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Overview of UV/Vis spectrometry

Solutions by GO Systemelektronik



Introduction to UV/Vis Spectrometry

Parameters & Measurement Ranges

Functions & Features

Calibration Monitoring

UV/Vis Spectrometer Product Solutions

Vergleich von ISA & BlueScan Plus

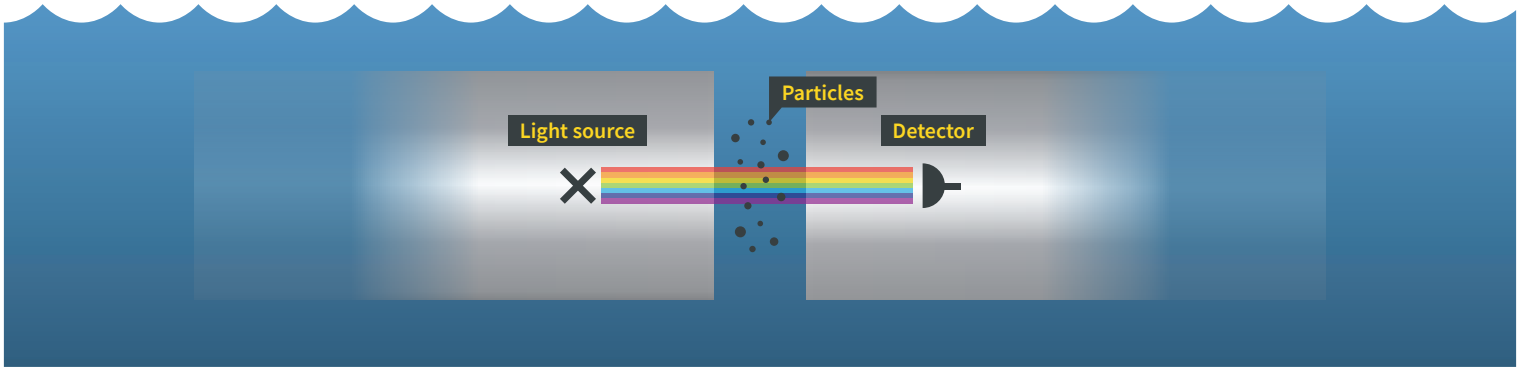
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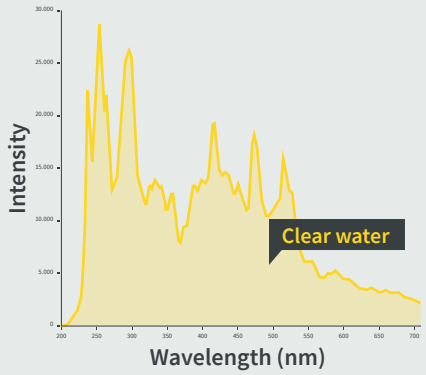
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Introduction to UV/Vis spectrometry

When light radiates onto a medium - such as water - various effects such as reflection, scattering or absorption occur. Lambert-Beer's law states that the absorption of light at a certain wavelength depends on the concentration of the substance to be measured. UV/Vis spectrometers make use of this effect. Light with wavelengths in the UV and visual range radiates onto the medium, hence the name UV/Vis spectrometry. The substances in the water absorb light of different wavelengths and with different intensity. The remaining light is measured by a detector. The specific absorption per wavelength can then be used to calculate the concentration.

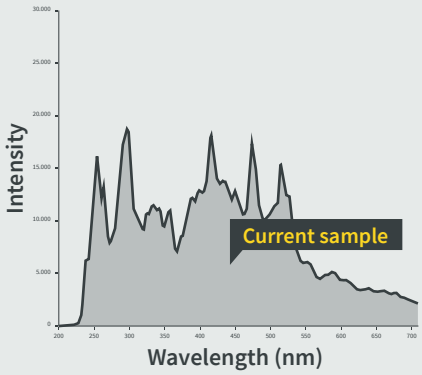


Clear Water Calibration



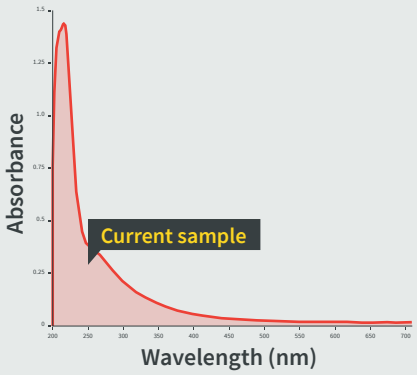
In order to correctly determine the absorption in water, a reference must first be defined. For this purpose, the intensity of the emitted light is recorded for the entire wavelengths in clear water. In order to calculate the ingredients correctly later on, double-distilled water should be used if possible. The clear water spectrum is stored as reference intensity I_0.

Current Raw Spectrum



With each measurement, the detector measures the remaining light that has not been absorbed by the measuring medium. This spectrum is also known as the raw spectrum and is stored as intensity I.

Absorption Spectrum



From the clear water calibration and the current raw spectrum, the absorption is finally calculated for each individual wavelength $A = lg(\frac{I_0}{I})$.

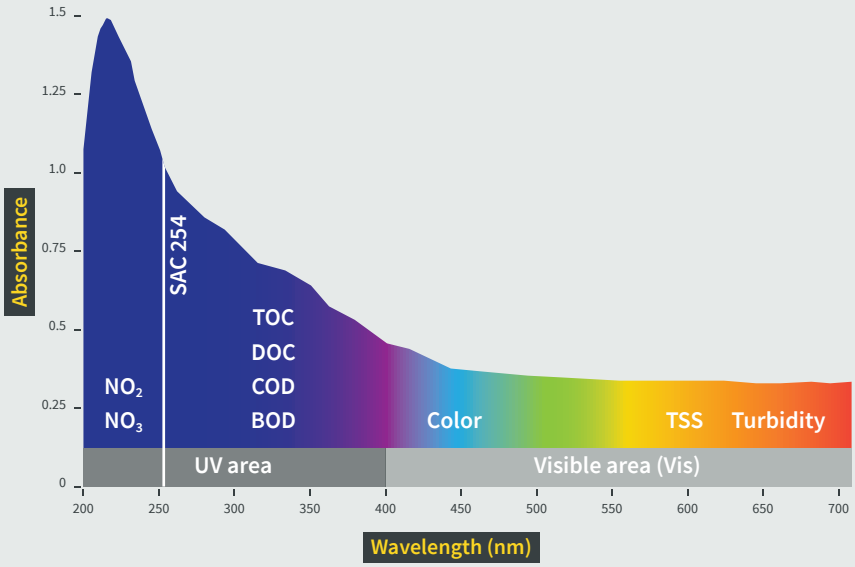
With the calculated values the whole absorption spectrum can be determined.

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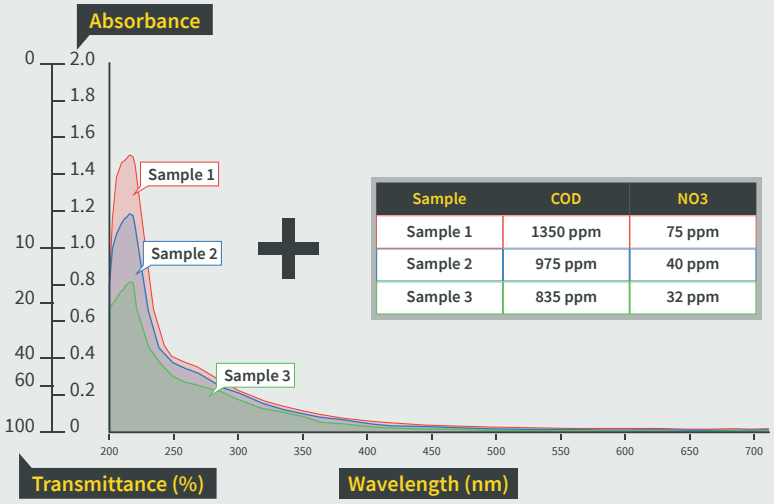
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Possible parameters with UV/Vis spectrometers

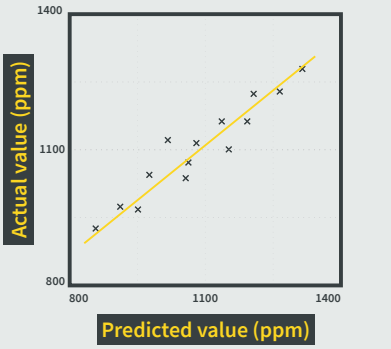
With a UV/Vis spectrometer different parameters can be measured simultaneously. The best parameters for the measurement are, of course, those that have an absorption of light in the UV/Vis range. Nitrate or COD values, for example, are often determined. However, other parameters that do not show any absorption themselves can also be detected under certain conditions. For a specific calibration, the concentration can also be determined as a function of the absorption of the entire water matrix and not on the basis of the absorption of the substance itself.



Specific calibration to various parameters



Sample	COD	NO3
Sample 1	1350 ppm	75 ppm
Sample 2	975 ppm	40 ppm
Sample 3	835 ppm	32 ppm



COD = - 5.05 + 388.44 * Absorbance (282 nm)
- 6123.48 * Absorbance (436 nm)
+ 5564.12 * Absorbance (448 nm)

To calculate the concentration of individual parameters based on absorption, a specific calibration must be performed. For the calibration it is necessary to take reference samples from which the laboratory values and absorption spectra are determined. From this data, a chemometric model can then be used to create a formula for calculating the respective parameter. The more reference values are available for the calibration, the better measurement accuracy can be achieved with this formula. The variance of different concentrations also optimizes the calibration.

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Parameters & Measurement Ranges - UV/Vis

The **Intelligent Spectral Analyser (ISA)** and the **BlueScan** are compact UV/Vis spectrometers that allows the simultaneous determination of a variety of parameters with a single optical sensor.

Parameter	Measurement range*	Measurement principle
Spectral Absorption Coefficient (SAC)	0 - 1500 1/m	Absorption single wavelength (254 nm)
UV-Transmittance (UVT)	0 - 100 %	Absorption single wavelength (254 nm)
Biochemical Oxygen Demand (BOD)	0,0 - 15.000 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Chemical Oxygen Demand (COD)	0,0 - 25.000 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Total Organic Carbon (TOC)	0,0 - 25.000 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Dissolved Organic Carbon (DOC)	0,0 - 15.000 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Total Suspended Solids(TSS)	0,0 - 5.000 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Total Nitrogen (TNb)	0,0 - 200 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Nitrate (NO3)	0,0 - 150 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Nitrite (N02)	0,0 - 75 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Color	0 - 500 Hazen	Absorption UV/Vis Spectrum (200 - 720 nm)
Turbidity	0 - 2000 FNU	Absorption UV/Vis Spectrum (200 - 720 nm)
Ammonium (NH4)	5,0 - 100 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)
Orthophosphate	5,0 - 100 mg/l	Absorption UV/Vis Spectrum (200 - 720 nm)

Single wavelength:
The absorption of individual wavelengths can be calculated with a UV/Vis Spectrometer. Thereby, it is possible to directly determine parameters like SAC or UVT without the need for a calibration.

Absorption UV/Vis:
Moreover, the measurement of the absorption across the entire UV/Vis range allows to develop chemometric models. With the help of these models it is possible to simultaneously determine a multitude of parameters. The UV/Vis Spectrometers of GO Systemelektronik continuously monitor the quality of these models and ensure the reliability of calculation.

* The mentioned measurement ranges present typical upper and lower limits. The specific measurement ranges and achievable accuracies depend on the composition of the water and the quality of the reference samples.

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Application Areas - UV/Vis



Wastewater

Influent, Process & Effluent of WWTP:
COD, BOD, TOC, TN, NO3, NO2, NH4, OP …
Effluent of industrial plants:
COD, BOD, TOC, TN, TSS …
Sewage network:
COD, BOD, TOC, TN, TSS …



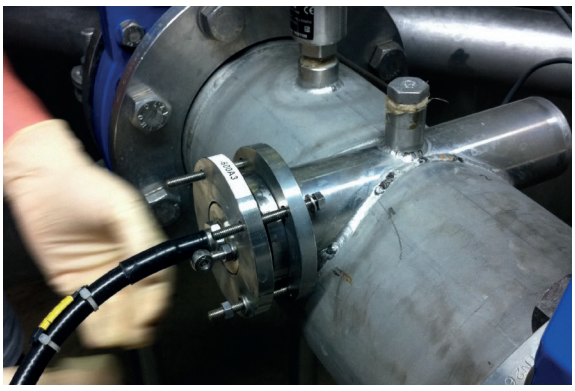
Drinking Water

Drinking water plant:
Fingerprint, SAC, Color, NO3, NO2,
DOC, COD, BOD …
Drinking water network:
Fingerprint, SAC, Color, NO3, NO2,
DOC, COD, BOD …



Environmental Monitoring

Lakes & River Monitoring:
Fingerprint, SAC, Color, NO3, NO2,
DOC, COD, BOD, TSS …
Sea water Monitoring:
Fingerprint, SAC, Color, NO3, NO2,
DOC, COD, BOD, TSS …



Process Monitoring

Influent of industrial plants:
Fingerprint, SAC, COD, BOD, TOC, TN …
Process of industrial plants:
Fingerprint, SAC, COD, BOD, TOC, TN …

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Functions & Features of our UV/Vis Spectrometers



Monitoring Function

The ISA and BlueScan Plus - UV/Vis Spectrometer Systems are capable of simultaneously detecting multiple parameters. With the corresponding calibration formulas, it is possible to calculate up to 99 different parameters.



ATEX Certified

The measurement head of the ISA UV/Vis Spectrometer System is ATEX certified and allow for the installation in potentially explosive atmospheres. The measurement head fulfils ATEX class III as standard. Optionally, ATEX class II is available.



Calibration Monitoring (SQI)

The Calibration Monitoring feature provides a real-time evaluation of the trustworthiness of measurement readings by means of a Spectral Quality Index (SQI). The SQI indicates the validity of the calibration. Thereby it is possible to determine how well the calibration fits to the current water matrix and to automatically select the most suitable calibration at all times. With this unique feature it is possible to obtain an on-line quality detection of the spectrometer results and ensure the proper operability of the system.



Adjustable Optical Path Length

The measurement head of the ISA - UV/Vis Spectrometer allows for an infinitely variable adjustment of the optical path length between 0.5 to 20 mm, which is a unique feature of the ISA Spectrometer. The optical path length of the BlueScan Plus measurement head can be adjusted in discrete steps between 1 to 30 mm. The path lengths can be changed directly in the field by using a simple screwdriver. The adjustment of the measuring path is an imperatively necessary feature for optimal adaptation to the local specific water matrix.



Automatic Cleaning

The ISA UV/Vis Spectrometer feature an integrated and automatically controlled compressed air flushing for the cleaning of the optical windows. The BlueScan Plus is equipped with an automatically controlled wiper brush system. With the cleaning solutions the service expenditure can drastically be reduced.



No Consumables

The UV/Vis Spectrometers do not require any reagents or other consumables and can be operated maintenance-free except for necessary cleaning on location (dependent on the installation). The calculated life-time of the flashbulb is > 10 years. In the case of a defect, service on location is possible because all electronic components are external to the submersible probe.





Deployable up to +110 °C

The ISA UV/Vis Spectrometer System measuring head features an extremely high-temperature durability of +80 °C (for short periods, up to +110 °C). This substantially extends the range of applications, particularly for industrial implementations. The temperature insensitivity of the ISA is an advantage for cleaning and sterilization of the probe head. Since there are no electronic components in the measuring head, temperature influences (drift) on the electronics, UV/Vis lamp, and Spectrometer unit are eliminated.



Intelligent Event Handling

With the help of the flexible communication possibilities of the BlueBox-System it is possible to transmit events locally or via telephone, network, mobile network, and satellite, if required through redundant paths, in a swift and reliable manner. All usual services like SMS, email, FAX and network protocols are available for the transmission. Response times for alarms and events can thereby be minimized and the reliability of operation can be optimized.



Cloud Data Service (BlueGate)

The BlueGate cloud data service automatically backs up all data and provides remote access via any web browser. The service offers a live data view, visualisations, and the and ability to export all measurement data. BlueGate also allows to set up alarms such as notifications for the exceedance of thresholds. All communications over public networks between BlueBox - BlueGate - and customer systems are encrypted.



Remote Access & Control

A connection via internet or mobile networks facilitates the transmission of measurement data and results at any time and allows for remote access and control of the system. Thereby it is possible to change settings or transmit calibrations remotely.

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Calibration Monitoring (SQI)

The **Calibration Monitoring** feature provides a real-time evaluation of the trustworthiness of measurement readings by means of a **Spectral Quality Index (SQI).** The SQI indicates how well the calibration fits to the current water matrix. The lower the SQI value the better the calibration will fit to the water matrix. A calibration with a SQI above the **threshold value of 4** leads to a lower measurement accuracy. The feature enables the determination of the **Validity of the Calibration** and allows for the A**utomatic Selection of the most Suitable Calibration**. With this unique feature for all of our UV/Vis Spectrometer Systems, it is possible to obtain an on-line quality detection of the spectrometer results and ensure the proper operability of the system.

SQI Threshold



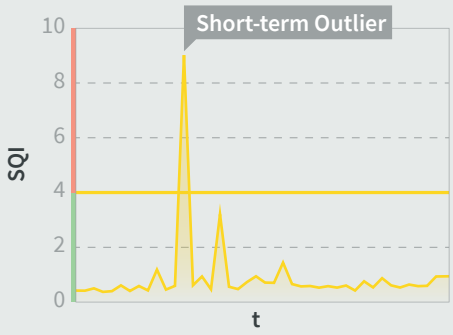
Available for the Following Products

- ISA - UV/Vis Spectrometer
- BlueScan Plus - UV/Vis Spectrometer

Validity of the Calibration

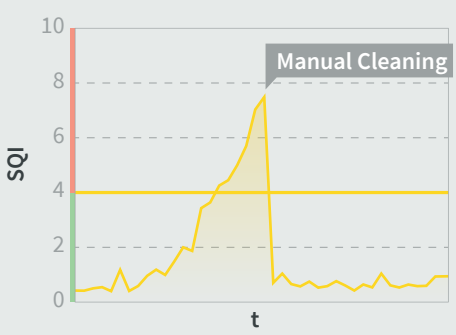
The SQI serves as a quality index that allows to determine how likely it is that the calibration is correct. Based on this information it is possible to distinguish between the occurrence of 3 potential cases and to assess whether action is required.

Short-term Measurement Error



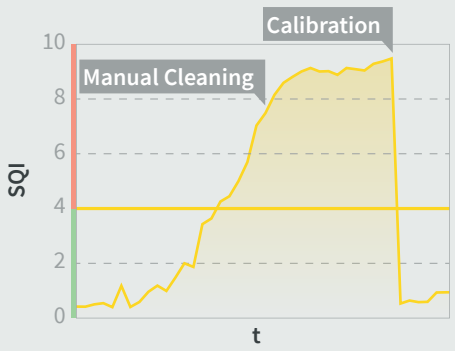
A **temporary spike** in the SQI can occur as a result of **air or particles caught in the measurement path**. The Calibration Monitoring feature allows to effortlessly identify short-term outliers and gives the opportunity to ignore measurements exhibiting a higher SQI.

Contamination



A **prolonged exceedance** of the SQI threshold value may be an indication for a **contamination of the measuring head**. In these instances, it is advisable to perform a **manual cleaning** of the measurement head. If the cleaning resolves the issue the SQI should drop back down to a lower level.

Changing Water Matrix



If the SQI remains at an elevated level, even after a **manual cleaning**, it may be an indication that the current calibration does not cover the water matrix anymore. The issue can be resolved either by **improving the existing calibration** through the **addition of reference values** or by **creating a new calibration**.

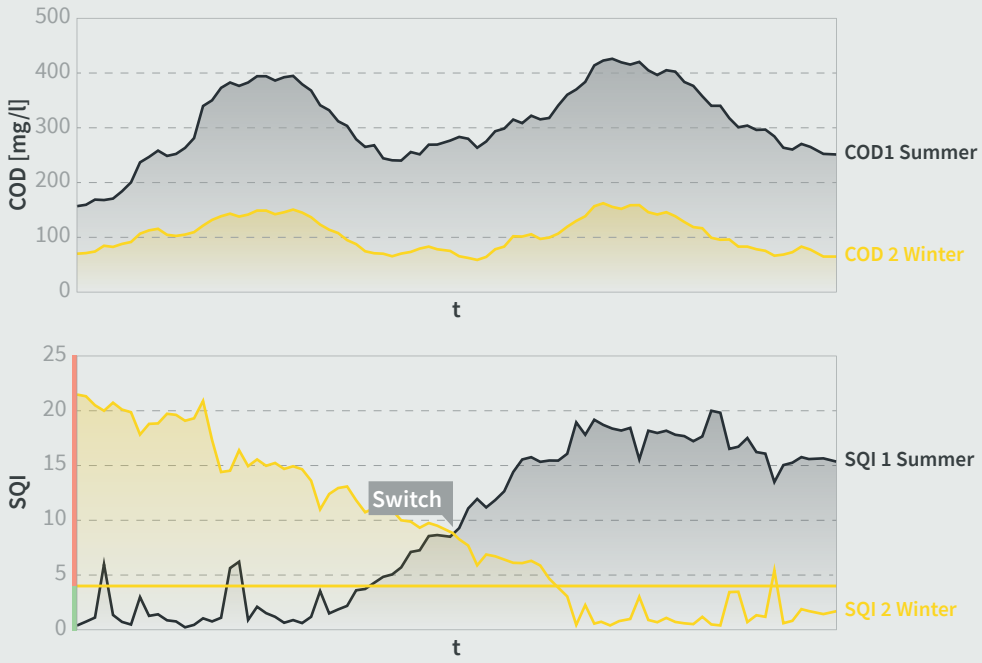
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Automatic Selection of the most Suitable Calibration

Based on the SQI it is possible to set up an automatic selection of the best suitable calibration settings. Thus, ensuring the optimal adaption of the system to changing conditions, by enabling the intelligent switch between different calibrations for different water matrices.

Calibration Monitoring for COD Measurement



In this example, the UV/Vis Spectrometer simultaneously measures the COD using two calibrations. The measurement values of the COD1 Summer calibration are shown in grey and the values of the COD2 Winter calibration are shown in yellow.

The system also tracks the SQI for both calibrations and is able to automatically determine the most suitable calibration for the current water matrix. In the example, the automatic switch occurs once SQI 1 Summer exceeds the value of SQI 2 Winter.

Configuration of the Automatic Switch

The associated software offers the opportunity to set up individual decision rules to configure the switch between the stored calibrations. Hereby, it is possible to automate the selection of the best fitting calibration. The decision rules can be defined according to the desired specifications by using simple formulas. The formulas can, for example, be based on the simple exceedance or number of instances and may include time delays, set events, etc.

Example: Simple Exceedance

```
COD_1_Summer = [ISA011073];
SQI_1_Summer = [ISA011073.SQI];

COD_2_Winter = [ISA011074];
SQI_2_Winter = [ISA011074.SQI];
COD_opt = 0;

if (SQI_1_Summer < SQI_2_Winter) COD_opt = [ISA011073];
if (SQI_1_Summer > SQI_2_Winter) COD_opt = [ISA011074];

COD_opt;
```

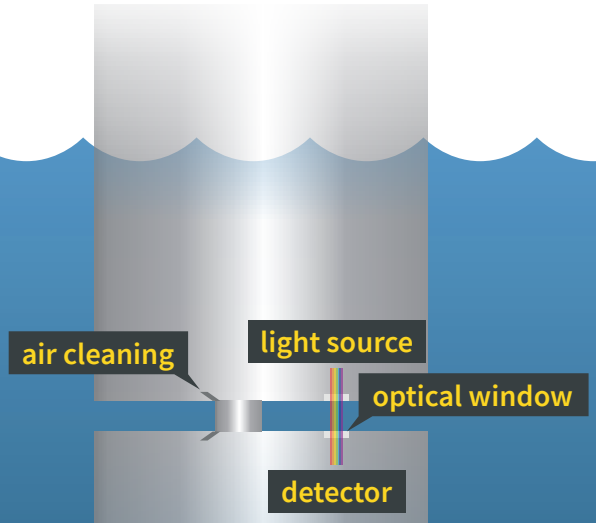
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Comparison of ISA & BlueScan Plus

The **Intelligent Spectral Analyser (ISA)** and **BlueScan Plus** are compact UV/Vis spectrometer systems that allow the simultaneous determination of a variety of parameters with a single optical sensor.
Each system contains a light source that emits light every 2 nm between 200 - 710 nm. The medium in which the sensor is located absorbs this light depending on the concentration of certain parameters. How strongly the medium absorbs is measured with a detector. An adjustable measuring path allows the adoption of the system to different applications. In order to minimize the maintenance effort, the optical windows of the spectrometers can be cleaned automatically with compressed air or with a brush.

ISA UV/Vis Spectrometer

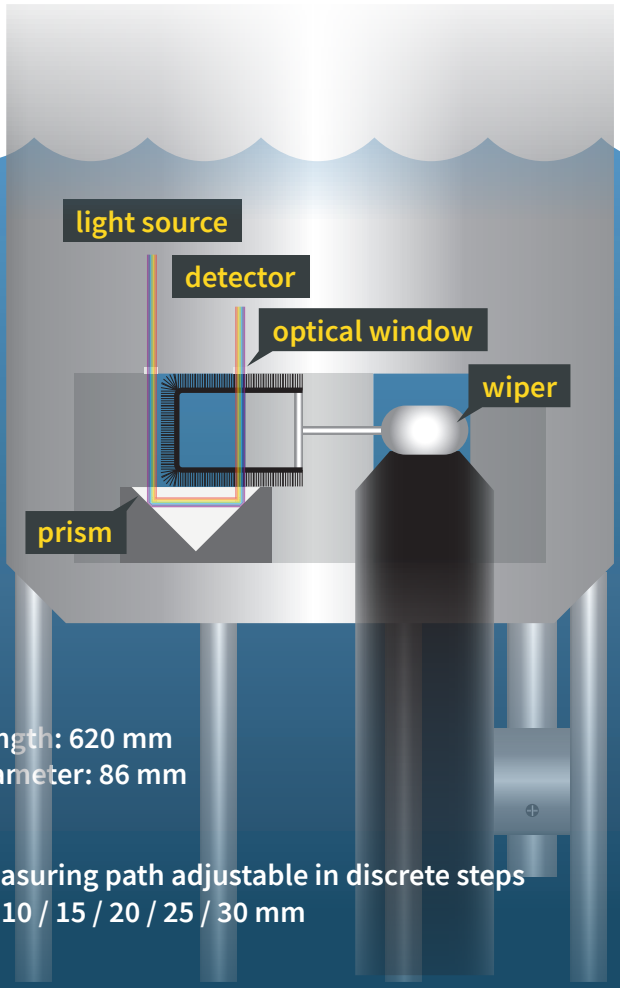


Length: approx. 230 mm
Diameter: 44 mm

Measuring path continuously adjustable
0.5 - 20 mm

Particularly suitable for applications in highly polluted water (e.g. wastewater)

BlueScan Plus UV/Vis Spectrometer



Length: 620 mm
Diameter: 86 mm

Measuring path adjustable in discrete steps
5 / 10 / 15 / 20 / 25 / 30 mm

Particularly suited for applications in clear water (e.g. drinking water or environmental monitoring)

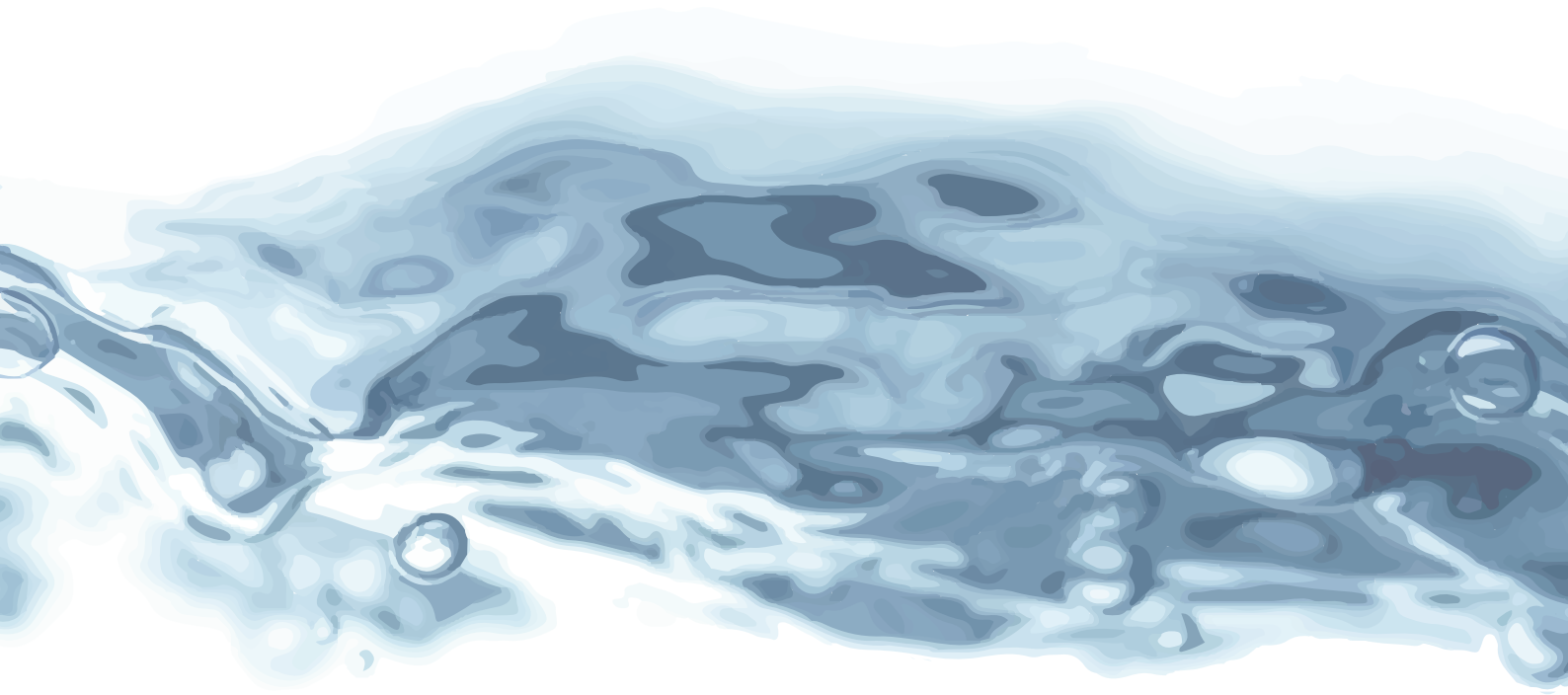
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	ISA UV/Vis Spectrometer	BlueScan Plus UV/Vis Spectrometer
Dimensions	Compact design due to external electronics, located in associated module.	Larger dimensions due to integrated electronics.
Optical path	The optical path length can be continuously adjusted with a simple screwdriver, allowing for an optimal adaption to the medium.	The optical path length can be adjusted in discrete steps with a simple screwdriver and by placing spacers between the bottom cap and the prism
Application	Particularly suited for applications in highly polluted water and harsh application conditions (e.g. wastewater), due to the minimal measuring gap (0.5 mm) and small areas requiring cleaning.	Particularly suitable for applications in clear water (e.g. drinking water) due to the maximum measuring gap (30 mm) and for environmental monitioring (e.g. rivers & lakes) due to equipped automatic brush cleaning and extended cable lengths.
Parameters	The ISA and BlueScan Plus Spectrometers allow the calculation of an unlimited number of parameters, which makes it possible to simultaneously determine COD, BOD, TOC, NO3, NH4, PO4 and many more parameters. GO Systemelektronik GmbH focuses on custom calibrations based on on-site samples to provide the best possible calibration for the respective water matrix.	
SQI	The Calibration Monitoring provides real-time evaluation of trustworthiness of measurement readings by means of a Spectral Quality Index (SQI). Furthermore, the Calibration Monitoring allows for an automatic selection of the best suitable calibration settings. Thereby enabling the intelligent switching between different calibrations for different water matrices.	
System	The ISA measurement head has no integrated electronics. As a result the measurement head has a high temperature durability of 80°C (for short periods, up to 110°C) and features an ATEX certification as standard. All electronics are housed in the associated measurement & control system (BlueBox RS) or module. The BlueBox RS takes over the subsequent task of evaluating measurements and serves as a data logger and control unit.	The BlueScan Plus Spectrometer features integrated electronics, which allows for extended cable lengths. The BlueScan Plus can be connected to any any BlueBox controller (BlueBox R1, BlueBox RS & BlueBox Panel), which serves as a data logger and control unit.

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