening the spectra window

- ② You can offset the maximum values curve and the minimum values curve at specific wavelength ranges. Right mouseclick in the spectra view field opens an offset selection menu. In [Set high offset] and set [Set low offset] you can determine a wavelength range and an offset value. If you are in zoom mode, the wavelength range will shift accordingly.



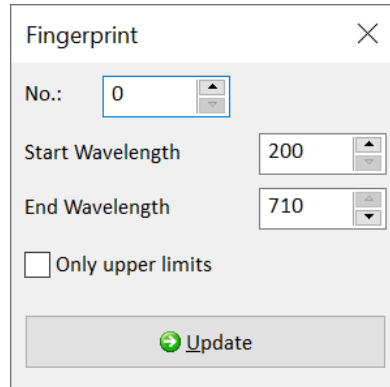
Save fingerprint



Click on <Save fingerprint> <To file> opens a window in which the storage path can be selected. The fingerprint is saved as an fp file.

Click on <Save fingerprint> <To BlueBox> opens a menu:

Click on <Update> saves the fingerprint on the BlueBox.



No.: Saves the current fingerprint with an identification number (0, 1, 2, 3).
With this identification number you can call up a fingerprint with AMS Formula.

Formula entry: **ISA.FP**(*identification number*)

– greatest deviation in percent from the fingerprint

ISA.FP(*identification number,wavelength*)

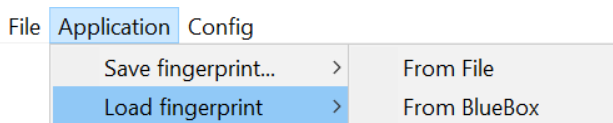
– deviation in percent from the fingerprint at a wavelength

The previous formula entry **ISAFP**(*n*) is no longer valid.

Start Wavelength Limits the enveloped area of the fingerprint to a wavelength range.
End Wavelength

Only upper limits The minimum values curve is not taken into account. The enveloped area of the fingerprint ranges between the maximum values curve and the x-axis (y=0). see above

Load fingerprint



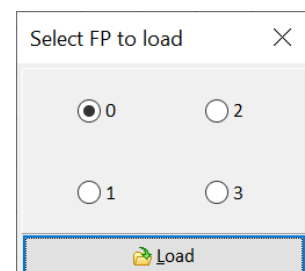
Click on <Load fingerprint> <From File> opens a window in which you can select the storage path of a fingerprint saved as an fp file.

The fingerprint appears in the Min-Max spectral values view.

Click on <Load fingerprint> <From BlueBox> opens a menu:

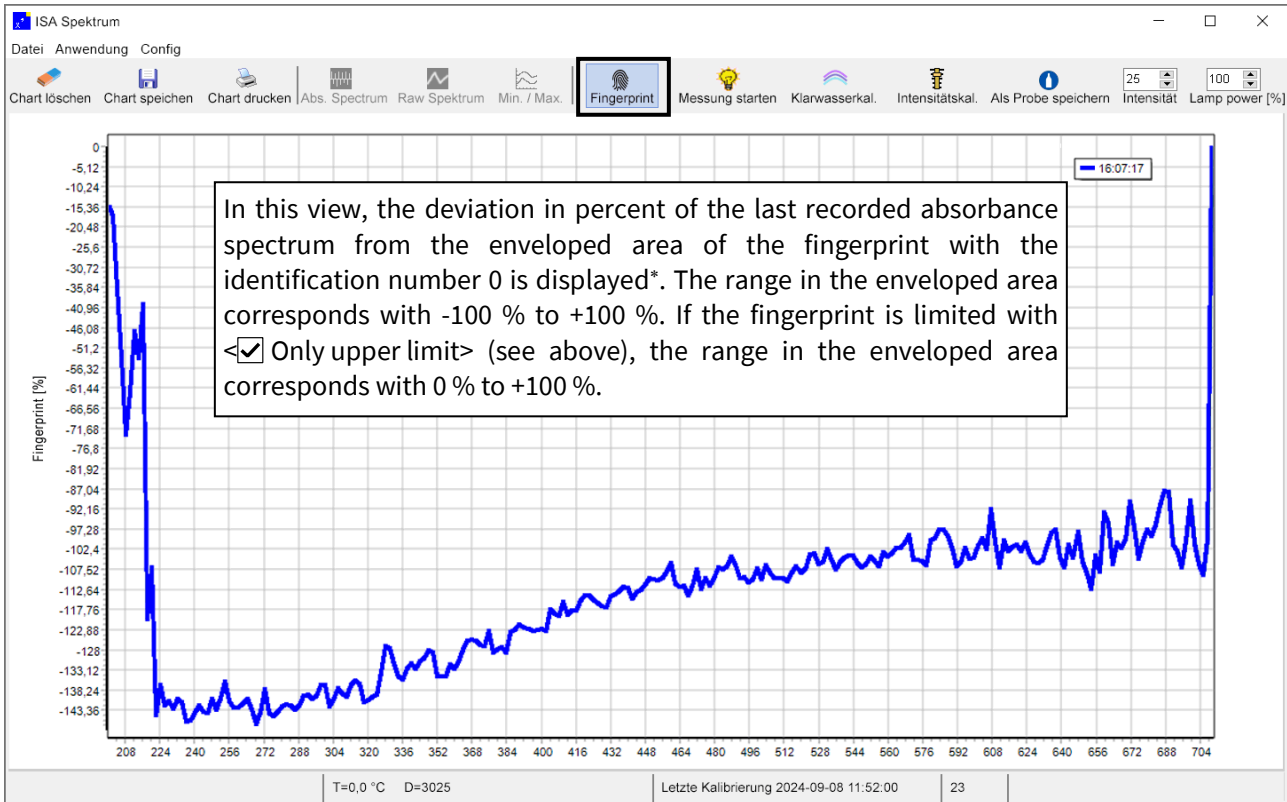
Use the radio buttons to determine the identification number (see above) of the fingerprint.

Click on <Load> loads the fingerprint in the Min-Max spectral values view.

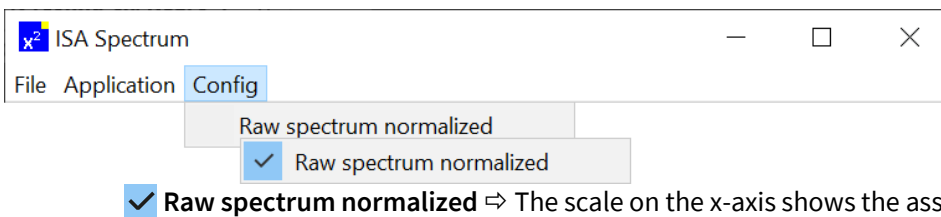


Applying a fingerprint to an extinction spectrum

Click on the fingerprint button applies the fingerprint with the identification number 0 (see above) to the last recorded absorbance spectrum.



9.2.2.7 Displaying Raw Spectrum Normalised to Wavelength



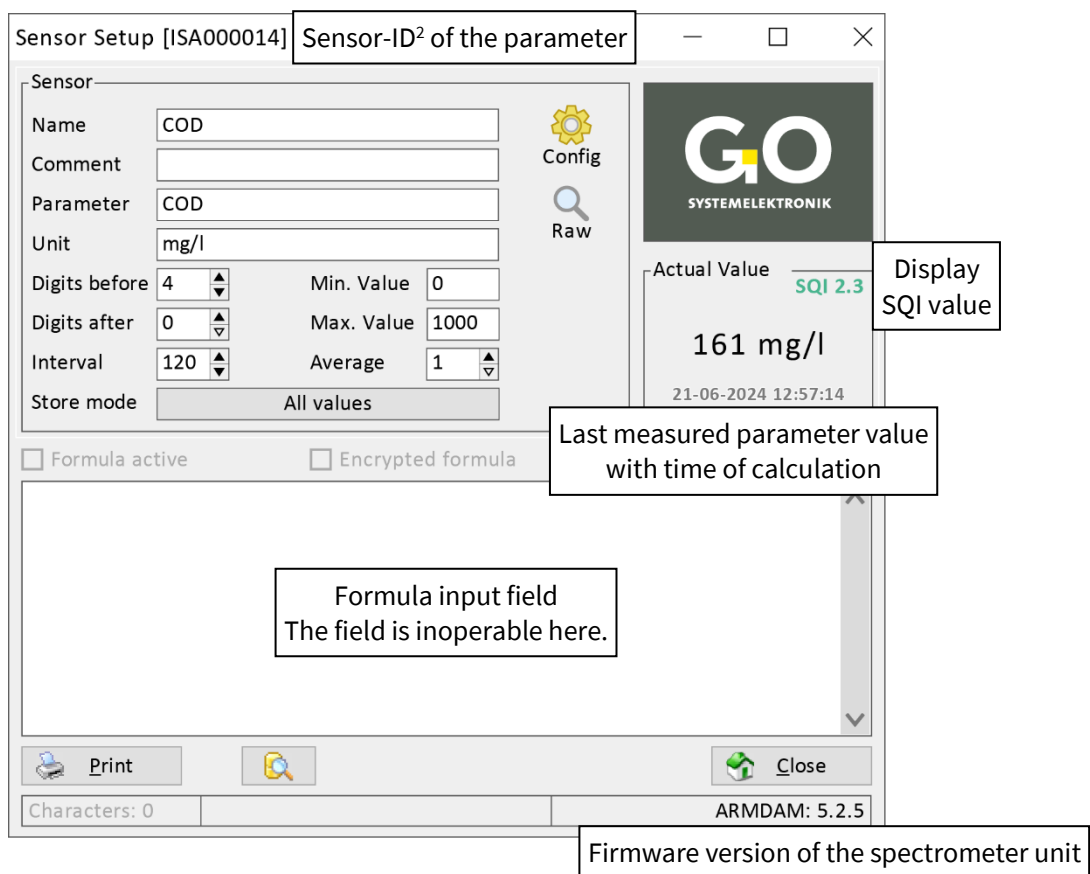
9.3 The Sensor Setup Window of an Application-Specific Parameter

The application-specific parameters generated from spectral data are, such as virtual sensors (see *13 Virtual Sensors*), calculated parameters. The main difference to virtual sensors is the type of calibration that allows a continuous calculation of the **SQI**¹ (Spectral Quality Index).

AMS handles the application-specific parameters such as sensors. By default, each spectrometer is configured with SAC254 as an application-specific parameter. In addition, there are three free parameters which can be customized configured. For more information on customer specific application parameters, please contact GO Systemelektronik.

Example customized parameter COD:

➔ **COD** Double-click in the AMS start window opens the sensor setup window.



Name, Comment, Parameter and Unit: Entries take effect after the Enter key on the PC keyboard is pressed or an active window element (not –□×) is clicked.



Config

Opens the configuration window of the parameter.
see 9. 3.1 *The Configuration Window of an Application-Specific Parameter*



Raw

Opens a window with the display of the last recorded single value of an averaged measurement value.³

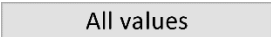
¹ SQI (Spectral Quality Index) see *Appendix B – SQI (Spectral Quality Index)*

² CAN-ID + sensor number (uniquely defined for each sensor, factory preset)


³ Is useful in some cases for testing purposes.

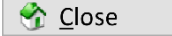
ISA - Operation with AMS

Name	Name of the virtual sensor, is queried by other BlueBox programs.	max. 20 characters
Comment	Any comment text for AMS and BlueBox SQL software*	max. 20 characters
Parameter	Name of the measured parameter	max. 20 characters
Unit	Unit of the output value More than 5 characters can't be displayed at the BlueBox display.	
Digits before	Number of displayed pre-decimal places	
Digits after	Number of displayed decimal places	
Interval	Time period in seconds between the calculations The minimum interval is the spectrometer interval. The interval of an application-specific parameter can only be an integer multiple of the spectrometer interval, in this example 120, i.e. in case of a spectrometer interval of 60 the calculation of the sensor value takes place at every second spectrum capture. Other values are taken as the next largest integer multiple of the spectrometer interval.	
Min. Value	Lower value limit	
Max. Value	Upper value limit	
Average	Number of single calculations for averaging	

 **All values** Opens a menu where you can define how the parameter values are stored in the database. see *Manual BlueBox PC Software* there *5.4.1 Sensor Setup* there *Display and save mode*

 **Print** Opens a window for to print the sensor-settings.

 Opens a list of the current variables with their current values.

 **Close** Closes the sensor setup window.

* In older software versions, here it was also possible to determine how a measurement value is stored in the database. The setting is now made via the <All values> button.

9.3.1 The Configuration Window of an Application-Specific Parameter



Sensor setup window of the parameter

The out greyed area does not apply here.

Calibration

Information on the imported calibration

Name Name of the calibration

Modified Modification time

The name and modification time are imported when the calibration data is generated with the 'ISA plus manager' program.

Options

Normalised 1/m

The calibration is calculated using absorbance spectra that are normalised to 1/m.

These normalised spectra have intensity values that refer to a normalised measurement path of one meter in length.

First derivate

The calibration is calculated with the values of 1. derivation* of the absorbance spectra.

Value < 0 = 0

A measurement value <0 is set to 0.

SQL settings

Opens the quality settings window, only visible if the SQL is being calculated.

The SQL calculation values are displayed and set in this window.

Only the value for **Max h** is of interest for operation, h is the **value of the SQL**. If **Max h** is exceeded, the measured value is shown in square brackets in the sensor setup window and in the BlueBox Display and the sensor symbol in the AMS start window becomes a warning sign ⚠.



Sets all settings to zero.

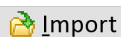


Transfers the settings to the spectrometer unit.

SQL (Spectral Quality Index)

The SQL is a degree of the statistical reliability of measurement values and is calculated continuously for each parameter. Precondition is the creation of a corresponding calibration file in the xml format.

see *Appendix B – SQL (Spectral Quality Index)*



Imports ISA Plus calibration data in txt-format, cal-format and xml-format.





Transfers the settings to the spectrometer unit.

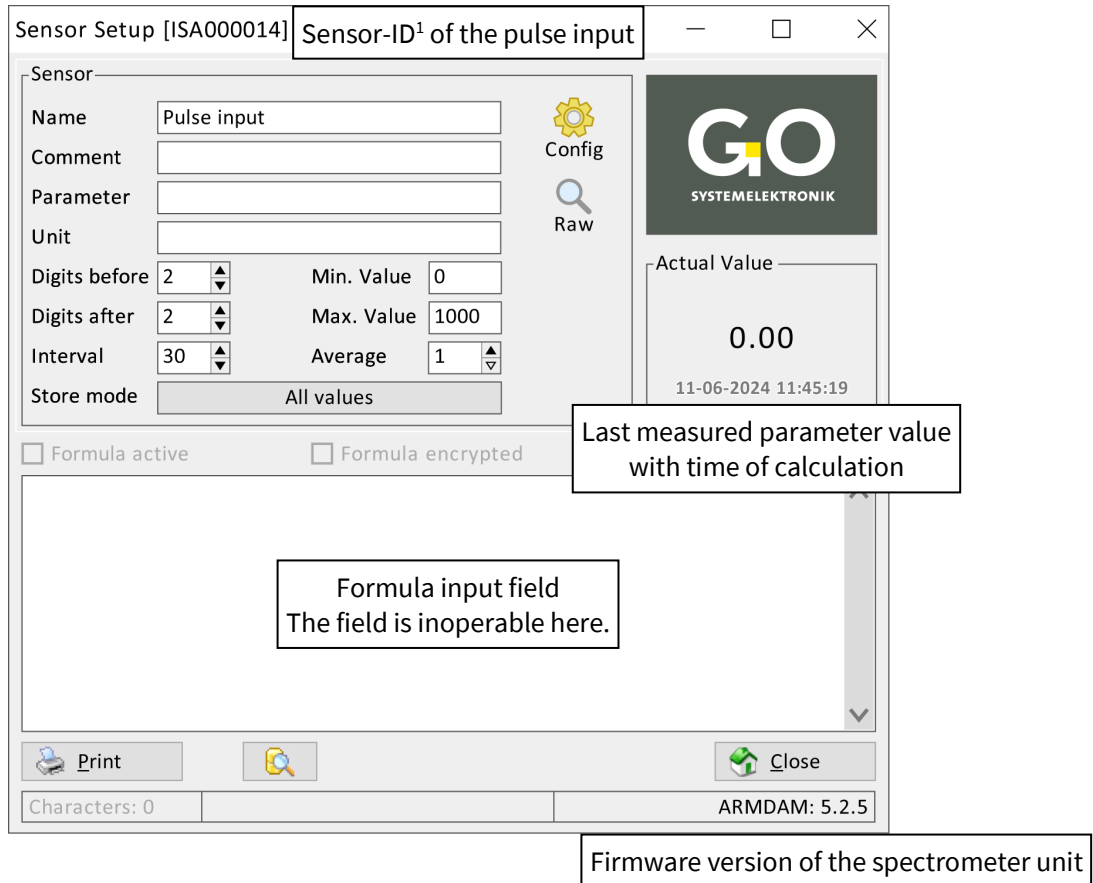
* means the differences of the adjacent absorbance values


9.4 The Sensor Setup Window of the Pulse Input

Setup of a pulse input

The pulse input is not set up in the standard factory setting. The setup is carried out via the AMS start window. Click on a grey sensor status symbol  in the AMS start window opens a sensor setup window, see below. Click on  opens a configuration window, see next page.

 **Pulse input** Double-click in the AMS start window opens the sensor setup window.



Name, Comment, Parameter and Unit: Entries take effect after the Enter key on the PC keyboard is pressed or an active window element (not ) is clicked.



Opens a configuration window of the pulse input.
see 9.4.1 *The Configuration Window of the Pulse Input*

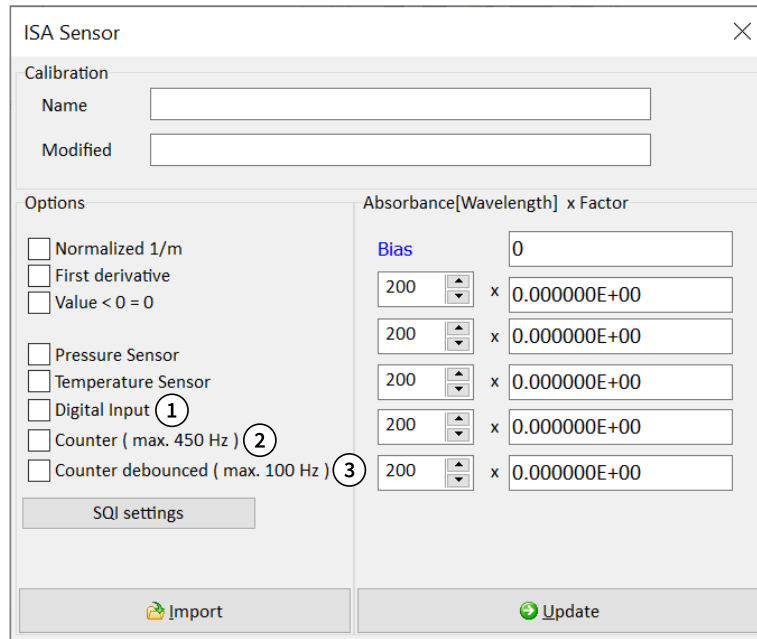


Opens a window with the display of the last recorded single value of an averaged measurement value.²

¹ CAN-ID + sensor number (uniquely defined for each sensor, factory preset)

² Is useful in some cases for testing purposes.

9.4.1 The Configuration Window of the Pulse Input

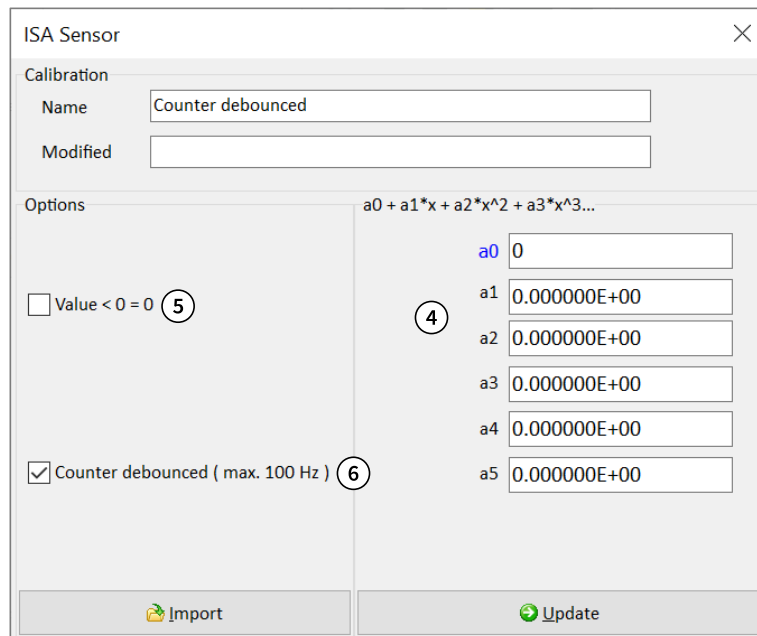


Name Input field for the sensor name of the pulse input

Time of setup

- ① Selection Digital input – Static input
- ② Selection Frequency (edge trigger) – Triggering on the rising edge, max. 450 Hz
- ③ Selection Frequency (debounced) – Triggering on the rising edge with debounce, max. 100 Hz

After setting a check mark, the window changes to the view of the calibration coefficients.



- ④ Input fields of the calibration coefficients
- ⑤ Selection of whether values less than zero are set to zero or not.
- ⑥ If the check mark is removed, the configuration view reappears



Imports calibration data.

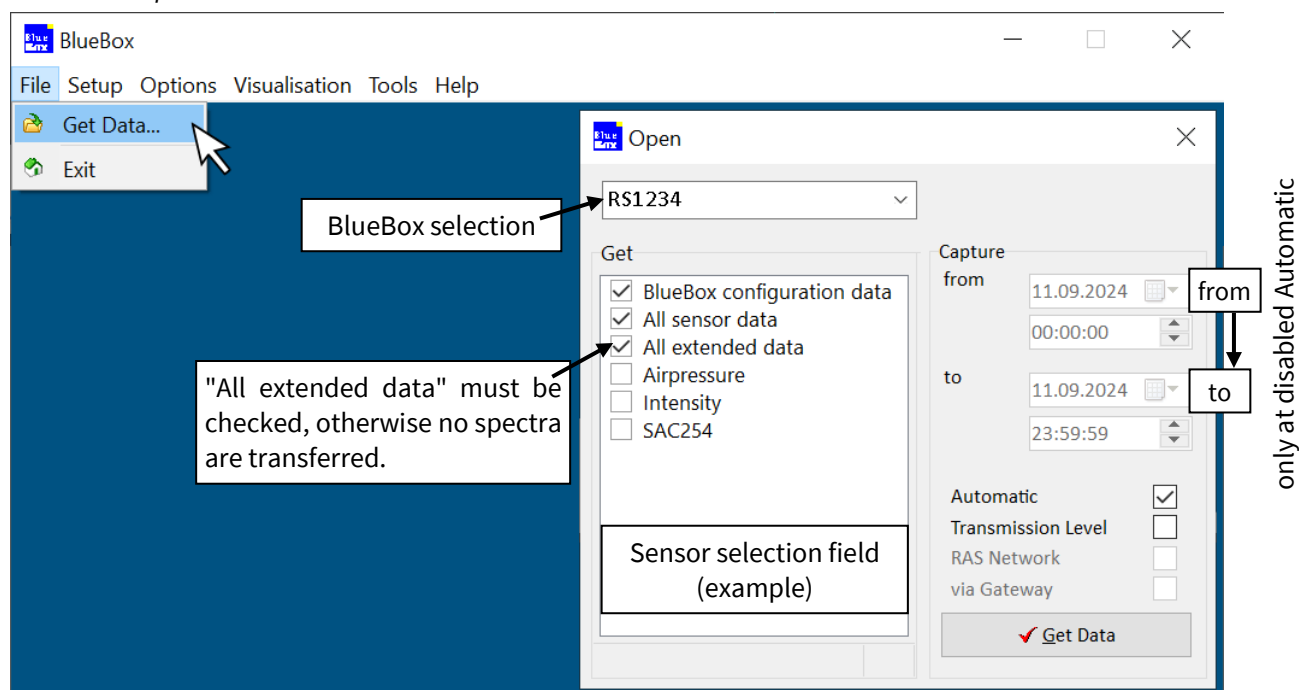


Transfers the settings to the spectrometer unit.

10 Transmitting the Data to the PC with the program BlueBoxSoft

Software version 4.5

To transfer the data from the BlueBox to the PC, call-up <File> <Get Data> in BlueBoxSoft.
see also 11 *Spectrum Visual*



When checkboxes in the sensor selection field are ticked, the following data is transferred to the PC:

- BlueBox configuration data** configuration data of the BlueBox
- All sensor data** the measurement data of all connected sensors
(in case of spectrometers the MVR's* of the raw spectrum)
- All extended data** the raw spectra and the absorbance spectra
- Air Pressure** the measurement data of all connected sensors
- Intensity** (for the spectrometer (Intensity) the MVR* of the raw spectra)
- SAC254**

- Automatic** If this check box is ticked, all those values are transmitted automatically, which had been recorded since the point in time of the last data transmission. This point in time is determined by the most current data set of the data base.

- Transmission Level** Only for measurement data.
If this check box is ticked, only those values are transmitted, which differs from the previous value for a certain degree.
The value of this difference is determined in: BlueBox SQL <Options><Sensor Details> "Data transmission level" (see *Manual BlueBox PC Software*).

- RSA Network** Only active, if the connection is established via modem or gateway.
- via Gateway**

- Get Data** Transmits the data to the PC.

* **MVR** = Maximum digital Value of a Raw spectrum

11 Spectrum Visual

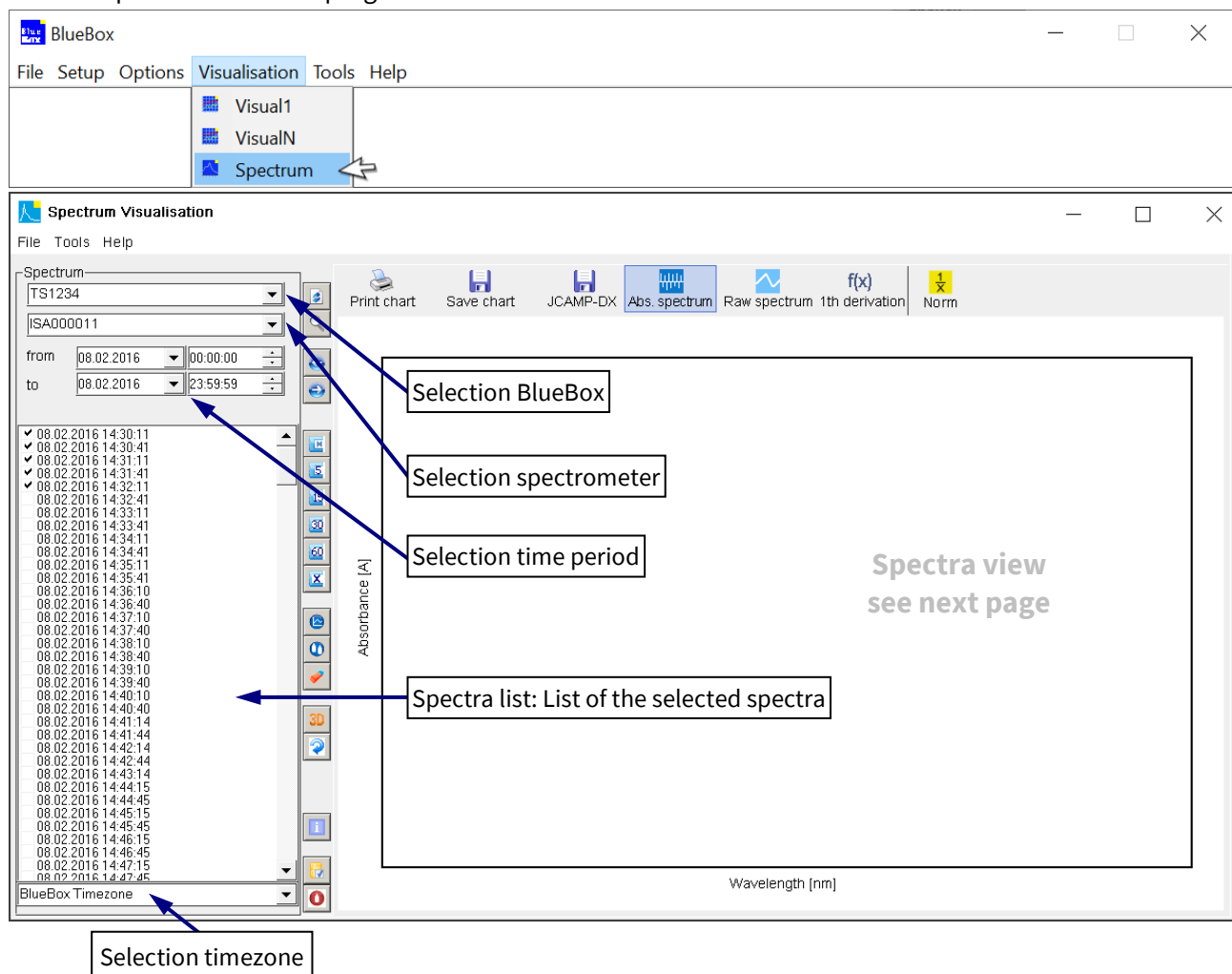
Software version Spectrum Visual: 4.6

The program Spectrum Visual

- displays graphically the spectra stored in the database on your PC,
- assigns sample numbers to spectra,
- stores spectral graphics in common graphic formats,
- exports spectral data into common formats,
- generates a fingerprint* from selected spectra,
- imports spectral data,
- and applies application calibrations to spectra in the database.

11.1 Call up and Display the Spectra

The call up is made with the program BlueBoxSoft.



Select a BlueBox, a spectrometer, a time period and a time zone. The selected spectra are listed in the spectra list.

There are two ways of marking spectra in the spectra list:

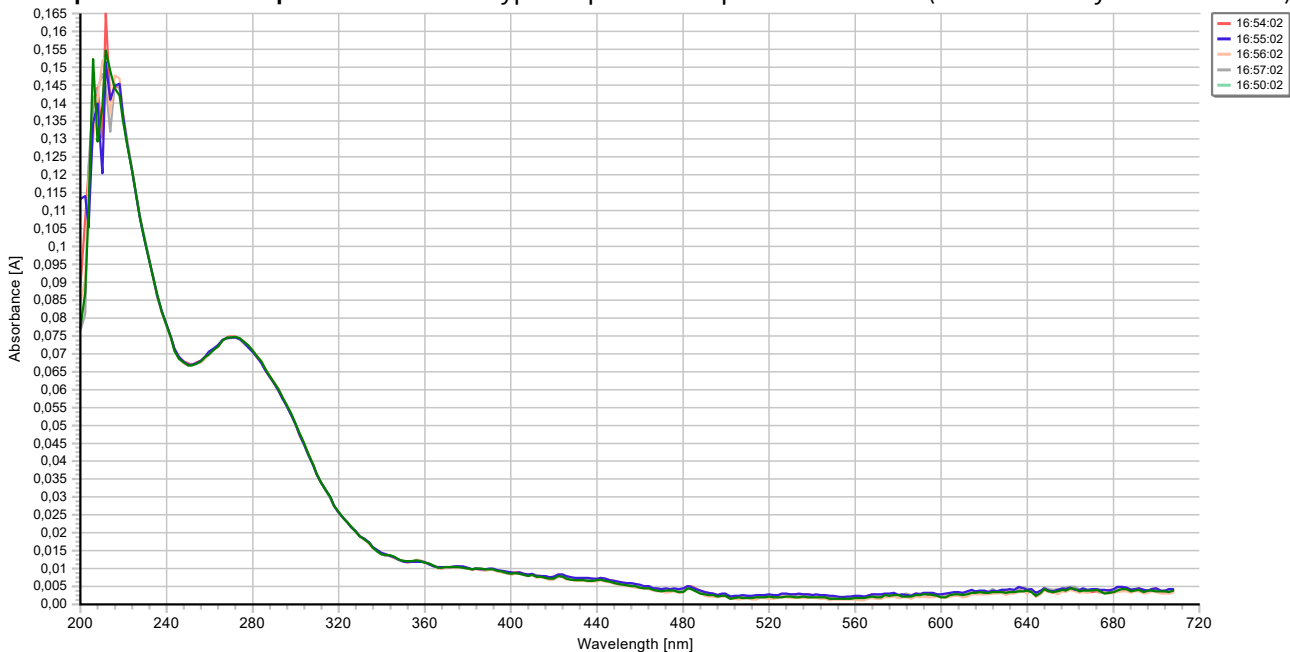
1. With the **checkbox**: The spectrum is checked and therewith **marked**. A multiple marking is possible, checked spectra are displayed as a line diagram.
2. **Click on time information** to the right of the checkbox: The time of a selected spectrum is highlighted in blue and therewith **marked**.

* see 9.2.2.6 Fingerprint

Marked spectra are displayed as a line graph (max. 500):

Example absorbance spectra

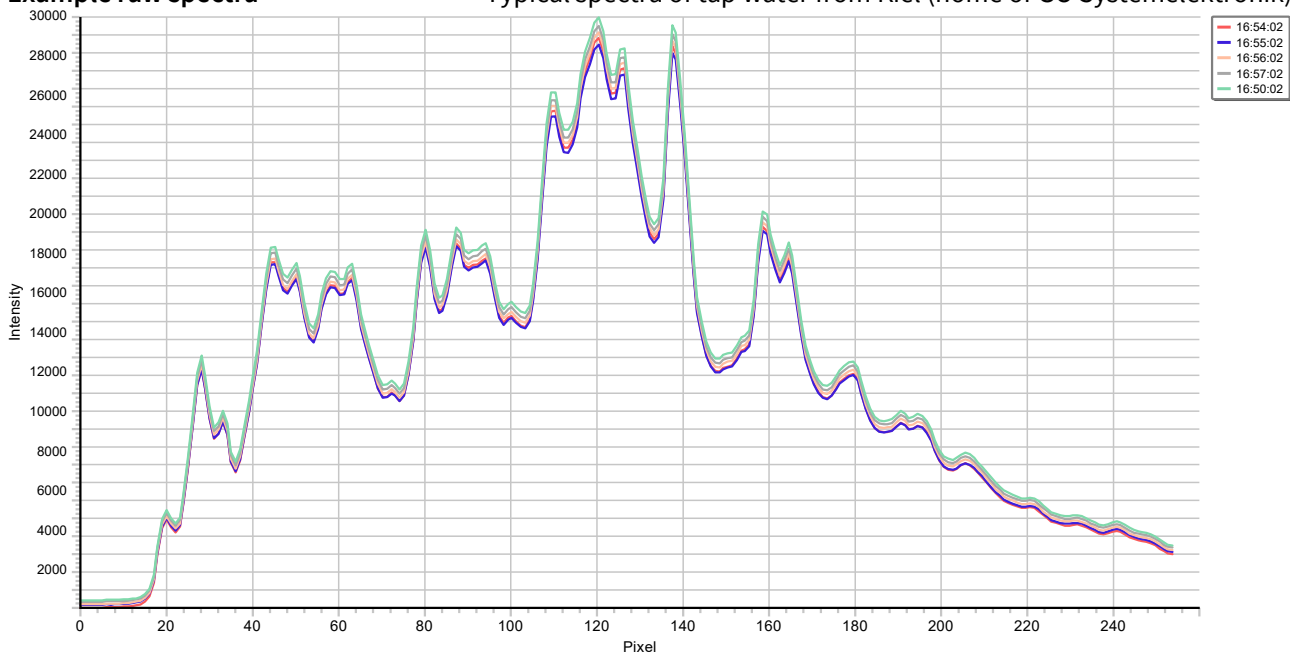
Typical spectra of tap water from Kiel (home of GO Systemelektronik)



The marked absorbance spectra are displayed as a line diagram in different colours. The values of the x-axis are the light wavelengths of 200 nm to 708 nm, the values of the y-axis the degree of absorbance.

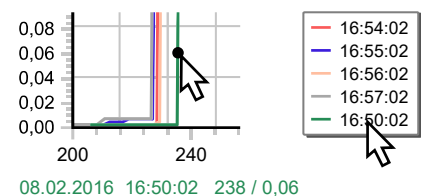
Example raw spectra

Typical spectra of tap water from Kiel (home of GO Systemelektronik)



The marked raw spectra are displayed as a line diagram in different colours. The values of the x-axis are the steps of the spectral resolution of the spectrometer (0 - 254), the values of the y-axis the counts of the AD converter (0 - 30000).

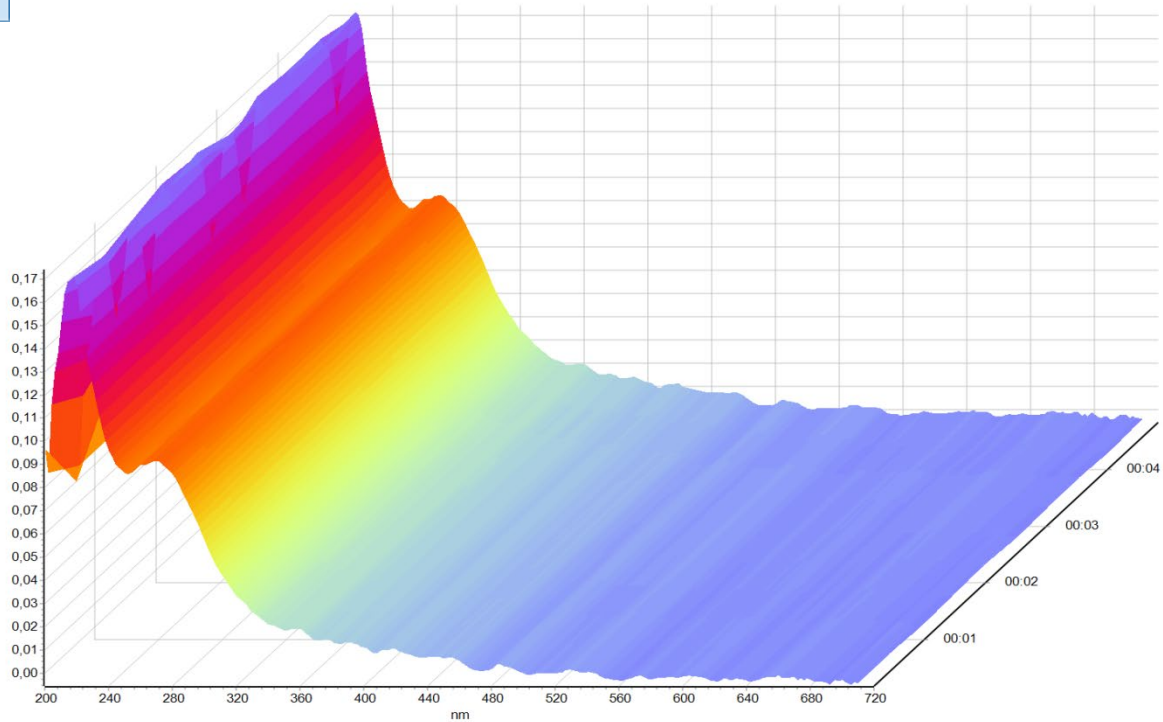
In the upper right the recording times of the spectra are listed with their line colour. Click on an entry activates the respective spectrum. You can then use the cursor to move to the single line points. On the bottom left the date and time of the spectrum recording and the xy-values of the line point are displayed.



ISA - Spectrum Visual

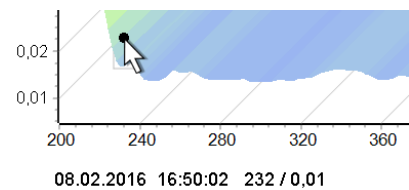
Example 3D view

Typical spectra of tap water from Kiel (home of GO Systemelektronik)



The values of the y-axis are displayed in different colours. The values of the z-axis are the recording times of the spectra.

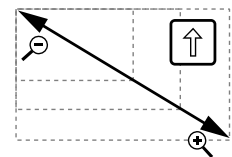
You can then use the cursor to move to the single points of the spectra surface. On the bottom left the date and time of the spectrum recording and the xy-values of the point are displayed.



You can enlarge or reduce the size of any spectra view by dragging a rectangle to the right or left while holding down the shift keys and holding down the left mouse button. Click on










for the normal view*.












* see vertical button bar

Functions of the horizontal button bar

-  Prints the spectra view.
 Print chart
-  Saves the diagram view as | .bmp | .emf | .wmf | .pcx | .gif | .jpg |
 Save chart
-  Exports the spectra data as a JCAMP-DX data format.
 see *11.3 Export Spectra Data*
 JCAMP-DX
-  Display of the absorbance spectra
 Abs. Spectrum
-  Display of the raw spectra
 Raw spectrum
-  Displays the graphs of the first derivation.¹
 Has no influence on the exported spectra data.
 1th derivation
-  Absorbance spectra² are displayed normalized to 1/m. These normalized spectra have intensity values related to a standardized measurement path of one meter length.
 Norm

Functions of the vertical button bar

-  Reload: Updates the spectra view.
 If, in the meantime, new spectra have been stored in the database, click on Reload loads the new spectra into the spectra list. Already marked spectra remain marked.
-  Back to the normal view
 If the spectra view is zoomed, click on this button switches back to the normal view.
-  Moves the selected time period by one day back.
-  Moves the selected time period by one day ahead.
-  Marks all spectra (max. 500).
-  Marks spectra (max. 500) at intervals of 5, 15, 30 and 60 minutes,
 Click again demarks all spectra.
-  Automatic Interval Markiert max. 500 Spektren gleichmäßig verteilt auf den ausgewählten Zeitraum.
-  Retrieves all ever captured spectra of the clearwater calibration.
-  Retrieves all ever defined reference spectra³ (Spectra with a sample number) auf.

¹ means the differences of the adjacent absorbance or raw values

² Does not work with spectra generated with older spectrometers.
 see 6.2 Notes on Current and Older Spectrometers

³ see Manual ISA and Process Spectrometer Commissioning – Maintenance – Service
 there 4.3 Application-Specific Calibration and following



Demarks all marked spectra.



Displays the spectra in a 3D diagram.



Below the next button a slider is displayed, with this slider you can adjust the display range of the z-axis of the 3D-diagram.

Click again to return to the 2D display.



The diagram display can be rotated around the x- and y-axis using the cursor and the pressed left mouse button.



Click again to return to the initial position.



Opens an info window with properties of the spectrum recording of a blue marked spectrum.



Marks all reference spectra (spectra with sample number) additionally to the already marked spectra.



Click again to return to demark all reference spectra.



Opens a window for entering a sample number for a blue-marked spectrum.

You can also double-click in the spectra list.

see *11.2 Enter and Delete Sample Numbers*

Menu bar functions

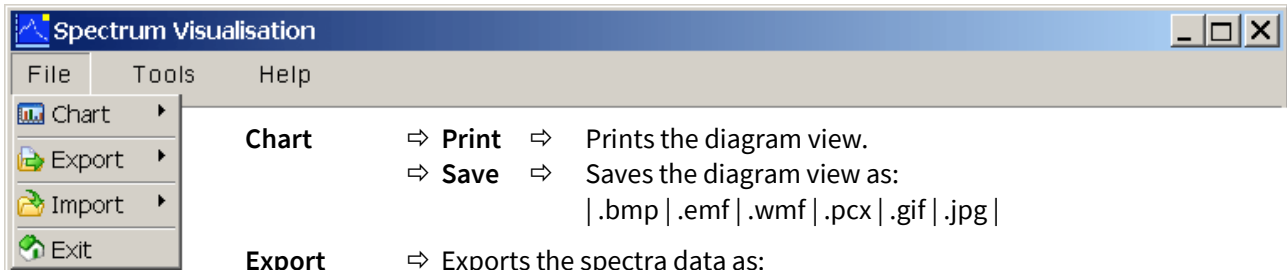


Chart	⇒ Print	⇒ Prints the diagram view.
	⇒ Save	⇒ Saves the diagram view as: .bmp .emf .wmf .pcx .gif .jpg
Export	⇒ Exports the spectra data as:	
	JCAMP-DX Text Format B+L Format BlueBox data base	see 11.3 <i>Export Spectra Data</i>
Import	⇒ Imports:	
	spectra data calibration data	see 11.4 <i>Import Spectrometer Data</i>
Exit	⇒ Closes Spectrum Visual.	




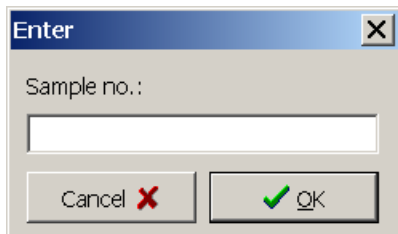
Export Fingerprint ⇒ Creates a fingerprint from the selected spectra and opens a window where the storage path can be selected. The fingerprint is saved there as an fp file. see also 9.2.2.6 *Fingerprint*



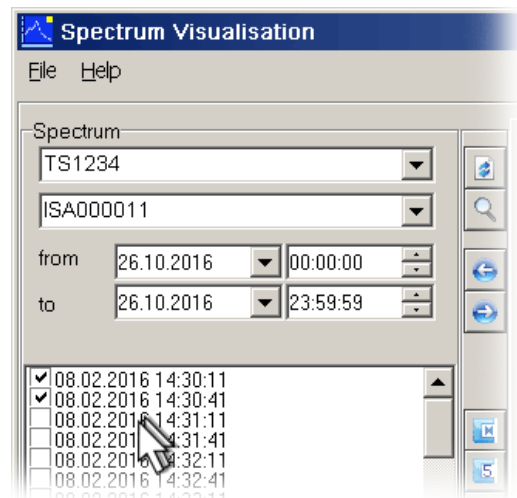
Opens an info window with the version number of Spectrum Visual.

11.2 Enter and Delete Sample Numbers

Click on  in the vertical button bar opens a window for entering a sample number* for a blue marked spectrum. You can also double-click in the spectra list.



Here you can assign a **sample number*** to a marked spectrum, entered commas are saved as point. A spectrum with sample number is a **reference spectrum** and is red marked in the spectra list.



You delete a sample number by clicking on <OK> without input.

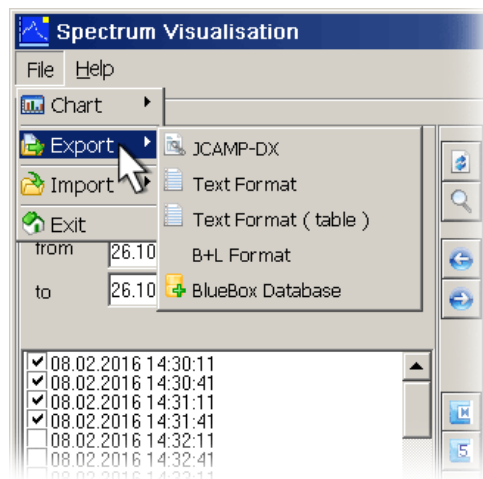
* Also called probe name or sample number. Character set: Standard ASCII
 The sample number is required for an application specific calibration in connection with a multi-parameter calibration, and is stored in the JCAMP-DX format together with the spectral data.
 see *Manual ISA and Process Spectrometer Commissioning - Maintenance - Service there 4.3 Application-Specific Calibration*

11.3 Export Spectra Data

You can export the selected spectra data of all spectra as one or various files.

Click on <File><Export> opens a selection menu.

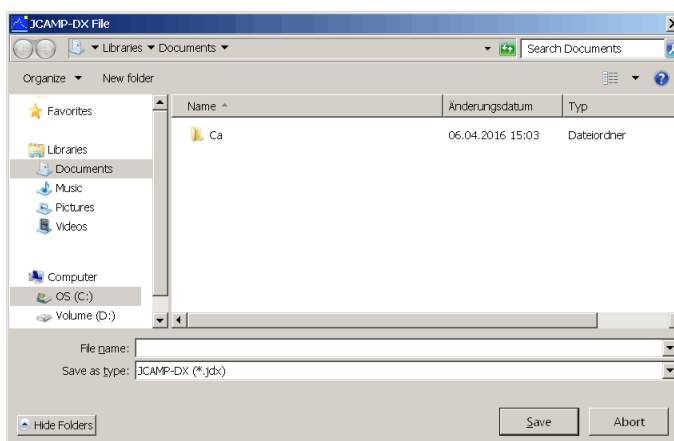
! If no spectrum is marked, all spectra of the spectra list are exported.



JCAMP-DX (with the extension *jdx*) is a standardized file format for exchanging spectra and related chemical and physical information between systems from different manufactures. The JCAMP-DX files are needed for calculating the calibration coefficients in the application-specific calibration (see *Manual ISA and Process Spectrometer Commissioning - Maintenance - Service* there 4.3 *Application-Specific Calibration*).

In the next window you specify name and memory location of the file. The file will then be saved with the file extension *jdx*.

The spectral data of the selected spectra are then summarized in a *jdx* file.



Text Format

The spectral data of each selected spectrum will be stored in a single *txt* file.

Text Format (table)

The spectra data of all marked spectra are saved in a *csv* file.

B+L Format

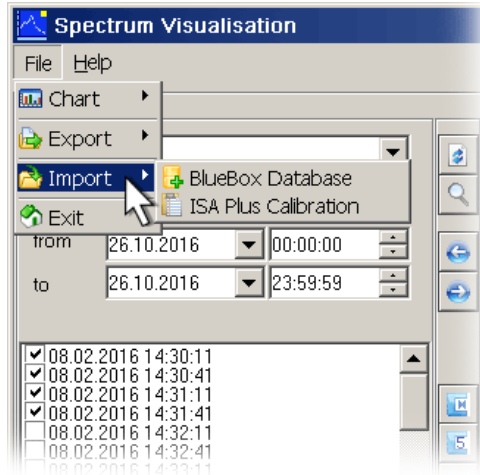
The spectral data of each selected spectrum will be stored in a single *asc* file. The modification date* of the file is the recording time point of the spectrum.

BlueBox Database

The spectral data of all selected spectra are stored in one file with the extension *isa*. With this *isa* file the spectra data could be imported from other computers (see 11.4.1 *BlueBox Database*).

* not the creation date

11.4 Import Spectrometer Data



11.4.1 BlueBox Database


Spectrum Visual can generate BlueBox export files with the isa file extension, see 11.3 Export Spectra Data. With these files you can export spectra data from a database (source database) to a database of the same name (target database) on another computer (target computer).

Prerequisite: If this database of the same name does not exist on the target computer, it must be set up.*

Setting up a database with the program BlueBox SQL:

see Manual BlueBox PC Software there 3.2.2 Setup of a New BlueBox

- ① Freely selectable name, does not have to match the BlueBox name on the source computer – Under this name (Selection BlueBox, see 11.1) you can call up the spectra from the imported database.
- ② Serial number of the BlueBox of the source database
- ③ Name of the source database, standard name is *bluebox*

Click on  creates the database on your computer.

Note on the time stamp: The record times of the spectra are stored in the database in Universal Time Coordinated (UTC), just like all other acquisition times. Changing the time zone, e.g. in Spectrum Visual, only changes the time stamp of the display, and not the time stamp in the database.

* The created database appears in the BlueBox PC Software as an actually existing BlueBox, to which direct access (e.g. retrieving data from the BlueBox or changing settings) is not possible.

11.4.2 ISA Plus Calibration – Apply Calibration Data to Existing Spectra

Here you can apply **ISA Plus calibration files** in the xml format and in the txt format to your spectra in the database.


i This import is not to be confused with the import of the calibration files to a BlueBox. see *Manual ISA and Process Spectrometer Commissioning - Maintenance - Service* there 4.3 *Application-Specific Calibration*


The calibration files are generated with an **application calibration**¹ and are used to calculate parameters of a specific application.


The parameter values are displayed as a line graph.


Import a calibration file:

Two additional buttons² appear in the horizontal button bar.



 **Calculated value** Displays the calculated parameter values as a line graph. You can then use the cursor to move to the single points of the line graph. On the bottom left date and time and calculated parameter value of the point are displayed. Beneath the name of the calibration file with date.


 **Quality [SQI]** Displays the SQI (Spectral Quality Index) of the calculated parameter values and the spectra. A third button appears.

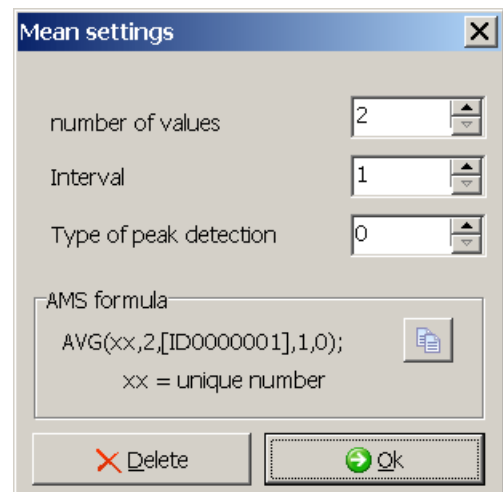
 **Ignore neg. values** Sets negative values to zero.

In the vertical button bar, another button appears ⇒ 

Click on this button opens the window of the mean value settings. Here you can determine how a moving average of the calculated parameter values is generated and how outliers are treated.

 **Delete** Cancels the effect of the mean settings. You can also click on 

 **Ok** Calculates the mean values and displays them graphically.



Number of values Number of parameter values from which the moving average is calculated, minimum is 2.

Interval Parameter values are calculated only from those spectra whose time difference, starting with the first marked spectrum, is greater than or equal to the interval.³

¹ see *Manual ISA and Process Spectrometer Commissioning - Maintenance - Service* there 4.3 *Application-Specific Calibration*

² and button **f(x)** disappears

³ Values less than/equal to the interval of the spectrometer are of no effect.

see 8.2.1 *General Settings* and 9.2 *The Sensor Setup Window of the Spectrometer*

Type of peak detection

0	No outlier detection
----------	----------------------

The measurement values determined with *number of values* (see above) are sorted by size.

1	The lower and upper 10 percent by number are removed and the arithmetic mean is calculated
2	The lower and upper 20 percent by number are removed and the arithmetic mean is calculated.
3	The lower and upper 30 percent by number are removed and the arithmetic mean is calculated.
4	The lower and upper 40 percent by number are removed and the arithmetic mean is calculated.
5	The calculated mean is the median of all n values.

AMS formula

This field displays the corresponding AMS formula entry.

AVG(xx,b,[Sensor-ID],d,e);


xx = Consecutive identification number of the moving average (0 to 9999)

b = Number of measurement values to be averaged.

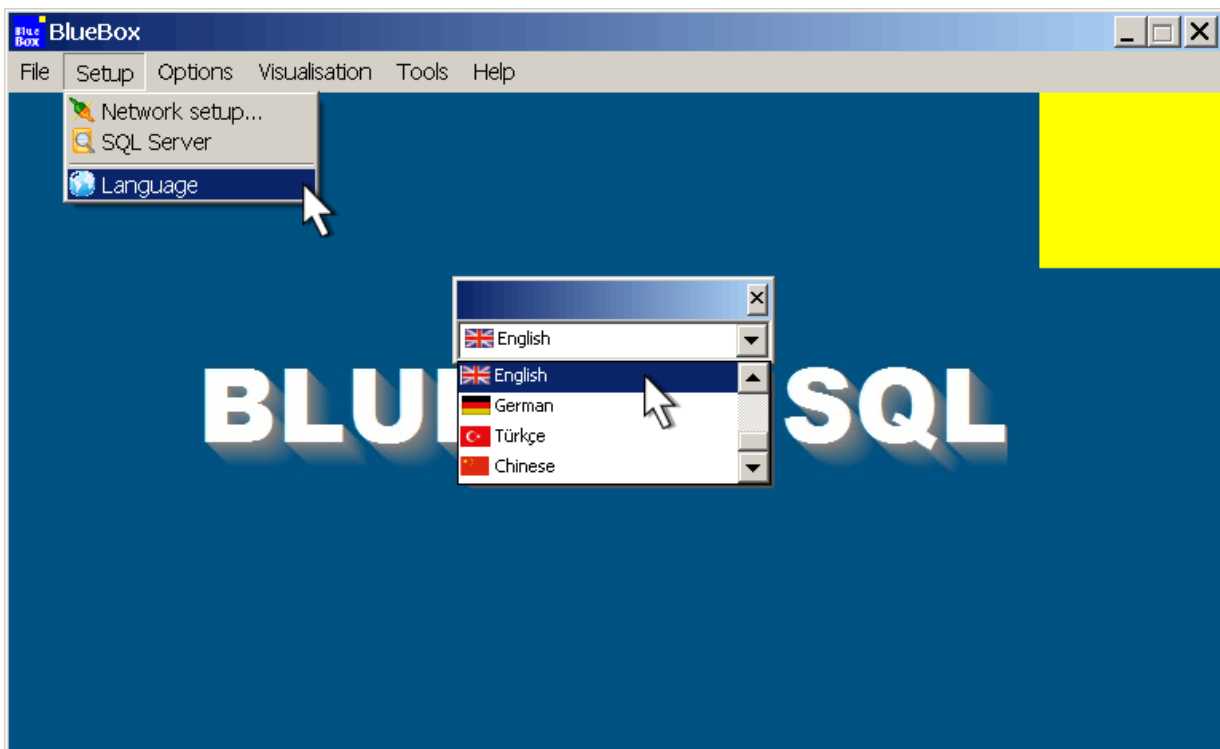
[Sensor-ID] = measurement value of the sensor

d = Interval

e = Type of outlier detection

Click on  copies the formula entry into the clipboard.

12 Language Options



13 Virtual Sensors

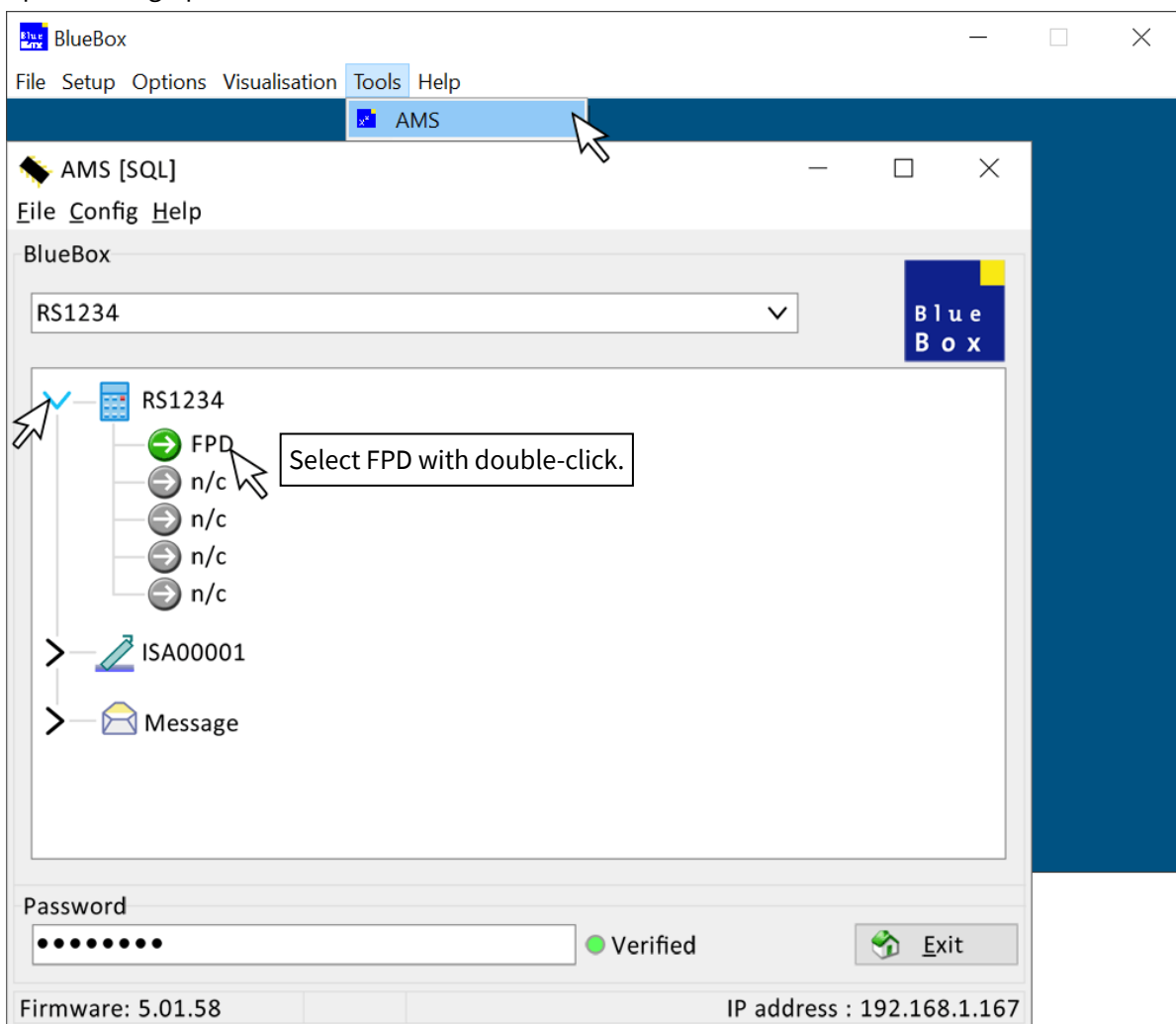
The BlueBox PC Software offers with AMS (Advanced Managing Software) the possibility to set up virtual (calculated) sensors. In combination with the ISA there are numerous possible applications. A description of the software AMS with its formula language AMS Formula can be found in the *Manual BlueBox PC Software*.

If more than one spectrometer is connected to the BlueBox, a spectrometer must be determined in the formula field with the entry `ISA="CAN-ID"`; to which the following ISA-specific formula elements refer.
 CAN-ID = CAN-ID of a spectrometer

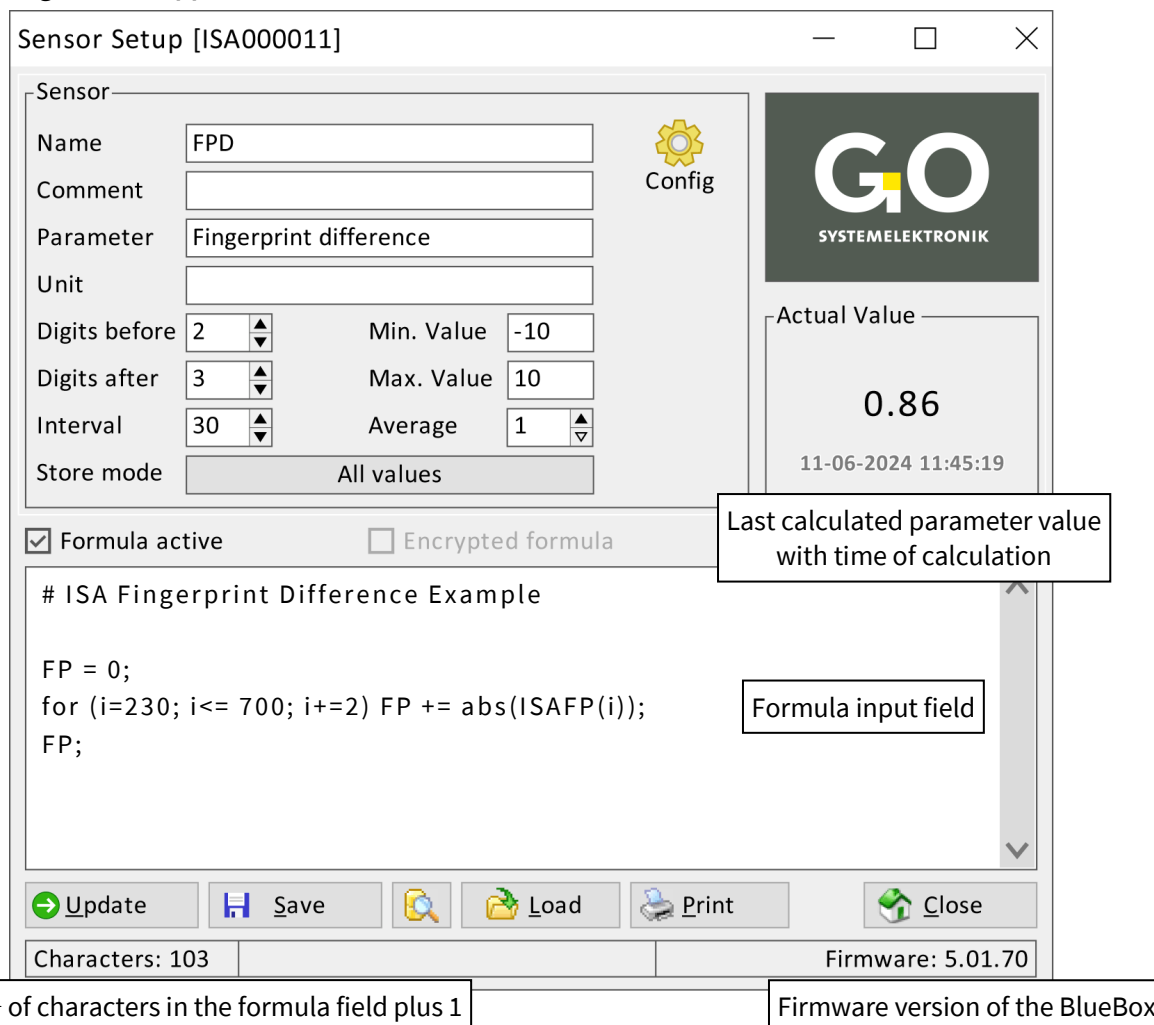
13.1 Example Calculation of a Fingerprint Difference

A fingerprint can be used as a reference to detect contamination in the measurement medium. In this formula, the sum of the absolute values of the differences between the current absorbance spectrum and a fingerprint is calculated at all even wavelengths from 230 nm to 700 nm. The frequency range can of course be freely selected.

Example of a Fingerprint difference with the name FPD:



The following window appears:



Sensor Setup [ISA000011]

Sensor

Name: FPD

Comment:

Parameter: Fingerprint difference

Unit:

Digits before: 2

Digits after: 3

Interval: 30

Min. Value: -10

Max. Value: 10

Average: 1

Store mode: All values

Formula active Encrypted formula

ISA Fingerprint Difference Example

```
FP = 0;
for (i=230; i<= 700; i+=2) FP += abs(ISA FP(i));
FP;
```

Actual Value: 0.86

11-06-2024 11:45:19

Characters: 103

Firmware: 5.01.70

Name, Comment, Parameter and Unit: Entries take effect after the Enter key on the PC keyboard is pressed or an active window element (not — \square \times) is clicked.



Opens the calibration window of the parameter.
see *Manual BlueBox PC Software* there 5.4.1.2.5 *Multi-Point Calibration*

Name	Name of the virtual sensor, is queried by other BlueBox programs.	max. 20 characters
Comment	Any comment text ²	max. 20 characters
Parameter	Name of the measured parameter	max. 20 characters
Unit	Unit of the output value More than 5 characters can't be displayed at the BlueBox display	
Digits before	Number of displayed pre-decimal places	
Digits after	Number of displayed decimal places	

¹ characters + spaces + line breaks

² In older software versions, here it was also possible to determine how a measurement value is stored in the database. The setting is now made via the <All values> button.

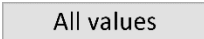
ISA - Virtual Sensors

Interval Time period in seconds between the calculations
 The minimum interval is the spectrometer interval.
 The interval of a virtual sensor can only be an integer multiple of the spectrometer interval, in this example 120, i.e. in case of a spectrometer interval of 60 the calculation of the sensor value takes place at every second spectrum capture.
 Other values are taken as the next largest integer multiple of the spectrometer interval.

Min. Value Lower value limit


Max. Value Upper value limit

Average The number of single measurements from which the arithmetic mean is derived.


 Opens a menu where you can define how the parameter values are stored in the database. see *Manual BlueBox PC Software* there 5.4.1 *Sensor Setup* there *Display and save mode*


Formula active/inactive Switches a formula entry active/inactive, effective by clicking on <Update>.


Formula encrypted or not optional Here you can add a password to the formula in the formula input field and encrypt it. Encrypted formulas can only be viewed and changed after entering the password.

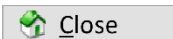
 **Update** Transfers the formula from the input field to the BlueBox.

 **Save** Opens a window to save the formula on the PC.

 Opens a list of the current variables with their current values.

 **Load** Opens a window to load a saved formula from the PC.

 **Print** Opens a window for to print these sensor-settings.

 **Close** Closes the sensor setup window.

13.2 ISA Formula Examples

Here are a few examples of how to calculate spectral data in virtual sensors.

ISA NO₃ example

In this formula the absorbance values at frequencies 284nm, 332nm and 628nm are used to generate a NO₃ value. A lower limit is also implemented. The exact coefficients are derived from ISA Soft software calculations.

```
# ISA NO3 (example)
```

```
Value = -0.06347;
Value += ISA(284) * 28.547863;
Value += ISA(332) * - 51.927711;
Value += ISA(628) * 30.110743;
```

```
if (Value < 0) Value = 0;
Value;
```

ISA SAK254

The formula calculates the Spectral Absorbance Coefficient (SAC) at 254 nm.

```
# ISA SAC254
```

```
SAC = ISA(254)*(1000 / ISA.Pathlength);
if (SAC < 0) SAC = 0;
SAC;
```

ISA SAK254 with turbidity compensation

```
# ISA SAC254 with turbidity compensation
```

```
offset = 0;
for(i=600; i<700; i+=2) offset += ISA(i);
offset /= 50;
# calculates the average of the absorbance spectrum drift
# in the range 600nm to 700nm
```

```
SAC = (ISA(254)-offset)*( 1000.0 / ISA.Pathlength );
if ( SAC < 0 ) SAC = 0;
SAC;
```

ISA Modbus export

This formula makes spectral data retrievable for a Modbus master device.

```
# ISA Spectrum Modbus-Export
```

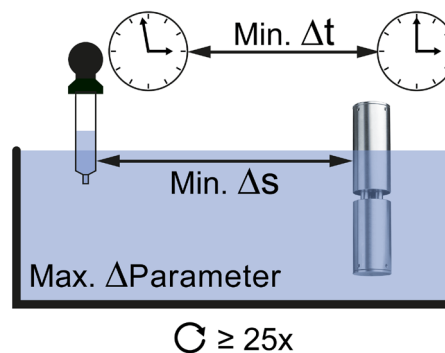
```
for (i=0; i<=255; i++) MODR(i) = ISA0(i);
```

14 Parameter Accuracy

Parameters, calculated with ISA spectral data can achieve the accuracy of 5% (typical 5 % - 10 %). In detail the accuracy can vary by the change of the water matrix. If the water matrix has higher variability, for example day/night or seasonal changes, this has to be analysed and a special calibration must be performed. In general, calibrations adapted to specific conditions can provide reliable measurements even under difficult conditions. Changes in the water matrix can be detected by other parameters (conductivity, pH value, temperature etc).

1. The accuracy of spectral data calculated parameters always is influenced by the quality of calibration. A higher number of calibration points will have the result of a more accurate calibration!
2. The range of the reference value pairs* must cover the entire measuring range evenly distributed as possible. The minimum number of reference value pairs is 25, a smaller number reduces the quality of the calibration and may subsequently lead to erroneous measurements.
3. The right choice of the analytical method and the care in the procedure are the most important requirements for the accuracy of the calculation. The accuracy of the ISA parameter calibration is depending upon the specific accuracy of the chemical method for the parameter.
4. After the calibration, the calibration has to be checked and (when appropriate) adjusted over a longer period (for example, one week). This increases the stability of the measurement.
5. Measurements with high accuracy over a longer period are only possible with correspondingly adapted maintenance, a maintenance schedule is highly recommended here.

In general, periodic cleaning and recalibration increases the measurement quality. The interval of the maintenance is determined by the measurement conditions and can last from several weeks to several months. see *Manual ISA and Process Spectrometer Commissioning - Maintenance - Service*



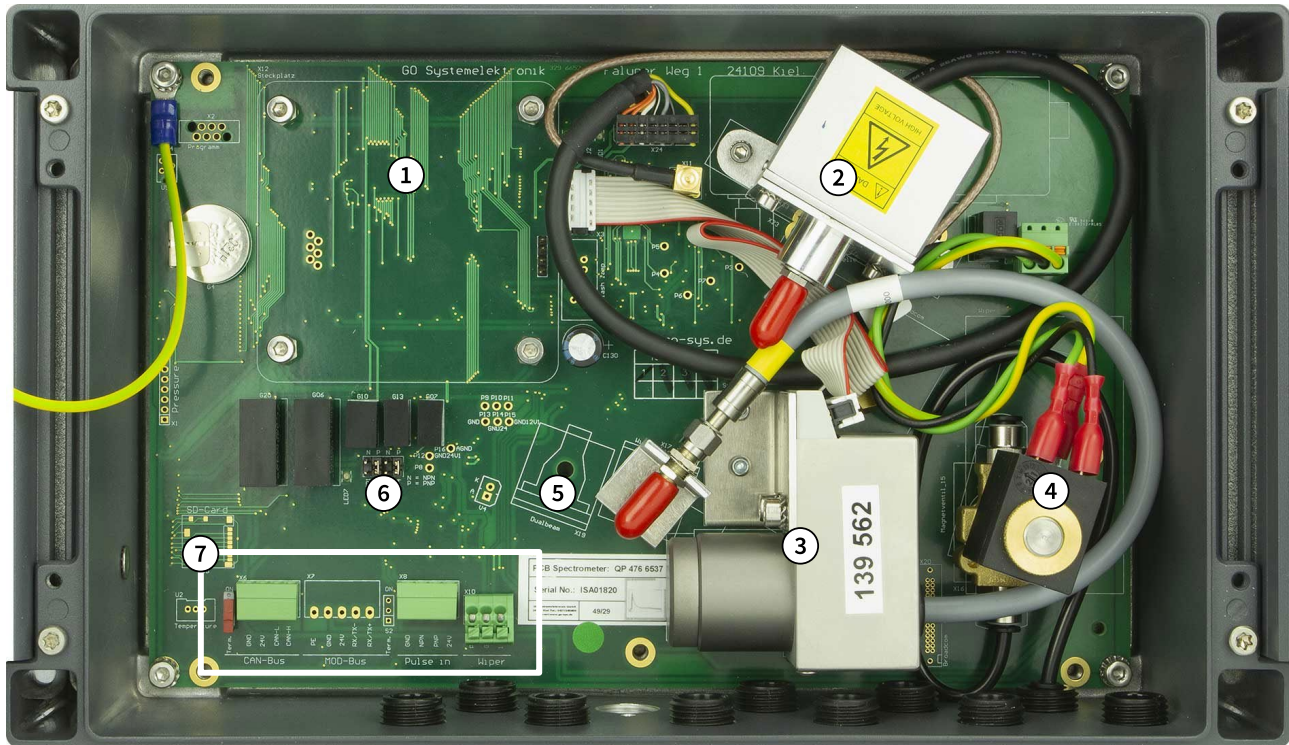
* For the calculation and calibration to the desired parameter of a specific application, it is necessary that for each parameter reference values from chemical laboratory analysis and the corresponding spectral values are provided. In case of a one-parameter calibration a spectrum is assigned to one reference value, in a multi-parameter calibration there is more than one reference value assigned. The spectral data of a spectrum plus one or more corresponding measurement values are called **reference value pair**.

ISA - Spectrometer Board

15 The Spectrometer Board

The spectrometer board is located in the BlueBox RS and in the Spectrometer Sensor Module.

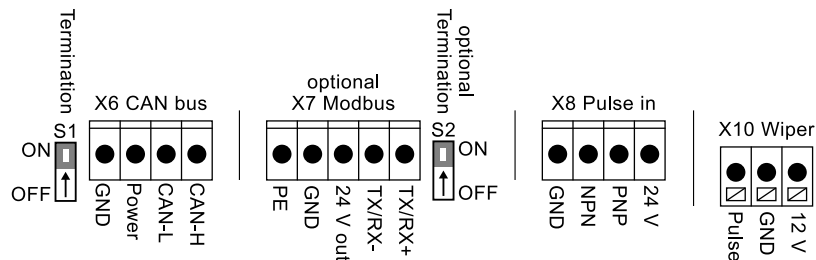
Example Spectrometer Module:



- ① Mounting place for an optional BlueConnect board
- ② Xenon flash lamp with fibre optic cable connector OUT
- ③ Spectrometer with fibre optic connector cable IN
- ④ Compressed air valve with electric switch. Alternatively, a wiper module can be mounted here.
- ⑤ Mounting place for the photometer of the optional DualBeam version
- ⑥ Jumper slots of the pulse input

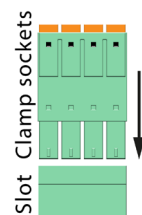
<input type="checkbox"/>	<input checked="" type="checkbox"/>	NPN	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
unassigned	assigned			PNP							

 Factory setting: PNP
 Jumper assignment
- ⑦ Cable connections and termination slide switches

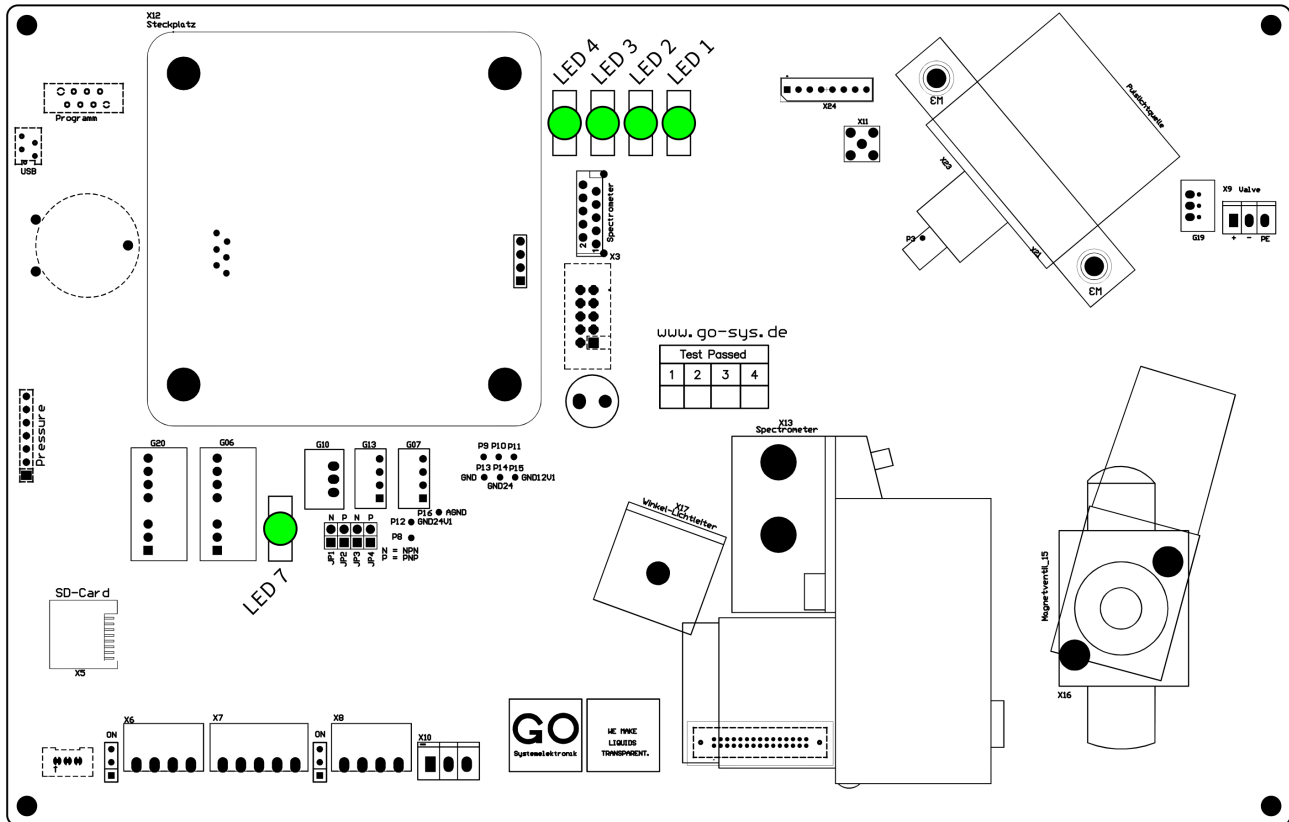


Slot X6, X7 and X8: The cables are connected to the slots by means of clamp sockets. Note that the slots lie flat, i.e. the clamp socket strips are plugged onto the slots from "above".

X10: There are cable clamps on the slot ex works.



ISA - Spectrometer Board





LED-Functions

- LED 1: Flashing – frequency 0.5 Hz; main processor is in operation
- LED 2: Cleaning with compressed air is carried out
- LED 3: Cleaning with wiper is carried out
- LED 4: Data transmission CAN bus
- LED 7: Supply voltage is present

16 Connections at the BlueBox RS


Housing Connections






-  Earth the BlueBox. This is the only way to ensure trouble-free measuring operation.  The earth connection is located on the left side of the housing.

LAN connection

USB Connection (MDI crossover)

-  Please note:
The USB port at the BlueBox is designed for data export and for firmware and license update.

Antenna connections

-  LTE Panel socket (female)  In case of doubt, differentiate the antenna connector as follows:
Panel socket = LTE (female) Panel plug (male) = WiFi
-  WiFi Panel plug (male)

PG glands M16

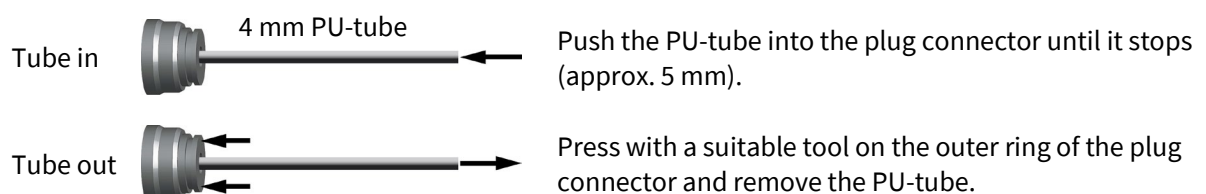
Via these glands the cables are led to the connections on the main board.

-  Ensure proper execution.

Socket of the sensor head cable

Compressed air line connection

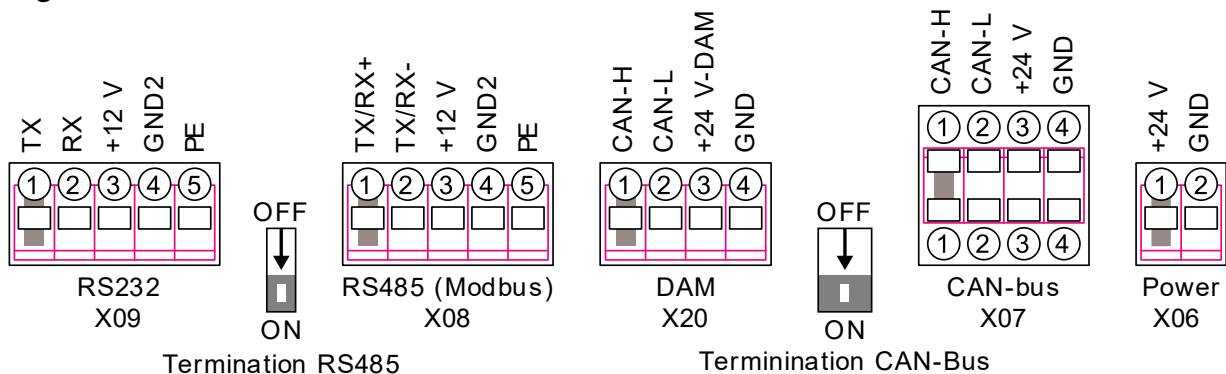
Quick connector for 4 mm PU-tube, 4 – 6 bar



Mainboard PIN Assignment and Termination

The internal spectrometer board is connected to DAM X20.

First generation mainboard



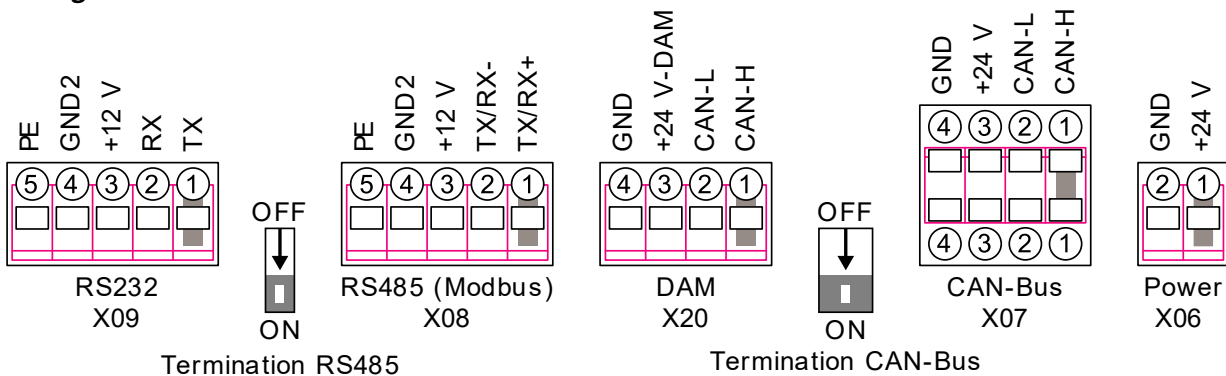
! The difference between the first- and second-generation mainboards is that the assignment of all slots has been "rotated".

You can see the difference in the assignment by looking at the mainboard labelling.



Caution: Reverse polarity can destroy the device.

Second generation mainboard



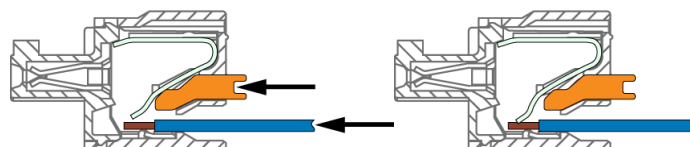
Note RS232 X09 and RS485 X08:

Only one of the two connections can be active, toggling is done via the AMS program. see *Manual BlueBox PC Software* there 5.3.3.2 *Custom Protocol Setup*

Note DAM X20:

Internal DAM connection to an internal BlueConnect Plus board or an internal spectrometer board.

Functionality of the cable clamp



17 The External Spectrometer Module

The Spectrometer Sensor Module is a CAN-bus module. It is connected to a BlueBox with a CAN-bus cable via the CAN-bus interface.

The current Spectrometer Sensor Modules have the
Article-No. 486 6000


The type plate is located at the right-hand side of the housing.

i Note on older versions of the Spectrometer Sensor Module
Second generation Spectrometer Sensor Modules (Article-No. 486 6002 and 486 6004) are compatible to the current BlueBox System.
see Page 3 *Notes on the Compatibility of Older and Newer Spectrometers*
see also 4.2 ATEX Notes




Housing Connections



 Earth the Spectrometer Sensor Module.

This is the only way to ensure trouble-free measuring operation.

 The earth connection is located on the left side of the housing.



PG glands M16

Via these glands the cables are led to the connections on the main board.

i Ensure proper execution.

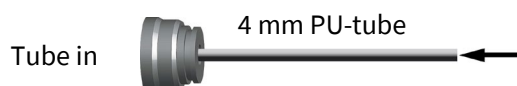


Socket of the sensor head cable



Compressed air line connection

Quick connector for 4 mm PU-tube, 4 – 6 bar



Push the PU-tube into the plug connector until it stops (approx. 5 mm).



Press with a suitable tool on the outer ring of the plug connector and remove the PU-tube.



PIN Assignment and Termination at the spectrometer board see *15 The Spectrometer Board*

Configuration Data Sheet

Appendix A – The Configuration Data Sheet

The configuration data sheet contains the necessary settings to run the BlueBox.

Example BlueBox RS:

 		Configuration Data Sheet Product: BlueBox	Page: 1/1 Date: 2023-02-07
1. BlueBox R1:			
Serial Number	RS1234		
Display PIN	xxx		
Storage Device	8 GB		
2. Network:			
IP Address	192.168.1.167		
Netmask [CDIR]	24		
Gateway	0.0.0.0		
Port	14111		
Login Name	bluebox		
Password	xxx		
3. Hardware			
LAN MAC-Address	xx-xx-xx-xx-xx-xx		
WLAN MAC-Address	xx-xx-xx-xx-xx-xx		
4. BlueBox BlueGate Settings:			
Host	bluegate.go-sys.de		
Password BlueGate	xxx		
5. BlueBox PC Software - BlueGate Settings:			
Host	datagateway.go-sys.de		
Username	xxx		
Password Windows	xxx		
This document contains confidential information.			
<small>© GO Systemelektronik GmbH Faluner Weg 1 D 24109 Kiel Telephone: +49 431 58080-0 Fax: +49 431 58080-11 Internet: www.go-sys.de</small>			

1. BlueBox R1:

Serial Number	R11234
BlueBox Password (PIN)	xxx
Storage Device	8 GB

Serial Number

Serial number of the BlueBox
 With this serial number the BlueBox is identified by the BlueBox PC Software.

⇒ set at the factory, not changeable

BlueBox Password (PIN)

Password of the BlueBox
 Is required to change the BlueBox system settings.

⇒ set at the factory, not changeable

Storage Device

Size of the internal BlueBox memory, here 8 GB

⇒ set at the factory, changeable by replacing

2. Network:

IP Address	192.168.1.167
Netmask [CDIR]	24
Gateway	0.0.0.0
Port	14111
Login Name	bluebox
Password	xxxxx

- IP Address** IP address of the BlueBox
At this address, the BlueBox is addressed on the network.
⇒ set at the factory, changeable
- Netmask [CDIR]** Netmask of the BlueBox
⇒ set at the factory, changeable
- Gateway** Standard gateway of the BlueBox
⇒ set at the factory, changeable
- Port** Default gateway of the Blue Box
⇒ set at the factory, not changeable
- Login Name** User name for a modem connection
⇒ set at the factory, not changeable
- Password** Network password of the BlueBox
Is needed to access the BlueBox via the AMS software.
⇒ set at the factory, not changeable

3. Hardware:

LAN MAC-Address	xx-xx-xx-xx-xx-xx
WLAN MAC-Address	xx-xx-xx-xx-xx-xx

- LAN MAC-Address** ⇒ set at the factory, not changeable
- WLAN MAC-Address** ⇒ set at the factory, not changeable

4. BlueBox BlueGate Settings:

IP Address	bluegate.go-sys.de ¹
Password BlueGate	xxxxx

- IP Address** IP address of an Internet Gateway
⇒ can be configured at the factory, changeable ²
- Password BlueGate** Password of an Internet Gateway
⇒ can be configured at the factory, changeable

5. BlueBox PC Software – BlueGate Settings:

Host	datagateway.go-sys.de ¹
Username	xxxxx
Password Windows	xxxxx

If the BlueBox is accessed via a gateway (e.g. with an UMTS connection), you have to enter these access data in the BlueBox SQL Software.

¹ default address of GO Systemelektronik

² changeable only at the default address

Appendix B – SQI (Spectral Quality Index)

Precondition for the calculation of the SQI is a corresponding calculation, see *Manual ISA and Process Spectrometer Commissioning – Maintenance – Service*.

In Situ spectrometers are used for decisions in the fields of food processing, chemical process cycles, drinking water monitoring, as well as in the field of wastewater treatment plant control and flow control.

Functional principle: The measurement method of in situ spectrometer, like the ISA, is based on absorbance spectra. Multiple calibrations can be created with these spectra and so different chemical ingredients can be measured online by calculation. No chemicals are needed for this measurement method – it is not predicated on any laboratory test or an existing DIN standard.

Based on the time behaviour of the spectral data in combination with associated analytical laboratory tests, an algorithm is determined with a chemometrical process, to calculate the different parameters. This chemometrical process is a statistical method which can develop specific prediction algorithms for the particular parameters.

A statistical method specially developed for the ISA allows the progressive adaptation of the calibrations, **quality monitoring in the calculation of the algorithm** has been given special consideration. Thus, an improvement of the algorithm by statistical parameters is already possible during the model development.

The aim is to expand a general algorithm by **on site specific** data and so to generate **user-specific** algorithms.

Every determination which is not DIN standard brings the risk of incorrect determinations. These failures cannot be eliminated completely by using statistically developed algorithms. When there are temporary situations which are not included in the statistical data set, the measurement reliability cannot be furthermore approved.

For this reason, **online quality detection** and thus **quality documentation** of these calculations are essential for the use of spectral sensors especially.

For this purpose, the Spectral Quality Index (SQI) is determined and saved for each calculated parameter by the ISA Spectrometer. The scaling of the SQI is as follows – under a value of 3.5 a measurement reliability of 95% can be assumed. Up to a value of 4.0 a certainty of 90% is given. However, when there is a permanent SQI above 4 determined over a longer time, it must be assumed that the spectral data set present in the range of the used wavelengths is no longer sufficiently statistically proven.

In this case a warning is issued, it is not recommended to use the calculated results for the process control. The system can be shifted to “emergency control signals” automatically. This process is similar to the failure of the lambda probe signal in the control of internal combustion engines.

A deviation of the SQI to values higher than 4 can also be caused by defects in the measurement system or by contamination or blocking of the optical measurement path.

In Figure 1 below we show results of measurements in the supply of a wastewater treatment plant. The red lines show the concentration gradient of the COD measurements. The green line visualizes the characteristics of the corresponding SQI values for this COD measurement. The given scales are shown on the left and right side of the application. High values of the SQI correspond with extreme changes in the value of the COD.

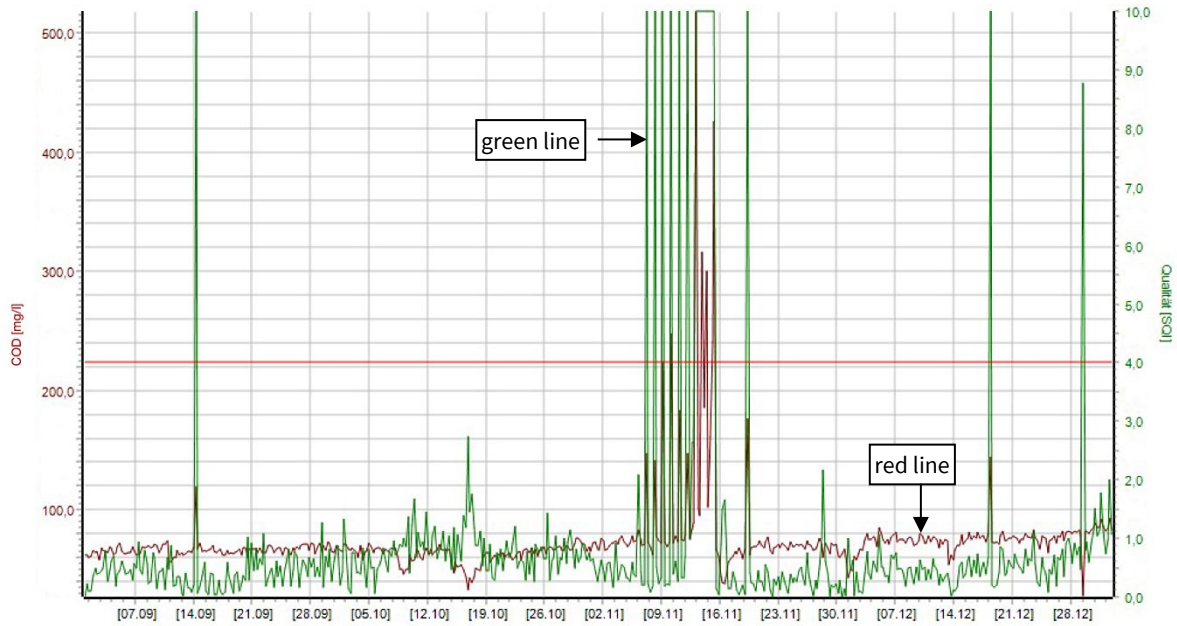


Figure 1* Concentration gradient of COD measurements (red) with the SQI (green)

Between the 12th and 16th of November a contamination could be determined, which was ascribed to a faulty compressor. By the use of the SQI the failure of the cleaning was detected very quickly and could be fixed without causing major damage. In October there was a brief single event – without recognized influences in the COD. At the end of the year, the water matrix varied due to strong temperature changes and caused a deterioration of the SQI values without leaving the acceptable range.

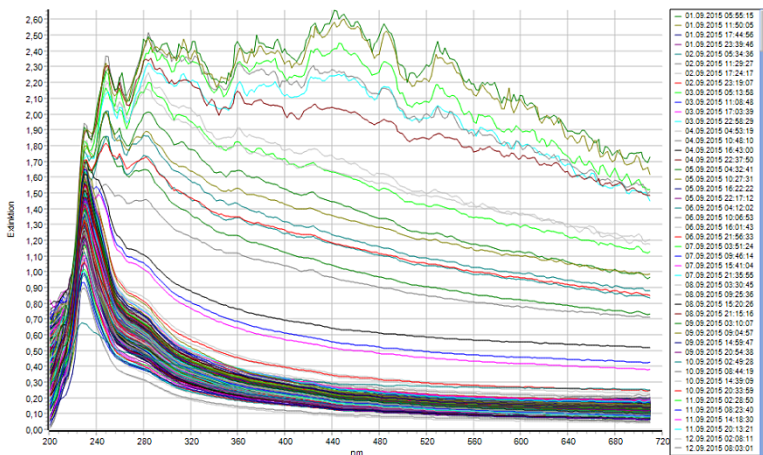


Figure 2* Absorbance spectra of the COD calibration

The function of the SQI as proof of quality and indication of malfunctions is easy to recognize in the Figure 1. The good performance of the SQI can also be ascribed to the high-quality calibration created by 54 reference values, taken over six months. The absorbance spectra of this calibration are shown in Figure 2.

For further information please contact GO Systemelektronik.

* The Graphic is generated with Spectrum Visual.

Appendix C – Stainless Steel 1.4404 in Comparison with Other Steels

Standards and designations for 1.4404

| EN 1.4404 | DIN X2CrNiMo17-12-2 | AISI 316L | UNS S31603 |

Stainless steel 1.4404 is the most commonly used steel for applications in aggressive environments. In natural environmental media, in media with moderate chlorine and salt concentrations and in the food industry, 1.4404 is characterised by excellent corrosion resistance. Due to its low carbon content, 1.4404 is resistant to intergranular corrosion. (PREN = 23.1 - 28.5)

With the addition of 2 - 2.5 % molybdenum, the material 1.4404 offers significantly better corrosion resistance than **1.4301** or **1.4307**. Due to the lower carbon content compared to **1.4401**, the material 1.4404 is also characterised by good processing properties.

Stainless steel **1.4571** (AISI 316Ti) is comparable to 1.4404 in terms of corrosion resistance and mechanical properties. 1.4571 is stabilised by the addition of titanium, which results in carbon bonding. This makes 1.4571 resistant to intergranular corrosion even after welding.

However, the surface of 1.4571 is difficult to polish and is therefore unsuitable for contact with food.

The only material more resistant than stainless steel 1.4404 is **titanium**, which should be used for salt contents above 10 PSU.

The ISA sensor head of GO Systemelektronik is available in stainless steel 1.4404 and in titanium.

Triggers for corrosion and ⇒ Countermeasures

- Electric fields
 - ⇒ Earthed measuring medium ⇒ Earthed probe ⇒ potential-free probe
- Machining residues from turning chips or other metals
 - ⇒ Chemical removal of foreign metals by pickling
- Release of hydrochloric acid on contact with PVC
 - ⇒ Avoidance of contact with PVC
- Electrochemical potential difference

The electrochemical voltage series in natural salt solutions and seawater is significantly different from the voltage series in KCL to the reference hydrogen standard electrode, making it difficult to estimate the potential.

 - ⇒ Avoidance of PVC in the environment