

BreathSpec®



User Manual



**G.A.S. Gesellschaft für
analytische Sensorsysteme mbH**

BreathSpec® – User Manual

Version 4.02, February 2021

Valid from BreathSpec® Firmware Version 4.00

All data, texts, designs, images and other elements used in this user manual are protected by copyright law. Any infringement may be subject to legal action.

Passing it on to third parties and producing copies of any kind or form – on the whole or in parts - is not permitted without written agreement of G.A.S. Any infringement may be subject to legal action.

G.A.S. reserves the right to realize technical changes to the product without explicitly mentioning them.

BreathSpec® is a registered trademark. Any infringement may be subject to legal actions.

The BreathSpec® does not have a medical approval.

CE-Marking according to:

**International Standard EN ISO 17050-1:2004
Directive 2014/35/EU (Low voltage directive);
Directive 2014/30/EU (Electromagnetic compatibility);
Directive 2011/65/EU (RoHS);
Directive 2012/19/EU on waste disposal (Waste Electrical and Electronic Equipment – WEEE)**

© Copyright 2020

**G.A.S. Gesellschaft für analytische Sensorsysteme mbH
44227 Dortmund - Germany**

All Rights Reserved.

**G.A.S. Gesellschaft für analytische Sensorsysteme mbH
Otto-Hahn-Str. 15
D-44227 Dortmund
Germany**

**Phone: (+49) 231/9742-6550
Fax.: (+49) 231/9742-6555
E-Mail: support@gas-dortmund.de
Internet: www.gas-dortmund.de**

Table of Content

1	General Information	8
1.1	Information about the Manual	8
1.2	Explanation of Symbols	8
1.3	Notation for dialogs, elements and references	9
1.4	Scope of Supply BreathSpec® with Circular Gas Flow Unit (Version 4G1). 10	
1.5	Scope of Supply Special edition BreathSpec with Airsense μ TD Unit (Version 4G2) 16	
1.6	Liability and Guarantee.....	20
1.7	Copyright.....	21
1.8	Return and Disposal	21
1.9	Software Updates	21
1.10	Customer Service	22
2	Safety.....	23
2.1	Intended Use Only.....	23
2.2	Responsibility of Operator	23
2.3	Requirements of Personnel	24
2.4	Dangers.....	25
3	Transport, Packing and Storage	26
3.1	Inspection after Transport.....	26
4	Packing	26
4.1	Storage and Transport.....	26
4.2	Cleaning and Maintenance.....	28
4.3	Cleaning	28
4.4	Maintenance.....	28
5	Introduction	29
5.1	Working principle of IMS technologie	29
5.2	Purpose of the device.....	33
5.3	Principle setup and internal gasflow	35
5.4	BreathSpec® (Standard Edition) Housing Device with Circular Gas Flow Unit (CGFU).....	37
5.4.1	Front	37
5.4.2	Rear	39

BreathSpec® – User Manual

- 5.5 BreathSpec® (Version 4G2) Housing Device with Airsense μ TD..... 41
 - 5.5.1 Top..... 41
 - 5.5.2 Front 42
 - 5.5.3 Rear 44
- 5.6 Device Type / Serial Number Plate..... 46
- 6 Operating Interface 47
 - 6.1 Overview 47
 - 6.1.1 Windows Selection Bar 48
 - 6.1.2 Windows Display Area 49
 - 6.1.3 Status Bar 49
 - 6.1.4 View Control Bar 50
 - 6.1.5 Low/High Pressure Control 51
 - 6.1.5.1 Low Pressure Error 51
 - 6.1.5.2 High Pressure Error..... 52
 - 6.2 Spectra Window 53
 - 6.2.1 Overview 53
 - 6.2.2 Measurement modes 54
 - 6.2.2.1 Measurement with user defined programs 54
 - 6.2.2.2 Manually operated measurement 55
 - 6.3 Sequence Window..... 56
 - 6.4 Defaults Window..... 58
 - 6.4.1 Overview 58
 - 6.4.2 Drift Voltage 60
 - 6.4.3 Flow Controls and Heating Modules 61
 - 6.5 Substances Window 62
 - 6.5.1 Overview 62
 - 6.5.2 Managing Substance Entries 63
 - 6.5.3 Managing Modbus TCP Setup 65
 - 6.5.4 Substance Calibration Information Area 67
 - 6.5.5 Recognised substances window 68
 - 6.6 Programs Window 69
 - 6.6.1 Overview 69
 - 6.6.2 Create Measurement Programs..... 71
 - 6.6.3 Edit Measurement Programs 72
 - 6.6.4 Flow Ramps 74

6.7	System Window.....	76
6.7.1	System Info Window	77
6.7.2	System Plan Window	78
6.7.3	System Settings Window	79
6.7.3.1	Snapshot Window	84
6.7.3.2	Simplified View Window	88
6.7.4	System Transfer Window.....	89
6.7.5	System Modes Window	91
6.7.5.1	Trigger Mode Window	92
6.7.5.2	Remote Mode Window	94
6.7.5.3	ID Input Mode Window	95
6.7.5.4	Cleaning Mode Window.....	96
6.7.5.5	Standby Mode Window.....	97
6.8	Error Information Window.....	98
6.9	Additional Dialog Windows	99
6.9.1	Log Messages Dialog Window.....	99
6.9.2	IP Address Input Dialog Windows.....	100
6.9.3	Date and Time Input Dialog Window.....	101
6.9.4	Text Input Dialog Window	102
6.9.5	Number Input Dialog Window	103
7	Installation BreathSpec® Device (Version 4G1) with Ciruclar Gas Flow Unit (CGFU).....	104
7.1	Installation Requirements	104
7.2	Installing the device	105
7.3	Mounting the Mouthpiece holder	109
7.4	Connecting the Mouthpiece tube.....	110
7.5	Installation of Luer-Lock adapter [optional].....	114
7.6	Prepare the device for operation	117
8	Installation BreathSpec® Device (Version 4G2) with Airsense μ TD	121
8.1	Installation Requirements	121
8.2	Installing the device	122
8.3	Prepare the device for operation	128
9	System Operation	132
9.1	Measurement Requiurements	132
9.2	Measurement Program.....	132

BreathSpec® – User Manual

9.3	Workflow: Breath Sampling via Handheld Breath Sampler.....	133
9.3.1	Workflow: Installation of Disposable Reservoir Tube and Mouthpiece	133
9.3.2	Workflow: Execute a breath measurement using the Handheld	134
9.3.3	Workflow: Exchanging the inner syringe body	137
9.3.4	Workflow: Execution of an ambient air measurement using the Handheld	139
9.4	Workflow: Breath Sampling via Disposable Breath Sampler	139
9.4.1	Start a breath measurement using disposable breath sampler	139
9.4.2	Execution of an ambient air measurement using syringes	142
9.5	Workflow: Exemplary Breath sampling with a sample bag	143
9.6	Workflow: Measurement in Normal mode.....	145
9.7	Workflow: Measurement in Simplified mode.....	147
9.8	Workflow: Measurement in ID Input Mode.....	149
9.9	Workflow: Manual Measurement Recording.....	151
9.10	Workflow: Create a Measurement Program	152
9.11	Workflow: Start Sequence	154
9.12	Workflows: File Transfer Setup	156
9.12.1	Overview	156
9.12.2	Connecting to a Server in a LAN.....	157
9.12.3	Workflow: Manual Transfer of measurement files to USB-Stick.....	163
9.12.4	Workflow: Manual Transfer of measurement files to connected server	165
9.13	Workflow: Current Loop Setup (only available in Version 4G2).....	167
9.13.1	Introduction	167
9.13.2	Electrical Interface	167
9.13.3	Configuring the Current Loop.....	167
9.14	Workflow: Modbus TCP Setup	171
9.15	Workflow: Start Cleaning mode	173
9.16	Workflow: Start Standby mode	174
9.17	Workflow: Remove the Housing Cover.....	175
9.18	Workflow: Change Capillary Column.....	178
9.19	Workflow: Change sample pump unit.....	183
9.20	Workflow: Change high voltage circuit board	186
9.21	Workflow: Reinitialize the 6-Port-Valve.....	192
9.22	Workflow: Change filter set CGFU.....	195
9.23	Workflow Firmware Upgrade	197

9.24	Workflow: Creating diagnostic information for support	200
9.25	Workflow: Packing for return transport	203
9.26	Workflow: Manual modification of the sample description attribute.	205
10	Appendix.....	207
10.1	Technical data: BreathSpec®.....	207
10.2	Technical data: I/O Interface	210
10.3	Ionisation Source Specification.....	213
10.4	Technical drawing: Internal Gasflow.....	215
10.5	Current Loop Interface (optional).....	216
10.6	Modbus TCP Specification	217
10.7	Troubleshooting.....	220
10.7.1	Error message list.....	220
10.7.2	IMS-Spectrum Examples	226
10.7.3	Troubleshooting / How to...	228
10.8	Consumables / Spare Parts.....	232
10.9	Corresponding G.A.S. Documents and Tutorials.....	240
10.10	Table of Figures	241

1 General Information

1.1 Information about the Manual

This manual describes a safe and adequate handling of the device. Following the instructions of the indicated safety aspects and instructions as well as the national and/or local rules and general safety regulations concerning the prevention of accidents are absolutely imperative.

Before starting the work with the device read the manual completely and thoroughly particularly the chapter security and respective safety references. Assure that you/the operator comprehend the terms described.

The manual is part of the device. It must be stored together with and next to the device at any time.



INFORMATION!

The graphics in this user manual are schematic and may differ from the actual conditions. The firmware and PC software screenshots in this user manual may differ from the actual conditions.

1.2 Explanation of Symbols

Important and safety-relevant references in this manual are characterized by symbols. These indications which are in-line with industrial safety must be respected and followed at any time.



INFORMATION

This symbol calls information, which are to be considered for efficient and perfect handling of the equipment.



WARNING

This symbol indicates references, which can lead to damages, malfunctioning and/or loss of the device.



DANGER

This symbol marks references, which can lead to health impairments, injuries, lasting body damages or to death due to electric current.



DANGER

This Symbol marks paragraphs, which describe potential dangers and damage due to exposure to radioactive radiation.



DANGER

This symbol marks references, which describe working procedures that demand special attention to avoid spreading of biohazard



WARNING

This symbol marks references, which can lead to health impairments, injuries due to pinching.

1.3 Notation for dialogs, elements and references

Example Dialog:

System > **Connections** > **LAN File Transfer** > **Settings...** > **Test Connection**

Example Elements:

Gas Out, **Sample gas in**

Example: References

Advanced User Manual, **Chapter 5.1 Installation Requirements**

Example: Information

keep the transport box

BreathSpec® – User Manual

1.4 Scope of Supply BreathSpec® with Circular Gas Flow Unit (Version 4G1)

Assure that you have received the full scope of supply. If there is any part missing, please contact the GAS-hotline immediately.

Standard Scope of Supply



BreathSpec® Device (1 piece)
including connected Circular Gas Flow Unit (CGFU) (1 piece)



Power supply with power plug (1 piece)



Mouthpiece Handheld holder arm with screws



Mouthpiece Handheld with
heatable Transferline



BreathSpec® Gas tube Kit (installed)

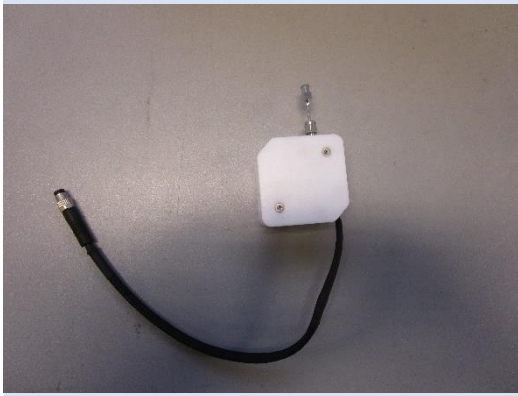
- Driftgas/Carriergas Adapter (1 piece)
- 0,6 m 3mm PFA Tubes with 3 mm Swagelok-Connector (2 pieces)



CGFU Connection cable (installed) (1 piece)



LAN Cable (1 piece)



Luer-Lock Adapter-Kit

- Luer-Lock Adapter (1 piece)
- Luer-Lock Adapter Heater (1 piece)



Disposable Breath Reservoir Kit

- Mouthpieces (100 pieces)
- Reservoir tube (100 pieces)



Inner Syringe Body (2ml syringe) (50 pieces)



Sampling Syringe (5ml syringe) (100 pieces)



BreathSpec® Blind plug Set (5 pieces)

(Swagelok 3mm Blind plug with red cap installed on device connectors)



Torx Tool Kit

- Torx Srewdriver 8 mm (1 piece)
- Torx Srewdriver 10 mm (1 piece)
- Torx Srewdriver 30 mm (1 piece)

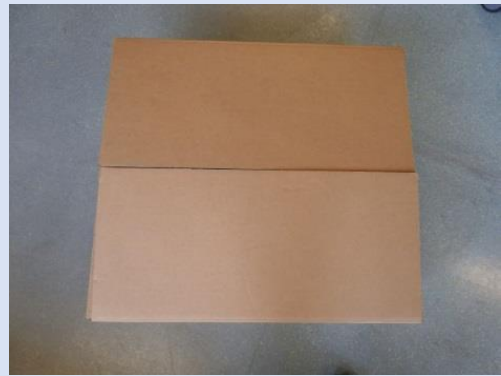


Document Map with Documents and Device User Manuals



USB-Stick Box with Software und Documents (1 piece)

BreathSpec® – User Manual



Transport box (1 piece)



Transport palett (60 x 80 cm)

Optional Scope of Supply (only available if ordered)



Laptop Computer (different design) including software for control and evaluation



CGFU-Filter Set (2 x Moisture-Trap, 1 x Hydrocarbon-Trap)

1.5 Scope of Supply Special edition BreathSpec with Airsense μ TD Unit (Version 4G2)

Assure that you have received the full scope of supply. If there is any part missing, please contact the GAS-hotline immediately.

Standard Scope of Supply



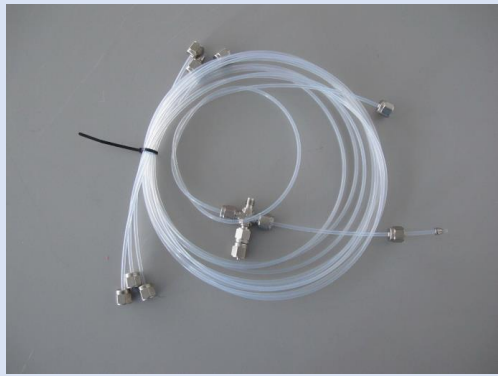
BreathSpec® Device (1 piece)



μ TD with accessories in transport case (1 piece)



Power supply with power plug (1 piece)



BreathSpec® Gas tube Kit

Driftgas/Carriergas/μTD Adapter (1 piece)

- 2 m 3mm PFA Tubes with 3 mm Swagelok-Connector (4 pieces)



Molecular sieve trap (200 ml) (1 piece)



LAN Cable (1 piece)



BreathSpec® Blind plug Set (7 pieces)

(Swagelok 3mm Blind plug with red cap installed on device connectors)



Torx Tool Kit

- Torx Srewdriver 8 mm (1 piece)
- Torx Srewdriver 10 mm (1 piece)



Document Map with Documents and Device User Manuals



USB-Stick Box with Software und Documents (1 piece)

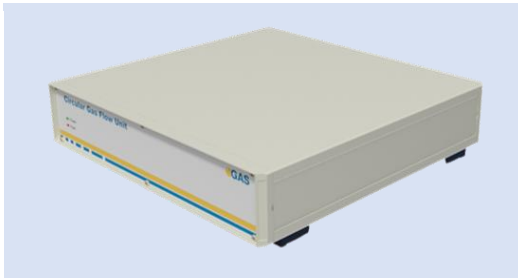


Transport box (1 piece)



Transport palett (60 x 80 cm)

Optional Scope of Supply (only available if ordered)



Circular Gas Flow Unit with accessories

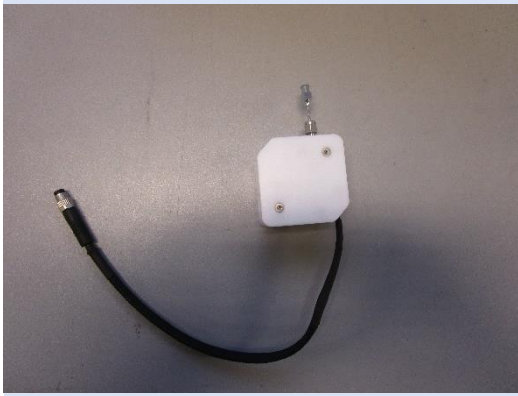


Nitrogen Generator with accessories
(example picture)



Laptop Computer (different design) including
software for control and evaluation

BreathSpec® – User Manual



Luer-Lock Adapter-Kit

- Luer-Lock Adapter (1 piece)
- Luer-Lock Adapter Heater (1 piece)



Sampling Syringe 5ml syringe for Luer Adapter) (100 pieces)

1.6 Liability and Guarantee

This user manual describes the safe and proper handling of the device.

All data and reference within this manual are compiled under the valid regulations, the state-of-the-art as well as G.A.S. experiences of several years.

This user manual must be stored together with and close to the device at any time and accessible to all persons, who operate or handle the device at any time.

This user manual must be read carefully before starting to work with the device. G.A.S. does not assume any liability for damage and disturbances, resulting from disregard of the instructions contained in this user manual. All claims of any kind related to damage from a not intended use of the device will be rejected.

G.A.S. reserves the right to realize technical changes of the product due to improvements without explicitly mentioning them.

1.7 Copyright

The manual is confidential. It is beyond doubt exclusively made and also meant for the personnel directly dealing with the equipment. All data, texts, designs, pictures and other representations within this manual are protected in the sense of the copyright law and are subject to further commercial patent rights. Each abusive is punishable by law.

Passing it on to third persons as well as duplications in any kind and form - also in part - as well as the use and/or report of contents are not permitted without written agreement of the manufacturer. Offences lead to payment of damages. We reserve ourselves all rights of the practice of commercial patent rights.

1.8 Return and Disposal

For an adequate disposal, the device or/and its equipment must be returned to the G.A.S. or to a third party authorized by the G.A.S.! For questions please contact G.A.S.

1.9 Software Updates

If there are any software updates customers will be contacted by G.A.S. Gesellschaft für analytische Sensorsysteme mbH as soon as the updates are available. The updates are free of charge within the first 12 month after delivery. Users will be provided with information about the changes and instructions for executing the updates.

1.10 Customer Service

For questions concerning G.A.S. products a customer service is available:

G.A.S. Gesellschaft für analytische Sensorsysteme mbH

Otto-Hahn-Straße 15

44227 Dortmund

Germany

Phone: +49 (0) 231 / 97 42 - 65 50

Fax: +49 (0) 231 / 97 42 - 65 55

support@gas-dortmund.de

The telephone hotline is available from monday to friday from 9:00 to 16:00 hours. In urgent cases or if you use fax or email please provide a telephone number for callbacks.

2 Safety

2.1 Intended Use Only



WARNING!

Usage other than described in this manual may damage the device and/or harm persons involved.

Do not use the device for other purposes. Damages due to misuse are not covered by the guarantee. Such damage claims will be rejected.

The device and its equipment are not certified for the employment in areas with explosive gas air mixtures.

All claims or requirements of any kind against the manufacturer and/or its authorized persons that arise due to damages from a not intended use of the device will be rejected. All damages that arise from a not intended use are of the operator's responsibility.

The intended use of the equipment and its correct handling according are described in the operating instructions of this manual. Other parts than the parts belonging to the scope of supply, may only be used after G.A.S. approval.

2.2 Responsibility of Operator

The device may only be operated in a perfect technical condition. Before putting the device into operation, the condition of the device and its equipment must be checked. The information and instructions provided in this manual must be followed at any time.

Besides the instructions provided in this manual the local rules for the prevention of accidents, general safety regulations - valid for the area of application of the device - as well as the valid environmental-protection regulations must be considered and respected.

The responsible technicians and operators must make sure a failure-free use of the device. Responsibilities among the involved persons regarding installation, operation, maintenance, and cleaning must be made clear.

The device can be used to analyze human breath. A hygienic operation must be ensured at all times. Ensure that human breath analysis does not conflict with local

ethical compliance. The breath analysis data might imply private information covered by data privacy protection that has to be obeyed.

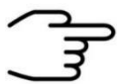
2.3 Requirements of Personnel

Only authorized and trained technical personnel may work with the instruments. The operator must have received an instruction over existing and all possible dangers and should be regularly instructed in safety procedures and environmental protection and that the personnel is fully aware of the complete operating instructions and particularly the safety notes. Personnel that might be under the influence of drugs or alcohol are to be kept off the device at any time.

Technical personnel in this context are defined as skilled employees who are knowledgeable due to their educational background. In case the foreseen personnel do not have the necessary qualifications to operate the instrument, it must be trained. Further to that non-authorized personnel should not operate the device.

The competencies for the work on and with the device must be specified and kept undoubtedly at any time so that with respect to security issues no unclear situation might come up.

Any changes of the equipment, which impair security of the personnel, must immediately be reported to the operator and every person dealing with it.



INFORMATION!

- Operators must be aware of local hygienic standards.
- Operators must be aware of local ethical compliances regarding human breath analysis.
- Operators must be aware of local privacy protection compliances.

2.4 Dangers

The device and its equipment is subject to an endangerment analysis. The construction and execution of the device corresponds to the today's state-of-the-art. The device is reliable in service when operated according to its intended use.



INFORMATION!

If the housing of the device is damaged, the device must not be used anymore and must be returned to the G.A.S. by using the original transportation case.



DANGER

The BreathSpec® device contains a radioactive radiation Tritium source of 75 MBq which in all EURATOM countries is below the exemption limit. Do not open the device! Do not try to recover malfunctions of the device! Malfunction recovery, repairs and any maintenance work may only be performed by G.A.S. or by qualified personnel authorized by G.A.S.



DANGER

The BreathSpec® and its equipment is not certified for the employment in areas with explosive gas air mixtures (Zone 0).



DANGER

Exercise great care in handling current-carrying parts like the power supply cord. Do not get directly in touch with current-carrying parts. Do not open the housing. Do not use damaged parts.



DANGER

All parts of the equipment that are in contact with human breath must either be disposed of or sanitized to prevent biohazard



DANGER

When Nitrogen is used as drift gas and helium as carrier gas, ignition of a helium plasma may occur due to the high voltage present in conjunction with a radiation source. This can damage the IMS.

3 Transport, Packing and Storage

3.1 Inspection after Transport

Check the supply immediately after delivery concerning its completeness and/or transport damages. If you detect externally visible transport damage, do not receive the supply, or only under reservation. State the extent of the damage on the provided delivery note and/or the transportation documents of the feeder. Generate a complaint. Lodge a complaint of covered defect immediately after recognizing, as claims due to transport damages can only be made valid within the complaint periods (usually 7 days).

4 Packing

If no return agreement regarding the packing was agreed upon dispose the packaging material always in an environmentally friendly way and according to valid local regulations. If necessary, ask a recycling company.



INFORMATION!

It is recommended to **keep the transport box** for a safety return transport.

4.1 Storage and Transport

Store the device only under the following conditions:

- **When not in use store the equipment in the supplied casing**
- **Prevent unauthorized access**
- **Do not store outside**
- **Protect the equipment from moisture and dust**
- **Put protective caps on all gas sockets**
- **Avoid mechanical vibrations**
- **Do not expose the equipment to aggressive substances**
- **Protect the equipment from direct sun light**
- **Storage temperature: 5 to 40 °C**

- **Relative Air Humidity: 0- 90%Rh, prevent condensation**
- **Instrument's position: Horizontal**

The equipment should be moved only within the provided carrying case. By this means, transport damages can be avoided. The above-mentioned values are considered for an instrument transported in its original new packing.



WARNING!

Protective caps should be put on gas sockets in case the device is stored or transported.

4.2 Cleaning and Maintenance

Natural aging and the wear of certain components of the equipment require a regular cleaning and maintenance.

4.3 Cleaning

Clean the device only with a dry or easily damp cloth.



WARNING!

Do not use cleaning agents, which contain solvents, acids or bases.

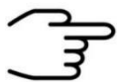
4.4 Maintenance



INFORMATION!

Maintenance of the device should only be carried out at G.A.S. or through specially trained and by G.A.S. authorized personnel.

The recommended **maintenance interval** for **BreathSpec®** device is **12 months** for **Circular Gas Flow Unit (CGFU)** is **6 months**.



INFORMATION!

Maintenance of the equipment must be carried out by G.A.S. or personnel authorized by G.A.S.

Please contact G.A.S. 6-8 weeks in advance to optimize the turn-around time!

5 Introduction

5.1 Working principle of IMS technologie

Ion Mobility Spectrometry (IMS) is an analytical technology to separately detect gaseous compounds in a mixture of analytes. The separation is based on the specific drift times, that ionized compounds need to pass a fixed distance (drift tube) in a defined electric field.

$$\text{Drift velocity: } v_d = KE$$

$$\text{Mobility: } K = \frac{L^2}{t_D U}$$

$$K = \frac{3}{16} \sqrt{\frac{2\pi}{\mu kT}} \frac{Q}{n\sigma}$$

Q	<i>ion charge</i>
n	<i>drift gas number density</i>
μ	<i>reduced mass of the ion and the drift gas molecules</i>
k	<i>Boltzmann constant</i>
T	<i>drift gas temperatures</i>
σ	<i>ion's collision cross section with the drift gas</i>

Figure 1: Ion Mobility Spectrometer - Basic Relations

Compared to other techniques e.g. TOF-MS, ions travel at atmospheric pressure versus a flow of inert drift gas. The drift time of each substance is determined by its ion mass and geometric structure, as slowing collisions with the drift gas molecules are more frequent for sterically demanding structures. Therefore, IMS can even differentiate isomeric molecules. For detection, the resulting ion current is measured by an electrometer as a function of time.

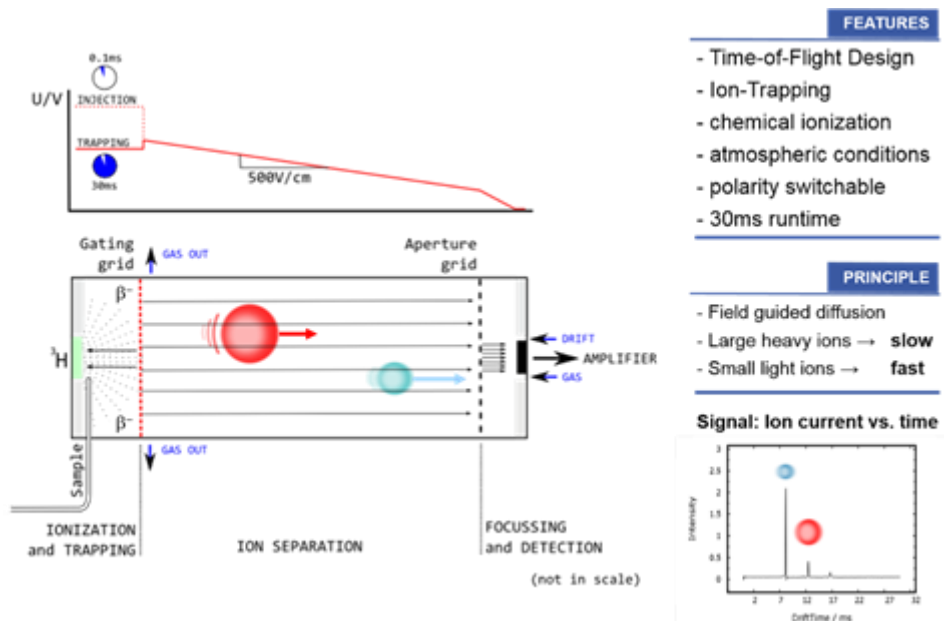


Figure 2: Ion Mobility Spectrometer -Working Principle

Atmospheric Ionization of molecules can be obtained by several techniques. G.A.S. uses photoionization with a 10.6eV UV-lamp or soft chemical-ionization initiated by a low-radiation tritium (H3) source (below exemption limits of EURATOM). While the first directly produces positive ions, the latter generates *reactant ions* with the gas atmosphere by a cascade of reactions following the collision of a fast electron emitted from the β -radiator H3. The so-called Reaction Ion Peak (RIP) representing the total of all ions available is formed as a first step. In nitrogen and air, resp., the *reactant ions* can be described as $H^+(H_2O)_n$ and $O_2^-(H_2O)_n$. Chemical ionization of analytes by *reactant ions* then result in the formation of specific analyte ions, when the affinity of the analyte towards the reactant ion is higher in case compared to water (using the positive ionization mode). The proton affinity of water is 691kJ/mol, so all molecules with a higher proton affinity will be ionized by a proton transfer, which is typically given for all heteroatom-organic compounds. The ionization takes place at ambient pressure, so that the analyte concentration is not diluted as compared to other analytical methods where a vacuum must be applied. Therefore, IMS is extremely sensitive. The detection limits typically are in the low ppb-range for *volatile organic compounds (VOC)*.

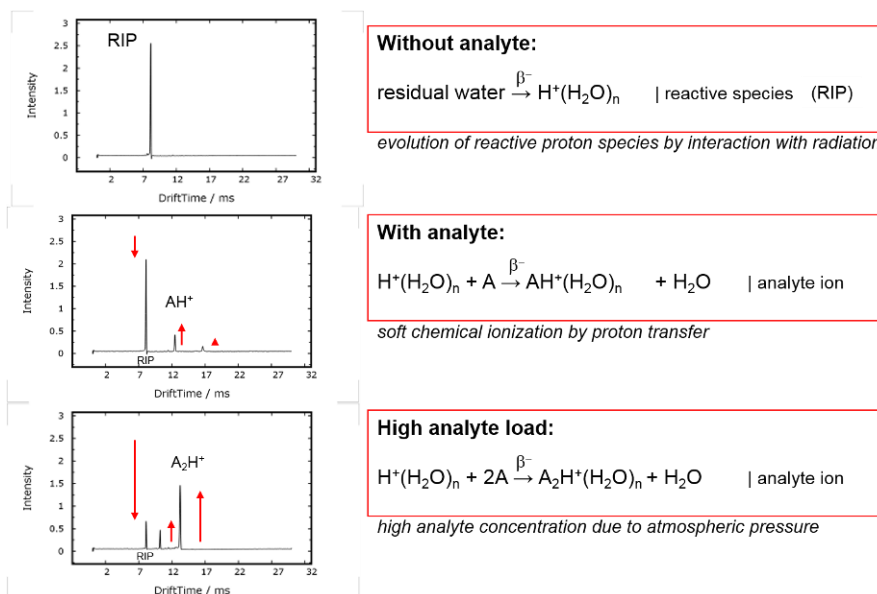


Figure 3: IMS Predominant Ionization (positive polarization)

The above figure exemplarily shows typical IMS spectra without analyte and with analyte. The RIP is formed as a sharp signal proving the cleanliness of the system and at a specific position that is used as internal standard. The spectrum containing analytes shows a decreased RIP, while new (analyte) peaks are correspondingly formed. The drift time is specific to an ion; therefore analyte identification is possible. The peak height and area correlate to the analyte concentration, so that a quantification is also possible.

Protone Affinities	Aromatic Amines	930.0 KJ/mol	Pyridine
	Amines	899.0 KJ/mol	Methyl Amine
	Phosphorous Compounds	890.6 KJ/mol	Trimethylphosphate
	Sulfoxides	884.4 KJ/mol	Dimethyl Sulfoxide
		853.6 KJ/mol	Ammonia
	Ketones	832.7 KJ/mol	2-Pentanone
	Esters	821.6 KJ/mol	Methyl Acetate
	Alkenes	805.2 KJ/mol	1-Hexene
	Alcohols	789.2 KJ/mol	Butanol
	Aromatics	750.4 KJ/mol	Benzene
		691.0 KJ/mol	Water
	Alkanes	543.5 KJ/mol	Methane

Source: Gary Eiceman & Zeev Karpas, *Ion Mobility Spectrometry*, CRC Press, 2005, ISBN 0-8493-2247-2

Protone affinities of various VOCs can be found at the NIST chemistry webbook
<http://webbook.nist.gov/chemistry/>

Figure 4: Protone Affinities of VOC's

BreathSpec® – User Manual

Complex analyte mixtures, like e.g. food flavours, often demand a second and independent separation step to separately analyse the multiplicity of compounds at low concentrations. Therefore G.A.S. -according to application- equips its IMS systems with gas chromatographic (GC) columns. The volatile compounds of samples under testing are pre-separated in time by a GC column. The discrete compounds are consecutively fed into the IMS ionization chamber, so that analyte and/or ion interactions are avoided.

Furthermore, a competition of analytes on the reactant ions is excluded, enhancing the sensitivity of the system for individual compounds.

The GC-IMS setup enables a twofold separation of analyte mixtures and the detection by the IMS electrometer. Since the IMS measurements are extremely fast (30ms / spectrum) a continuous and high-resolution recording of analyte signals is provided.

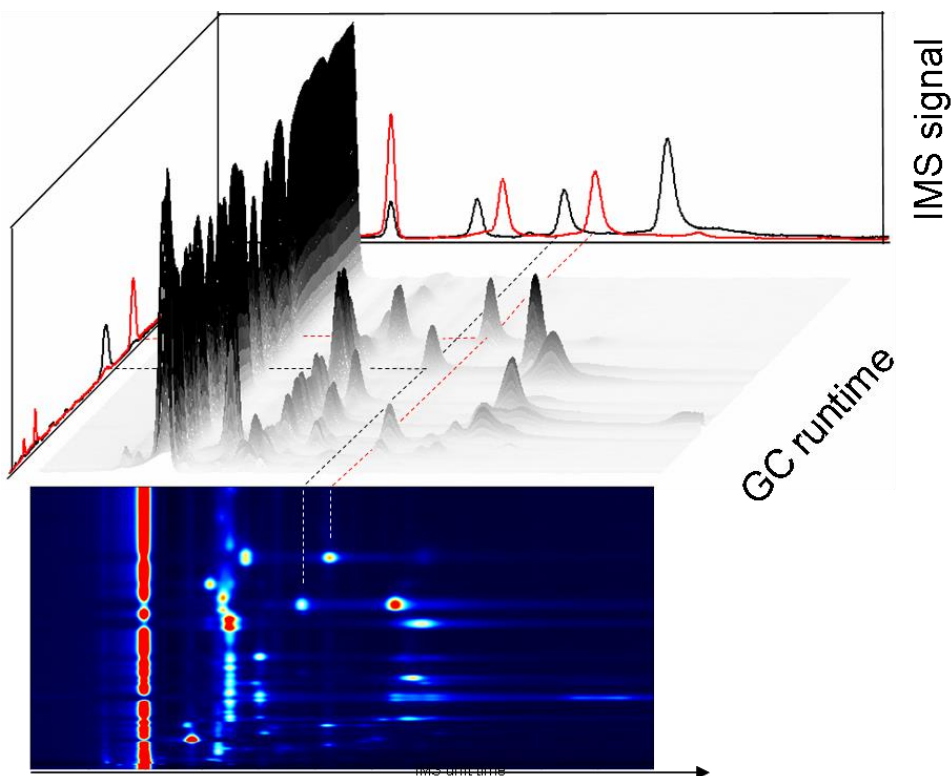


Figure 5: GC-IMS measurement 3D

The above figure sketches the GC-IMS measurement's 3D-dataset and the corresponding heatmap visualization.

5.2 Purpose of the device

The BreathSpec® represents the synergies of a fast gas chromatograph and the outstanding sensitivity of an IMS. Thus, traces of Volatile Organic Compounds (VOCs) even in highly humid matrices like the human breath become detectable without any special sample preparation. Its intended purpose is to:

Measure traces of volatile organic compounds in exhaled air of humans.

The device allows sampling of human breath directly by sucking in breath exhaled in a handheld breath sampler. The handheld sampler is equipped with disposable mouthpiece, sampling tube and sampling tip to minimize possible carry over of microbes. Furthermore, the device can be equipped with a Luer port to accept samples collected breath in a common disposable syringe. Sampling into a syringe - adsided from the device. -. can be done using a full disposable breath sampling setup.

Results are available within a few minutes and compounds are typically detectable even at ppbv-/pptv-levels. The technical configuration, its menu as well as its extremely easy.



WARNING!

The BreathSpec® device must not be operated by introducing aggressive gases or any kind of liquids or solids. The operational reliability is only ensured when the equipment is applied for this intended purpose.



INFORMATION!

Any use of the device, that differs from the intended purpose will be regarded as “out of purpose”. Any claims of any kind against G.A.S. or her associates that are related to damages from a use not covered by the aforesaid will be rejected.

The BreathSpec® contains several parameterized components that can be modified for optimizing measurement data in terms of separability of substances and clarity of resulting peaks.

The BreathSpec® can be operated in negative or positive drift voltage mode. The reactant ion peaks (RIPs) and analyte ion peaks (AIPs) in the positive drift voltage mode will be displayed as maxima in the spectra. In the negative drift voltage mode both will be shown as minima. One of these modes may be more suitable for specific substances.

BreathSpec® – User Manual

Measurement data can be acquired by employing user-defined measurement programs. In these programs the operational parameters of various components of the BreathSpec® can be modified at defined sequences of the measurement run.

Measurement data can also be acquired in a manual way using the “Recording” mode.

Acquired measurement data are stored in measurement files either on the internal storage volume of the BreathSpec® or – when activated – in a shared network folder. Stored measurement files can further be copied to a connected USB volume.

For using a shared network folder the BreathSpec® can be integrated into a local area network (LAN) by using the Ethernet socket at the rear side of the device.



INFORMATION!

The BreathSpec® does not have a medical approval.

5.3 Principle setup and internal gasflow

The schematic drawing shows the principle structure of the gas flow system of the BreathSpec® is shown. The system consists of the IMS coupled to a gas chromatographic column.

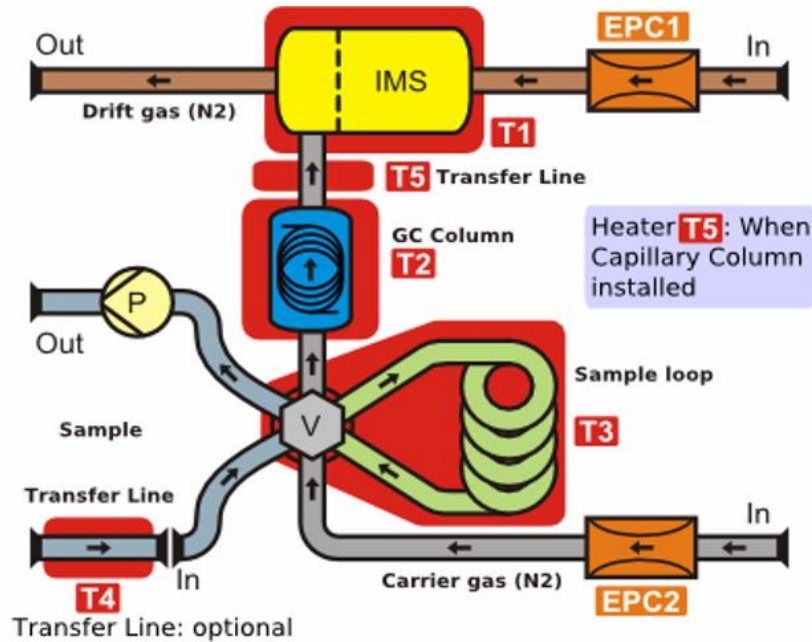


Figure 6: BreathSpec® device plan (exemplary)

The gas supply comes from a coupled circular gas flow unit and supplies the system with purified air. The drift gas for the IMS is supplied using an electronic pressure control unit (EPC1). The carrier gas for the column is supplied using a second electronic pressure control unit (EPC2). Both gases (carrier and drift gas) leave the device at the gas out and goes back again into the circular gas flow unit (Gas In).



INFORMATION!

To ensure correct measurements it is necessary to **connect the supplied exhaust tube** (Sample gas out).

The exhaust system must **not generate any negative pressure**.

IMS (T1), GC-Column (T2), 6-Port Valve with sample loop (T3) and Transferlines (T4 and T5) are heated.

The gas sample is introduced into the System by sucking it into the sample in port at the front of the housing.

BreathSpec® – User Manual

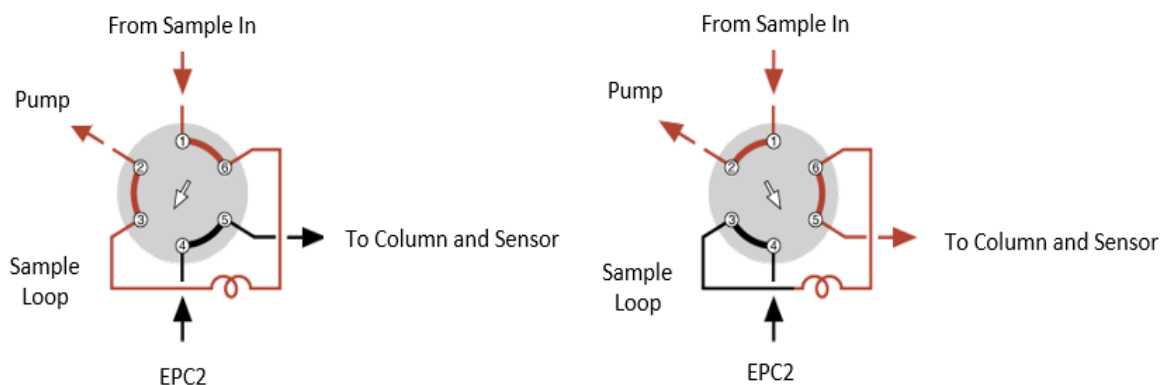


Figure 7: Six-Port Valve - Position Fill Loop and Inject

The sample is transferred via the heated 6-port-valve (T3) to the GC-Column. In the default position of the 6-port-valve the carrier gas permanently flushes the multi capillary column. The sample gas is pumped through the loop by the pump *P*. This phase is called “Fill Loop”. In this position the sample gas from the Sample In socket is directly routed to the Sample Out socket.

For routing the sample gas in the loop to the GC-Column and to the IMS, the 6-port-valve is switched to the second position. The carrier gas now transports the sample gas into the loop and further to the GC-Column, where the substances in the sample gas are separated by time. The eluting substances are introduced into the ionization region of the IMS and leave the system via the Gas Out socket.

The carrier gas stream now transports the sample gas to the multi GC-column, where the substances in the sample gas are separated by time. The eluting substances are introduced into the ionization region of the IMS and leave the system via the Gas Out socket.



INFORMATION!

In the event of a power failure, check the position of the valve position. The basic setting must be set to **Fill Loop**.

5.4 BreathSpec® (Standard Edition) Housing Device with Circular Gas Flow Unit (CGFU)

5.4.1 Front

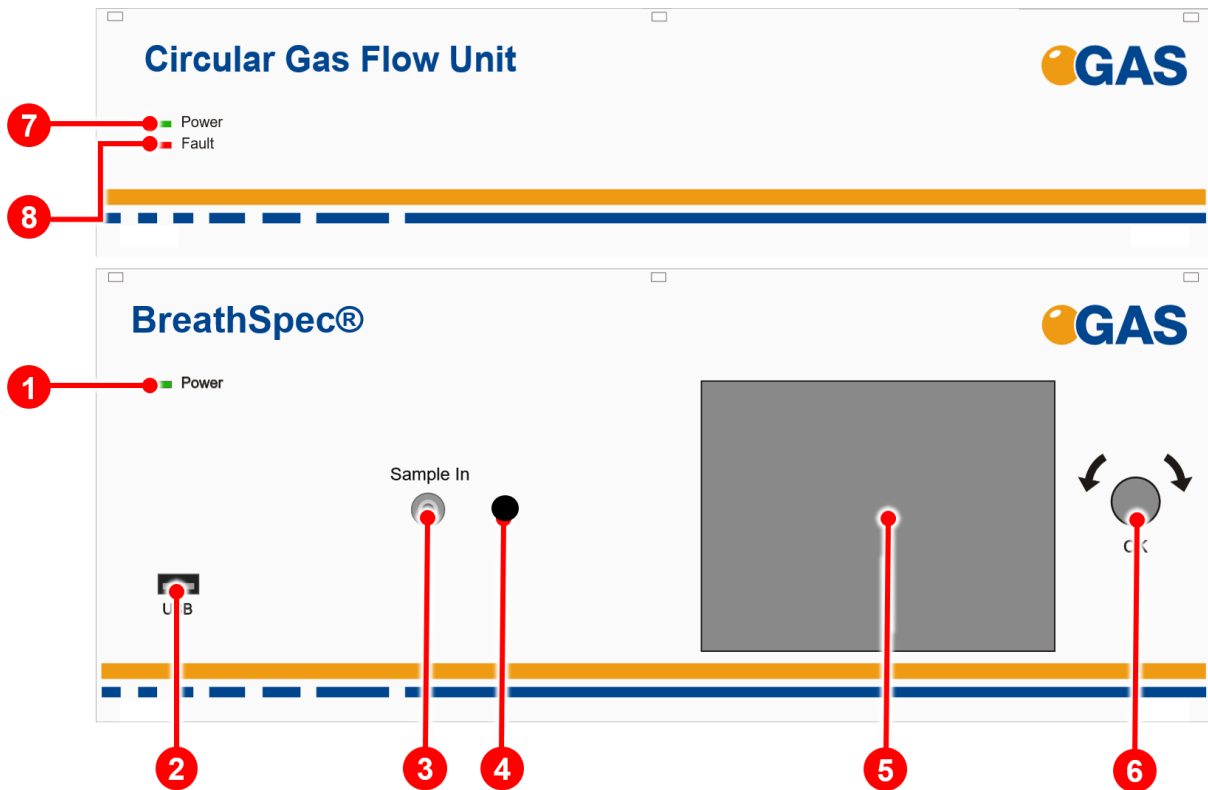


Figure 8: BreathSpec® (Version 4G1) - Housing of device - Front

<p>1</p>	<p>Power LED</p>	<ul style="list-style-type: none"> ■ Indicates whether or not the device is connected to a power supply and is switched on ■ Indicates an internal system error.
<p>2</p>	<p>USB Socket</p>	<p>USB socket for connecting external USB storage volumes. These volumes can be used for:</p> <ul style="list-style-type: none"> exporting measurement files importing sample name lists upgrading the device's firmware saving/loading system settings.

3	Sample in	3 mm Swagelok inlet plug for connecting the device to a gas source via <ul style="list-style-type: none">• Transferline or• Luer-Lock-Adapter.
4	Heater socket	Connector for heater current supply (Transferline or Luer-Lock Adapter).
5	Touch screen Display	Displays the graphical user interface and allows the control of the device by touch screen.
6	Pushable Rotary Knob	Input control for cycling through and activating the control elements of the graphical user interface.
7	Power LED	Indicates whether or not the device is connected to a power supply and is switched on
8	Fault LED	Indicates an internal system error.

5.4.2 Rear

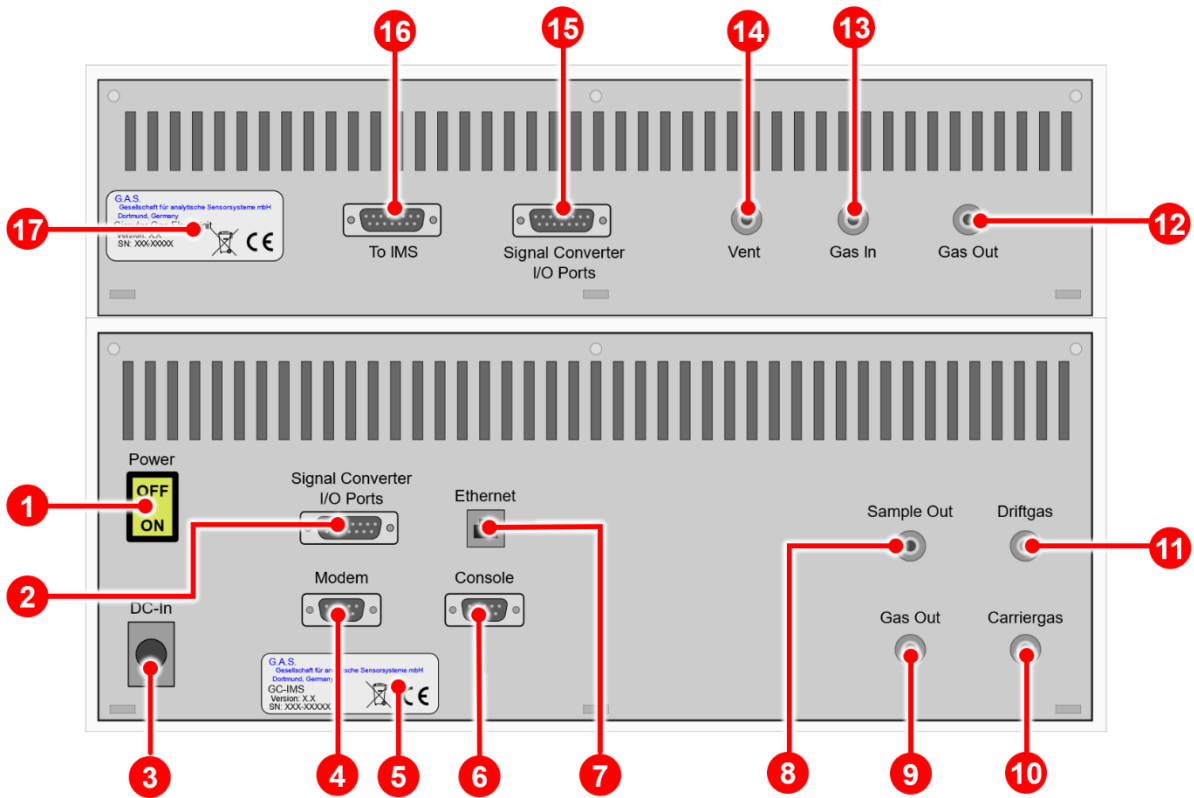


Figure 9: BreathSpec® (Version 4G1) - Housing of device - Rear

1	Power Switch	Switches the device on or off.
2	Signal Converter –I/O Ports	Socket for connecting a PLC (Programmable Logic Controller) or other devices.
3	DC-In	24V XLR-Connector for connecting the power supply.
4	Modem	Socket for connecting an external modem. For service purposes only.
5	Device Type/Serial Number Plate	Displays manufacturer identification, device type, serial number and version.
6	Console	Console interface socket. For service purposes only.

BreathSpec® – User Manual

7	Ethernet	Socket for connecting the device to a local area network (LAN) or directly to a computer.
8	Sample Out	3 mm Swagelok plug for connecting the device to an adequate laboratory waste gas ventilation system/fume hood.
9	Gas Out	3 mm Swagelok plug for connecting the device to the Gas In Socket 13 of the CGFU
10	Carriergas	3 mm Swagelok inlet plug for connecting the device to Gas Out Socket 12 of CGFU.
11	Driftgas	3 mm Swagelok inlet plug for connecting the device to Gas Out Socket 12 of CGFU.
12	Gas Out	3 mm Swagelok plug for connecting the device to Drift Gas In Socket / Carrier Gas In Socket 11 10 of BreathSpec®
13	Gas In	3 mm Swagelok plug for connecting the device to Gas Out Socket 9 of BreathSpec®.
14	Vent	Socket for the internal pressure compensation.
15	Signal Converter –I/O Ports	Socket for connecting a PLC (Programmable Logic Controller) or other devices.
16	To IMS	Sub D Socket to power supply and device control of CGFU via BreathSpec®. The To IMS socket of the CGFU must be connected to the connector Signal

		Converter I/O Ports of the BreathSpec®.
17	Device Type/Serial Number Plate	Displays manufacturer identification, device type, serial number and version.

5.5 BreathSpec® (Version 4G2) Housing Device with Airsense μTD

5.5.1 Top

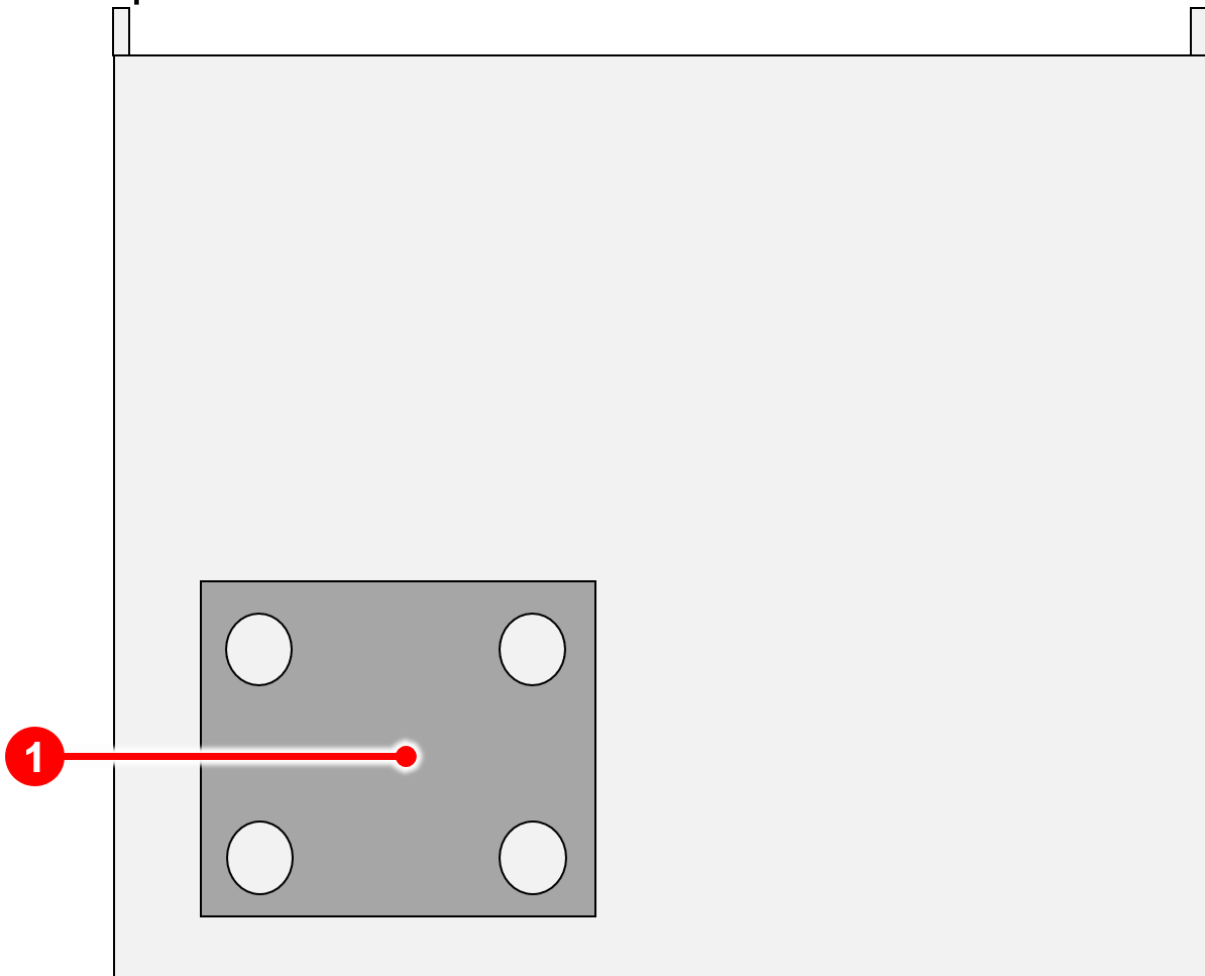


Figure 10: BreathSpec® with Airsense μTD (Version 4G2) - Housing of device - Top

1	μTD Mounting Plate	<ul style="list-style-type: none"> • Mounting plate for placing the μTD Unit
----------	---------------------------	---

5.5.2 Front

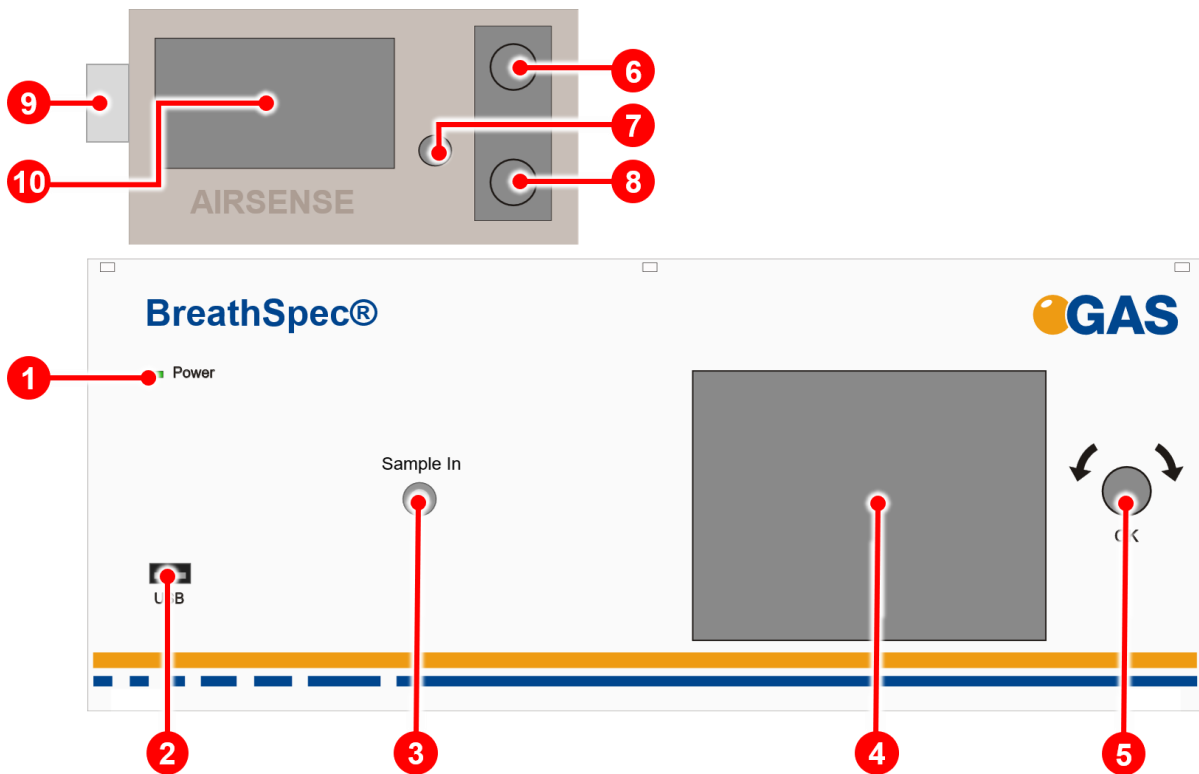


Figure 11: BreathSpec® (Version 4G2) with Airsense μ TD - Housing of device - Front

<p>1</p>	<p>Power LED</p>	<ul style="list-style-type: none"> ■ Indicates whether or not the device is connected to a power supply and is switched on ■ Indicates an internal system error.
<p>2</p>	<p>USB Socket</p>	<p>USB socket for connecting external USB storage volumes. These volumes can be used for:</p> <ul style="list-style-type: none"> exporting measurement files importing sample name lists upgrading the device's firmware saving/loading system settings.
<p>3</p>	<p>Sample in socket</p>	<p>3 mm Swagelok inlet plug for connecting the device to a gas source via</p> <ul style="list-style-type: none"> Bypass Adapter Transfer-line or Luer-Lock-Adapter.

4	Touch screen Display	Displays the graphical user interface and allows the control of the device by touch screen.
5	Pushable Rotary Knob	Input control for cycling through and activating the control elements of the graphical user interface.
6	Inlet Sampler Connector	Heated transferline for connection to a sample source
7	Start/Stop Button	Switches the μ TD device on or off.
8	Inlet Detector Connector	Heated transferline for connection to BreathSpec sample in connector
9	Adsorbens Tube Holder	The adsorbens tube can be installed.
10	Display	Displays the current phase of the desorption cycle

5.5.3 Rear

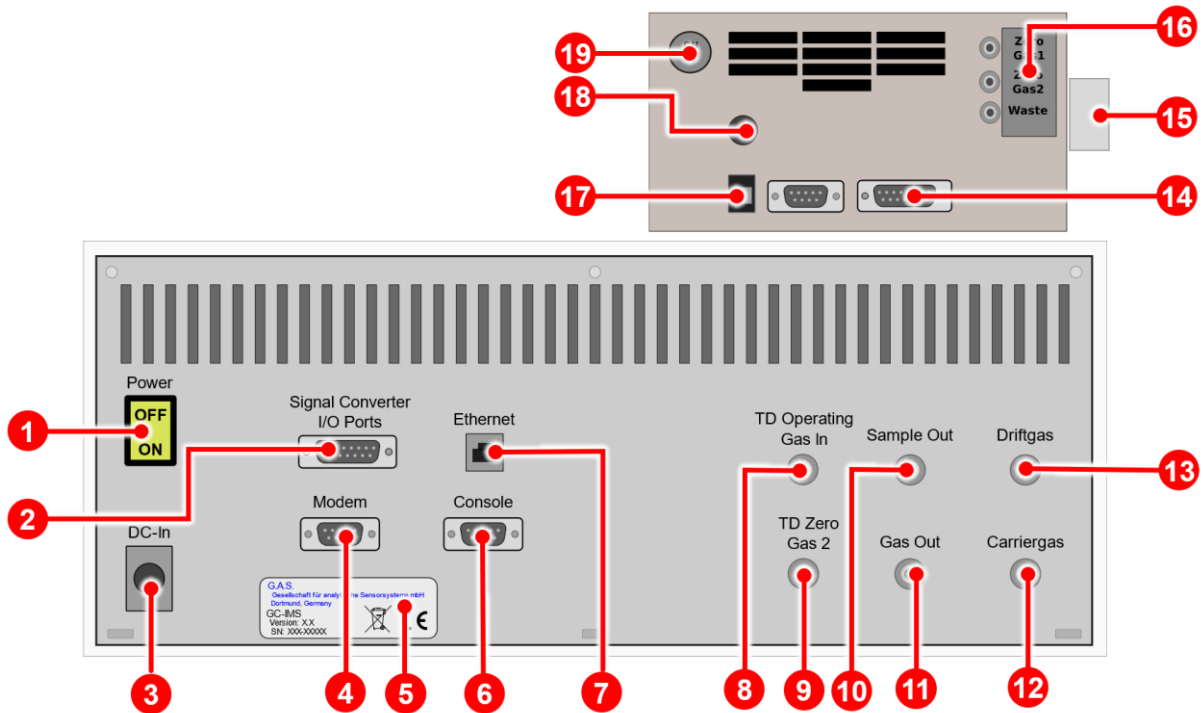


Figure 12: BreathSpec® (Version 4G2) with Airsence µTD - Housing of device - Rear

1	Power Switch	Switches the device on or off.
2	Signal Converter –I/O Socket	Socket for connecting a PLC (Programmable Logic Controller) or other devices.
3	DC-In Socket	24V XLR-Connector for connecting the power supply.
4	Modem Socket	Socket for connecting an external modem. For service purposes only.
5	Device Type/Serial Number Plate	Displays manufacturer identification, device type, serial number and version.
6	Console Socket	Console interface socket. For service purposes only.

7	Ethernet Socket	Socket for connecting the device to a local area network (LAN) or directly to a computer.
8	TD Operation Gas In	3 mm Swagelok inlet plug for connecting the device to an operating gas source.
9	TD Zero Gas 2	3 mm Swagelok inlet plug for connecting the device to the 3 mm Zero Gas 2 connector of the μ TD.
10	Sample Out Socket	3 mm Swagelok plug for connecting the device to an adequate laboratory waste gas ventilation system/fume hood.
11	Gas Out Socket	3 mm Swagelok plug for connecting the device to an adequate laboratory waste gas ventilation system/fume hood.
12	Carrier Gas In Socket	3 mm Swagelok inlet plug for connecting the device to a drift gas source.
13	Drift Gas In Socket	3 mm Swagelok inlet plug for connecting the device to a drift gas source.
14	Digital Port	Digital Port to connect the μ TD to the GC-IMS Signal Converter I/O Port with interface cable.
15	Tube Holder	Tube holder for adsorption tube
16	Gas connectors	3 mm Gas port Zero Gas1 , Zero Gas2 and Waste
17	USB Socket	Socket for connecting the device to a computer.

18	Power Supply Socket	Connector for connecting the μ TD power supply
19	Power Switch	Switches the device on or off.

5.6 Device Type / Serial Number Plate

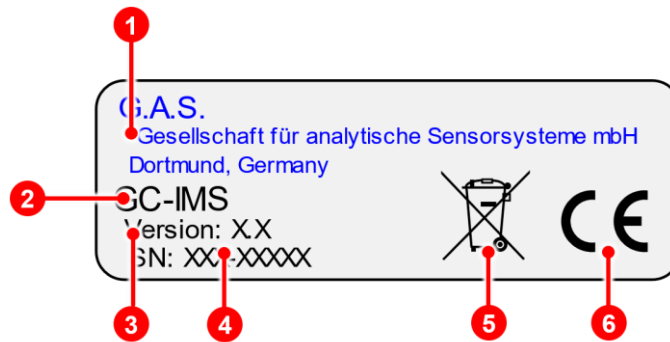


Figure 13: Device Type / Serial Number Plate

1	Manufacturer
2	Type Name
3	Version Number
4	Serial Number
5	Disposal Instructions This marking on the instrument indicates that they must not be disposed of in domestic waste. The disposal is carried out by return to the manufacturer or by the corresponding municipal authorities (see EU directive 2012/19/EU)
6	CE Marking CE, Communauté Européenne Instruments bearing this mark comply with the relevant European directives

6 Operating Interface

The graphical user interface of the device can be controlled by using the touchscreen in combination with the pushable rotary knob at the front of the device.

The selected control (button, input field etc.) element is marked blue. To activate it the knob can be pressed.



INFORMATION!

As the product is under continuously development, the screen shots in this user manual may differ from the actual conditions.

All possible functionalities of the firmware are described.

Depending on the hardware some functionalities are not available.

6.1 Overview

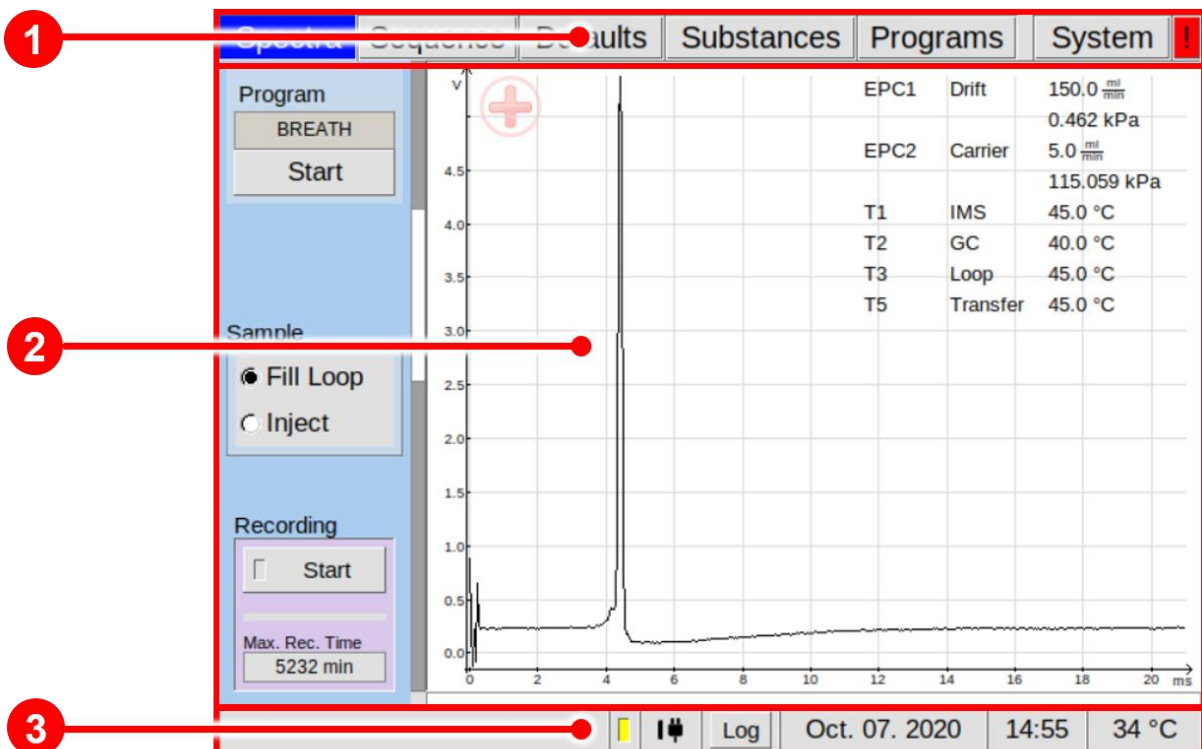


Figure 14: Operating Interface - Overview

1	Window Selection Bar	The main windows can be selected.
2	Window Display Area	The content of the selected main window will be displayed.
3	Status Bar	Status messages and system information are displayed.

6.1.1 Windows Selection Bar

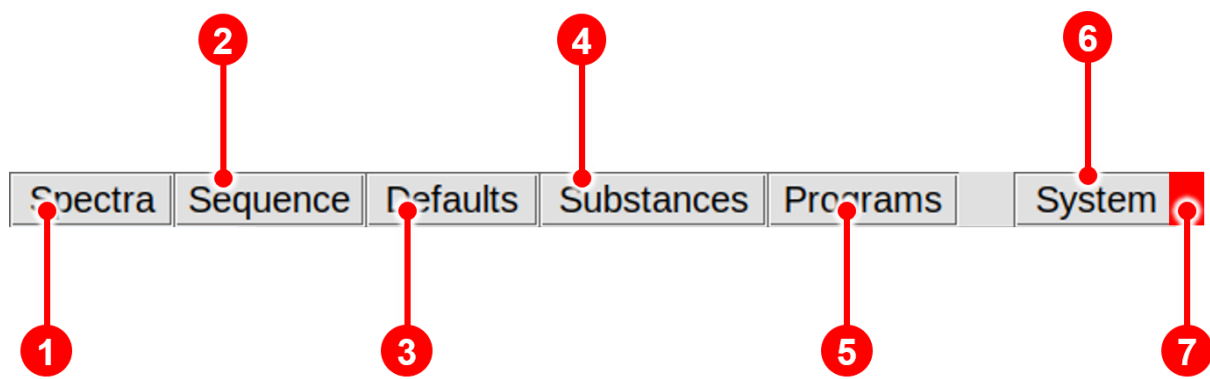


Figure 15: Operating Interface - Windows Selection Bar

1	Spectra Window Button	In Spectra Window the data acquisition process is controlled.
2	Sequence Window Button	In Sequence Window user created sequence files using the Sequence Designer software can be imported.
3	Defaults Window Button	In Defaults Window the default settings can be set.
4	Substances Window	In Substances Window a Substance list with assign search parameter sets can be managed.
5	Programs Window Button	In Programs Window user-defined measurement programs can be set.

6	System Window Button	In System Window system specific information are displayed system specific settings and can be set.
7	Errors Information Window Tab	In Error Information Window current error information are displayed.

6.1.2 Windows Display Area

In Window Display Area the content of the following main windows is displayed:

- Spectra Window
- Sequence Window
- Defaults Window
- Substances Window
- Programs Window
- System Window

6.1.3 Status Bar

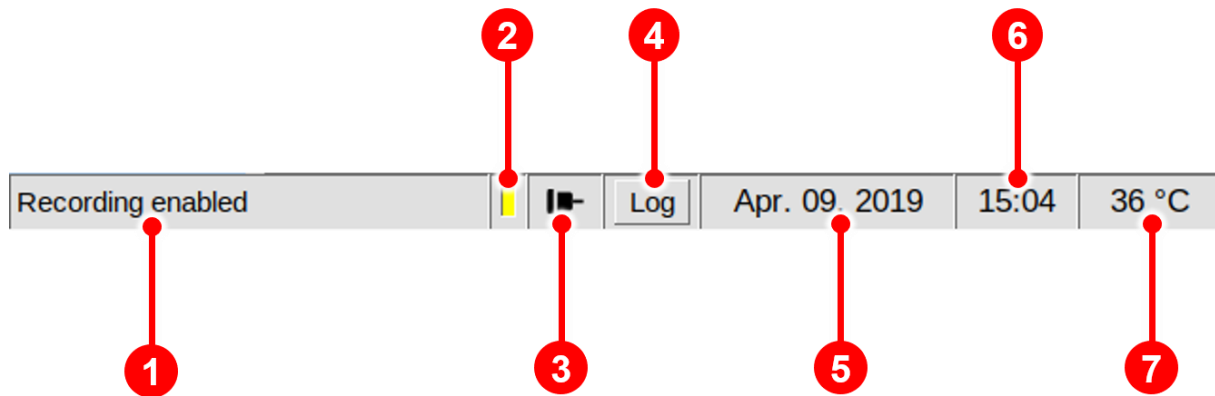






Figure 16: Operating Interface - Status Bar

1	Status Message Section	Device events information will be displayed.
2	Export Message Section	Displays the current connection status. Export on: <input type="checkbox"/> Export of <input type="checkbox"/>

<p>3</p>	<p>LAN Connection Section</p>	<p>Displays the current connection status: Connected:  Disconnected: </p>
<p>4</p>	<p>Log Section</p>	<p>Displays the current log status. New entry:  No modification:  Selecting this button will open the Log Section Window with a chronological list of system events</p>
<p>5</p>	<p>Date Section</p>	<p>Displays the current date of the device clock. It can be set in System Window.</p>
<p>6</p>	<p>Time Section</p>	<p>Displays the current time of the device clock. It can be set in System Window.</p>
<p>7</p>	<p>Temperature Section</p>	<p>Displays the current inner housing temperature of the device.</p>

6.1.4 View Control Bar

The view control bar function is available in the Spectra window and in the Defaults window. By touching the screen, the control bar is displayed underneath the displayed spectra.

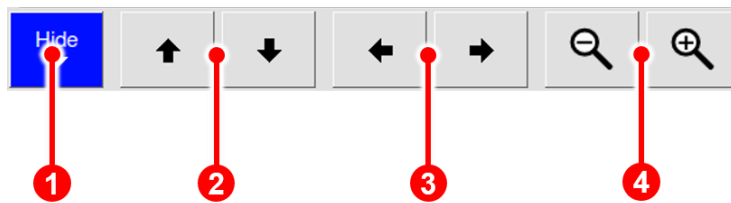


Figure 17: Operating Interface – View Control Bar

<p>1</p>	<p>Hide Button</p>	<p>The control bar can be hidden manually. After 3 seconds of inactivity it is hidden automatically.</p>
<p>2</p>	<p>Vertical Control Buttons</p>	<p>Moves the vertical position of the display area on the screen up or down.</p>

3	Horizontal Control buttons	Moves the horizontal position of the display area on the screen left or right.
4	Zoom Control buttons	Reduces or enlarges the view of the display area on the screen

6.1.5 Low/High Pressure Control

The device pressure is monitored. Two types of error are defined:

6.1.5.1 Low Pressure Error

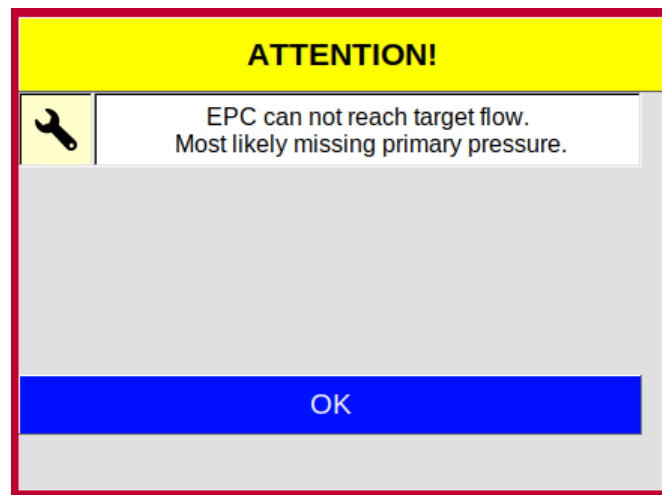


Figure 18: Operating Interface - Low Pressure Alarm Box

1. After 10 seconds a dialogue box is displayed and an acoustic alarm sounds.
2. After 5 minutes all temperature controllers are switched off.
3. When the pressure is reached again the alarm is switched off and all temperature controllers switch themselves on automatically

6.1.5.2 High Pressure Error



WARNING!

High pressure can destroy the device.

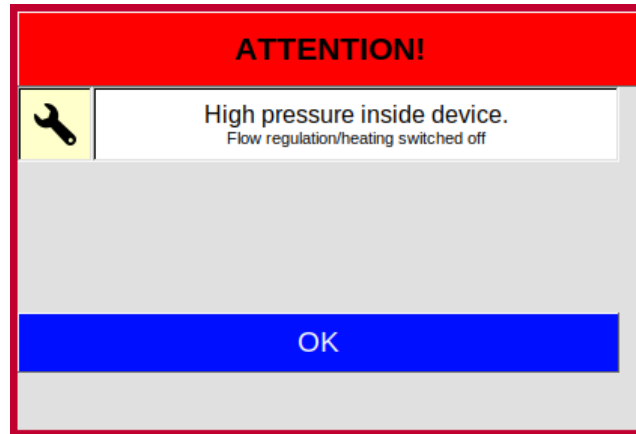


Figure 19: Operating Interface - High Pressure Alarm Box

1. If overpressure is detected, a visual and audible alarm is triggered immediately. At the same time all temperature controllers and flow controllers are switched off.
2. Before continuing to operate the unit, the cause of the spotlight must be eliminated.
3. By confirming the dialogue box or restarting the system, all temperatures and flows are reset to their normal values.

6.2 Spectra Window

6.2.1 Overview

After the device is switched on and the system start is completed the Spectra Window is displayed. In the Spectra Window the data acquisition can be controlled.

The current spectrum is displayed. The Recording Mode can be activated. The selected measurement program can be started.

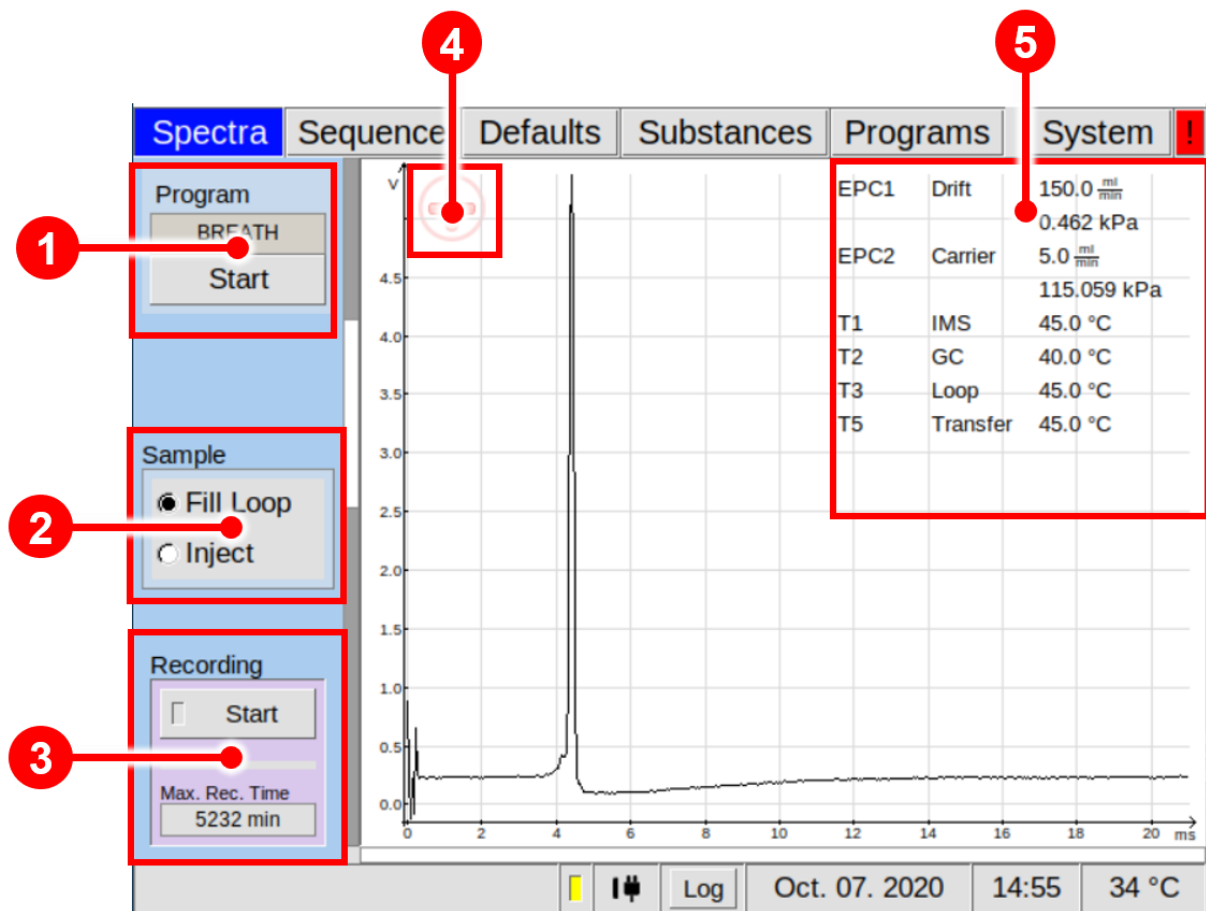


Figure 20: Operating Interface - Spectra Window

1	Program Start Button	By selecting this button the displayed program is started.
2	Switching Valve Button	The 6-port-valve can be toggled manually between Fill Loop and Inject Position . The basic setting must be set to Fill Loop .

3	Recording Check Box	The live monitoring of measurements can be recorded manually. The available storage capacity in minutes is displayed.
4	Drift Voltage Mode	Displays the current selected Drift Voltage state (positive / negative).
5	Device Parameter	Displays the current temperature, flow and pressure values.

6.2.2 Measurement modes

Two measurement modes are available:

- Measurement with user defined programs
- Manually operated measurement

6.2.2.1 Measurement with user defined programs

In this mode data acquisition with user-defined measurement programs can be started. The executable measurement program can be created and selected in the Programs Window. The name of the current selected program is displayed in the upper left of the Spectra Window. The selected measurement program can be started by activating the Program button in the upper left of the Spectra Window.

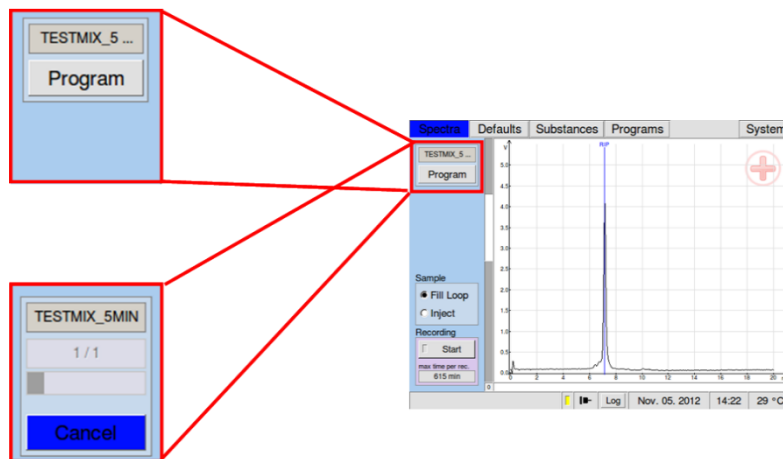


Figure 21: Start Program

6.2.2.2 Manually operated measurement

To record a measurement manually the Recording button can be switched on. If recording is not active the button is set to **START** and the checkbox is grey. If recording is active the button is set to **STOP** and the checkbox is yellow.

In this case a measurement file is generated from the recorded data and saved to the internal flashcard. The remaining time for data storage to the internal flashcard is shown. It depends on the number of measurement data that were released for export but were not yet exported and their file size depends on the value of spectra averages that are used.

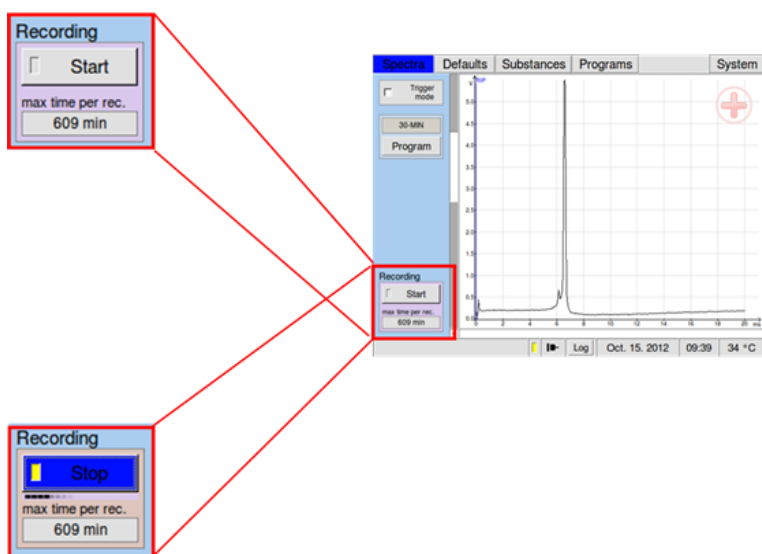


Figure 22: Recording Check Box

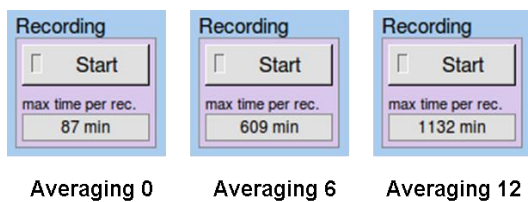


Figure 23: Recording Check Box

6.3 Sequence Window

In Sequence Window Sequence files can be imported and started by clicking on the Start Button. The processing status of a user created sequence file can be watched:

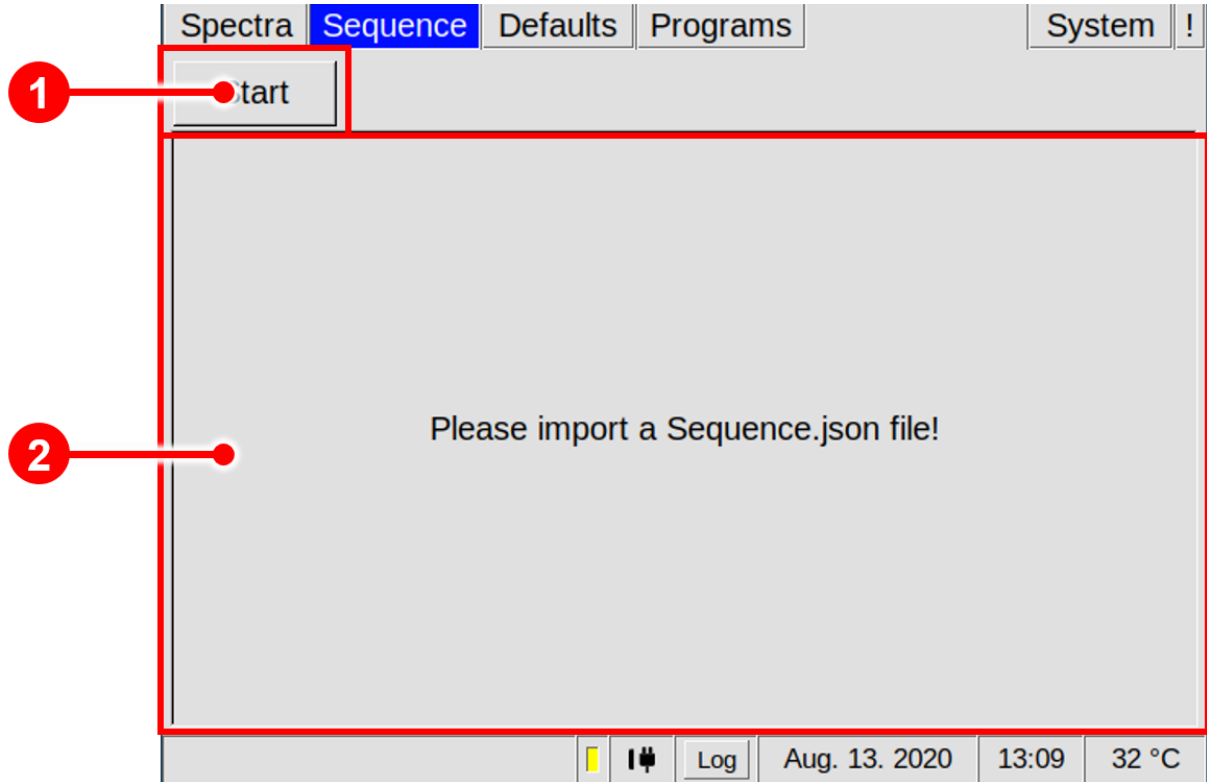


Figure 24: Operating Interface - Sequence Window

1	Start Button	A user created sequence files, created by G.A.S.Sequence Designer Software , can be imported.
2	Information Window	The live monitoring of measurements can be recorded manually. Displays the available storage capacity in minutes.



INFORMATION!

The sequence file must be named as **sequence.json**.

After selection, the software will try to import and analyse the sequence file. If the file could be imported and the analysis showed no errors, the sequence will be executed. The following figure shows the execution of a sequence:

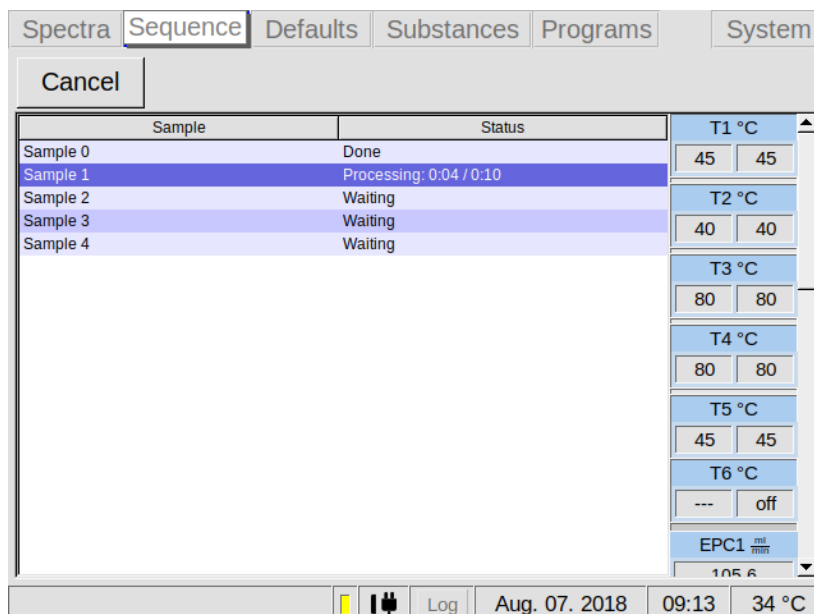


Figure 25: Operating Interface - Sequence Window - Processing

You will see the sequence being processed, one Sample after another. The time passed and the total time for each Sample are displayed, showing you the progress. The scrollable area on the right displays the current and the target device parameters for temperatures and flows, as well as some IMS specific values such as voltages and the trigger duration. Clicking on the cancel button will stop the Sequence, but still apply all the After Run Settings. Once the Sequence has finished, all Samples will be marked as done, the last After Run Settings are applied and the software will display the message Execution finished. The system is now ready for further sequences or manual operation.



INFORMATION!

The sequence file must be created with the **G.A.S. Sequence Designer Software**. For detailed Information refer to the **G.A.S. Sequence Designer Software Manual**.

6.4 Defaults Window

6.4.1 Overview

The Defaults window allows the monitoring and modification of various device component parameters. The electronic pressure controllers (EPC 1 and EPC 2) and the heating modules of the device can be controlled (T1 – T6). Further, the sample pump performance, averaging and drift voltage polarity can be switched manually.

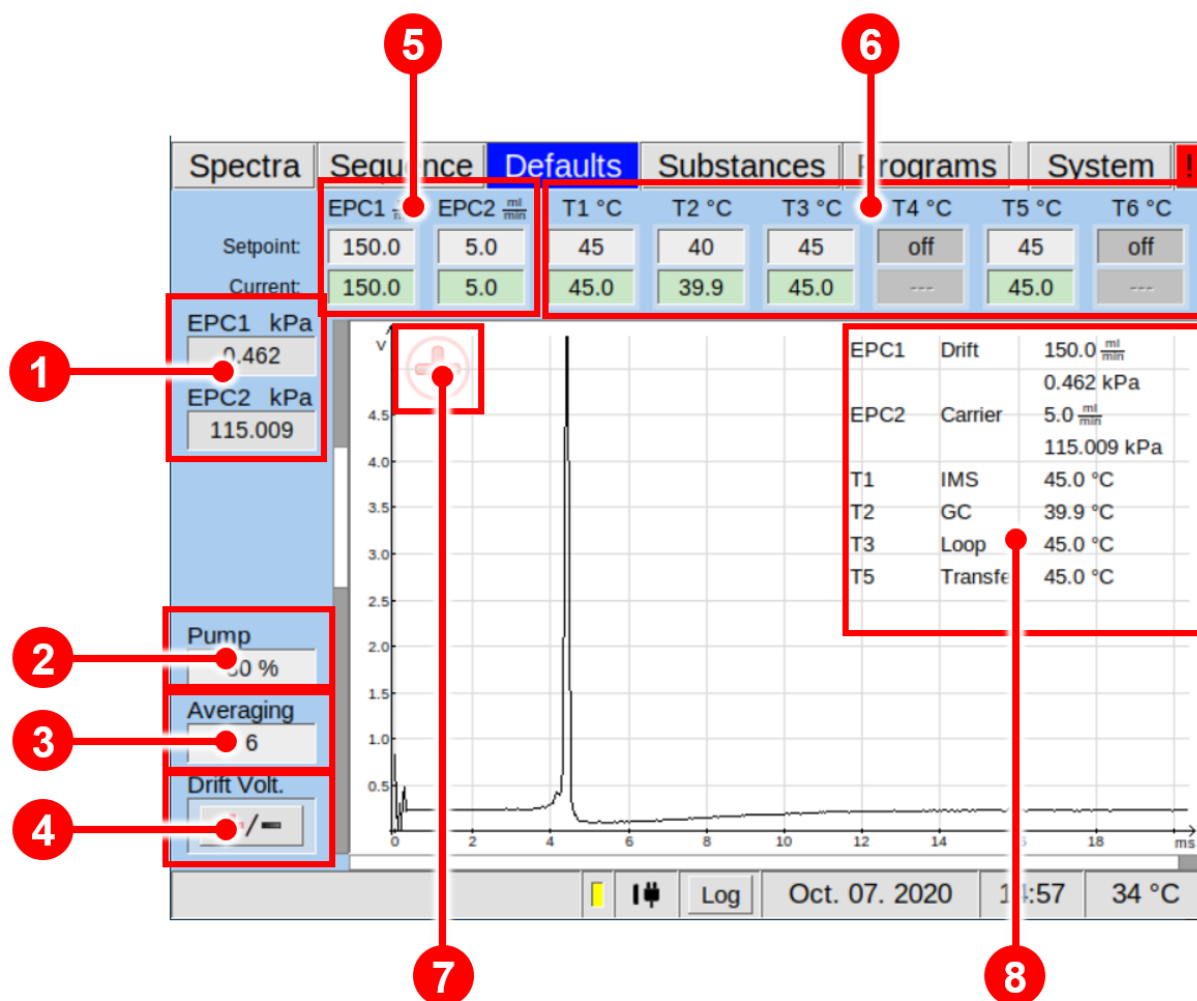


Figure 26: Operating Interface - Defaults Window

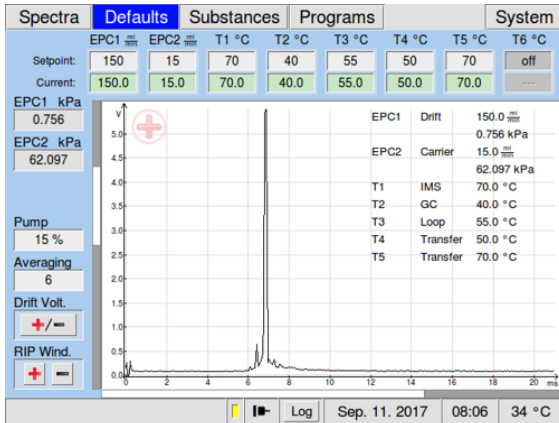
1	Pressure display	Displays the relative overpressure of the gas flow. EPC1 displays the current the overpressure of the drift gas flow. EPC2 displays the overpressure of the carrier gas flow.
2	Pump	The sample-in flow in percent of the pump power can be set here.

3	Averaging display	Displays the current average value. The averaging value determines how many raw spectra are averaged to generate one single spectrum as result in the stored measurement file. Modifying the averaging parameter affects the number of recorded spectra per time period. A typical average value is 6. The maximum is set to 99. A value of 0 (Off) disables averaging.
4	Drift-Voltage Button	Drift Voltage polarity can be selected and switched (positive/negative).
5	Flow display	In Input Field Setpoint the flowrate of Drift gas (EPC1) and Carrier gas (EPC2) can be set. The current flowrates for Drift gas (EPC1) and Carrier gas (EPC2) are displayed. The maximum value for EPC1 is 500 ml/min. The maximum value for EPC2 is 150 ml/min. The working value for EPC1 is 150 ml/min. The working value of EPC2 depends of the application measurement and is influenced by the build-in GC-Column (length, inner diameter).
6	Temperature display	In Input Field Setpoint the temperature values of the heating modules IMS (T1) , Column (T2) , Six-Port Valve with Sample Loop (T3) , internal Transferline (T5) and external Transferline (T4) can be set. The current Temperatures (T1–T5) are displayed. Temperature module T6 is currently not available. The maximum settable value is 80 °C.
7	Drift Voltage mode	Displays the current selected Drift Voltage state (positive / negative).
8	Device Parameter	Displays the current temperature, flow and pressure values.

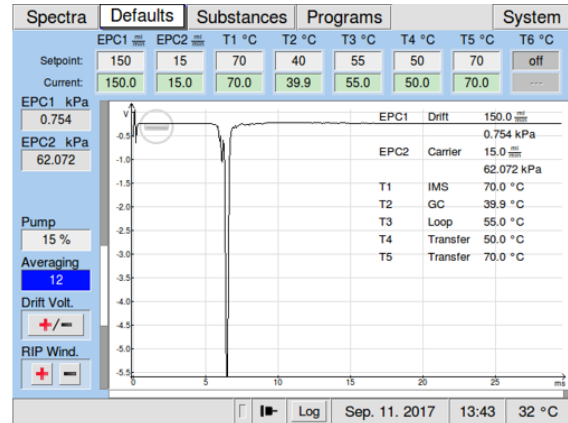
BreathSpec® – User Manual

6.4.2 Drift Voltage

The Drift Voltage can be switched between positive and negative drift voltage mode. One of these two modes may be more suitable for specific substances.



Positive Mode



Negative Mode

Figure 27: Drift Voltage Windows - positive and negative Mode

6.4.3 Flow Controls and Heating Modules

	EPC1 $\frac{ml}{min}$	EPC2 $\frac{ml}{min}$	T1 °C	T2 °C	T3 °C	T4 °C	T5 °C	T6 °C
Setpoint:	150.0	50.0	45	40	80	80	45	40
Current:	150.0	50.0	45.0	40.0	>80	---	45.0	---

Figure 28: Flow and Temperature Control (Example)

The component parameters are displayed and can be modified in the upper section of the window and in the left section of the window.

Above the spectra chart the flow rates of the drift and carrier gas controlled by the two electric pressure controllers (EPC 1 and EPC 2) and the temperatures of the heating elements of the device are managed. Unused elements are greyed out. The current flow rates and set-points for EPC 1 (drift gas) and EPC 2 (carrier gas) are displayed. The maximum value for EPC 1 is 500 ml/min. The maximum value for EPC 2 is 150 ml/min (Depending on the column used). The current temperatures and the set points of the IMS (T1), the column (T2), the 6-Port valve with sample loop (T3) and the inner heated transferline (T5) are displayed. The set points can be set using these controllers. The maximum adjustable temperature value is 80 °C. During the cleaning process the heating modules can reach temperatures up to 100 °C. These will be displayed as “> 80 °C”. Heating modules can be turned off by decreasing the respective value to “off”.

6.5 Substances Window

6.5.1 Overview

In the Substances window a list of **up to 50 substances** with assigned search parameter sets can be managed. This substance list is used for analysing the measurement data during a measurement program run. The result of this analysis is a subset of the substances in this list detected in the respective gas sample. It is stored along with the measurement data.

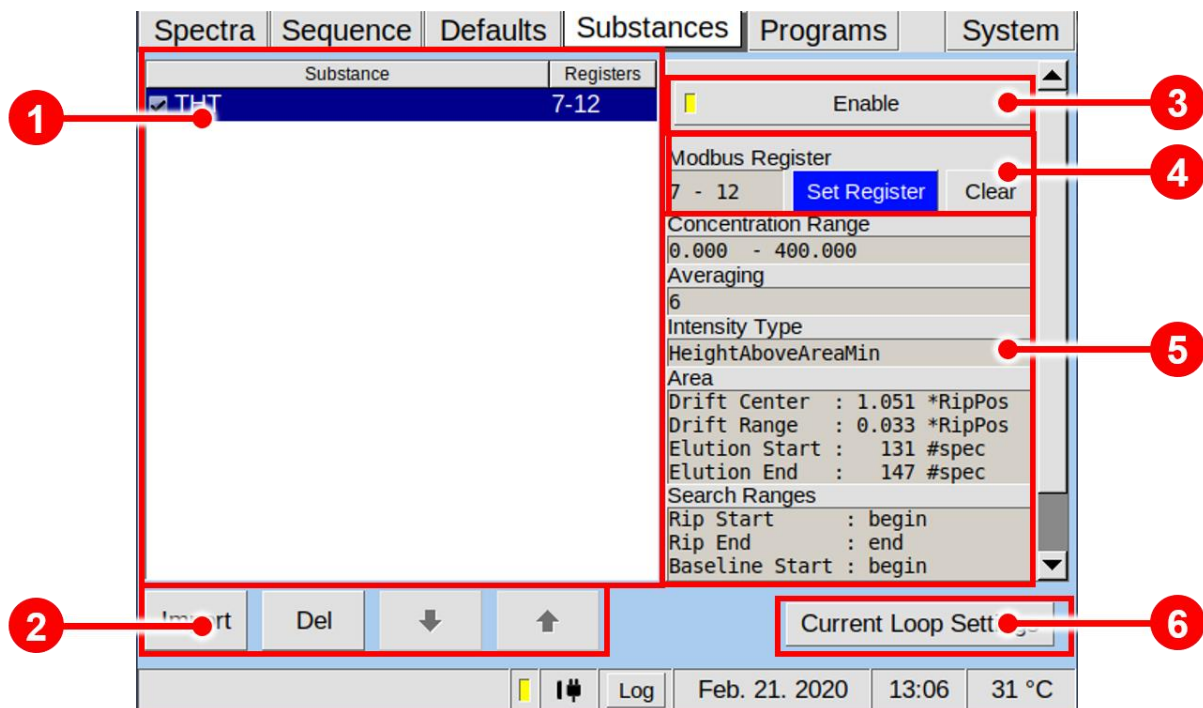


Figure 29: Operating Interface - Substances Window

1	Substances List window	All created substance entries are listed in this box by name. The highlighted substance is selected for modification.
2	Substances List Control Panel	Buttons for import, changing or deleting actions of the selected substances <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="border: 1px solid gray; padding: 2px 5px;">Import</div> <div style="border: 1px solid gray; padding: 2px 5px;">Del</div> <div style="border: 1px solid gray; padding: 2px 5px;">↓</div> <div style="border: 1px solid gray; padding: 2px 5px;">↓</div> </div> <p style="text-align: center;">Import Delete down up</p>
3	Enable Button	Enables or disables the selected substance as a candidate for the detection process.

4	Modbus Register	<div data-bbox="794 219 986 273">Set Register</div> opens the Modbus Register setup dialog. <div data-bbox="794 295 896 340">Clear</div> deletes set registers
5	Substance Calibration Information Area	Displays the substance specific calibration information such as used concentration range, average, intensity type, area, search ranges and the quantification model name.
6	Current Loop Settings (optional)	Opens the current loop setup dialog.

6.5.2 Managing Substance Entries



Figure 30: Substance List Control panel

The Substance List Control Buttons Panel contains buttons for importing (**Import**) and deleting (**Del**) substance entries. By pressing the buttons **Up** ↑ and **Down** ↓ the position of a selected entry in the substances list can be changed.

After importing a substance calibration file it is available in the Substance List window.

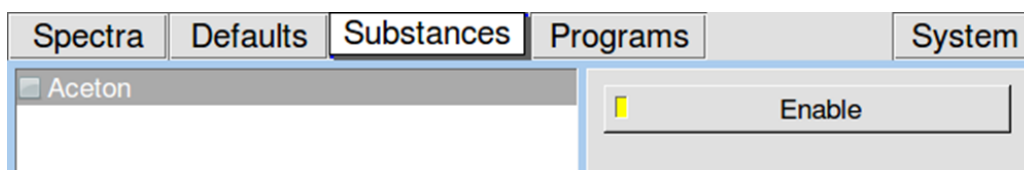


Figure 31: Substance selection 1

To make the substance active it has to be activated by pressing the Enable Button. The activated substance is marked.

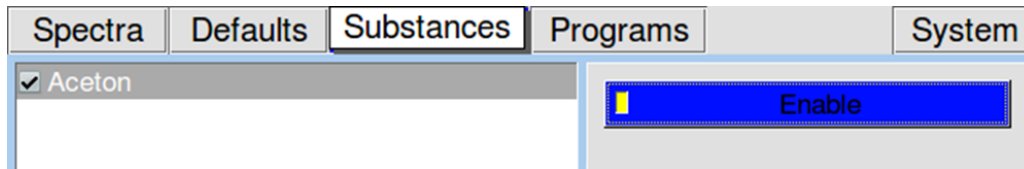


Figure 32: Substance selection 2

In case that the average between System setting and Substance data is different the relevant substance entry is labelled red and marked with an error symbol.

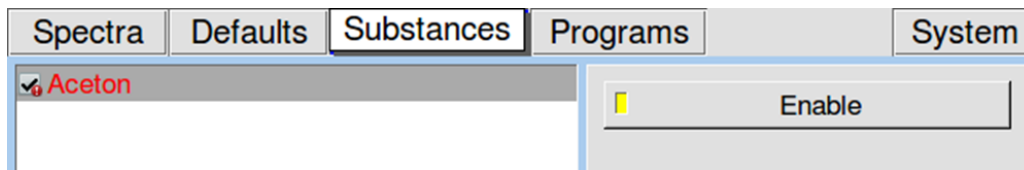
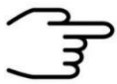


Figure 33: Substance selection 3

When the **Enable Button** for the selected substance is checked that substance entry will be included in the substance recognition process during the next measurement program run.



INFORMATION!

For detailed Information about the compilation of Substance calibration files (gsd-files) refer to the [VOCAL Tutorials](#).



INFORMATION!

The calibration file must be named as `calibration.gsd`

6.5.3 Managing Modbus TCP Setup

GAS Devices can output their results via the Modbus TCP protocol. The Registers can be set up on your device's **Substances page**. When selecting a substance from list on the left, information about it will be displayed on the right. This includes the registers it will be mapped to. Every substance will require a fixed set of registers, so the total of number substance information which can be transferred over the Modbus is limited. Registers for different substances cannot overlap. In case you try to overlap them, you will be informed by an error window, about which registers in specific have been assigned twice. Using the **Enabled** button, you can select or deselect substances for evaluation. Deselecting them will result in the designated status code in the corresponding registers. You can check the last Modbus TCP connection to your device in **System > Transfer > Modbus TCP**. It will give you information on when and from which IP the last connection was made and whether it is still active (Figure 35).

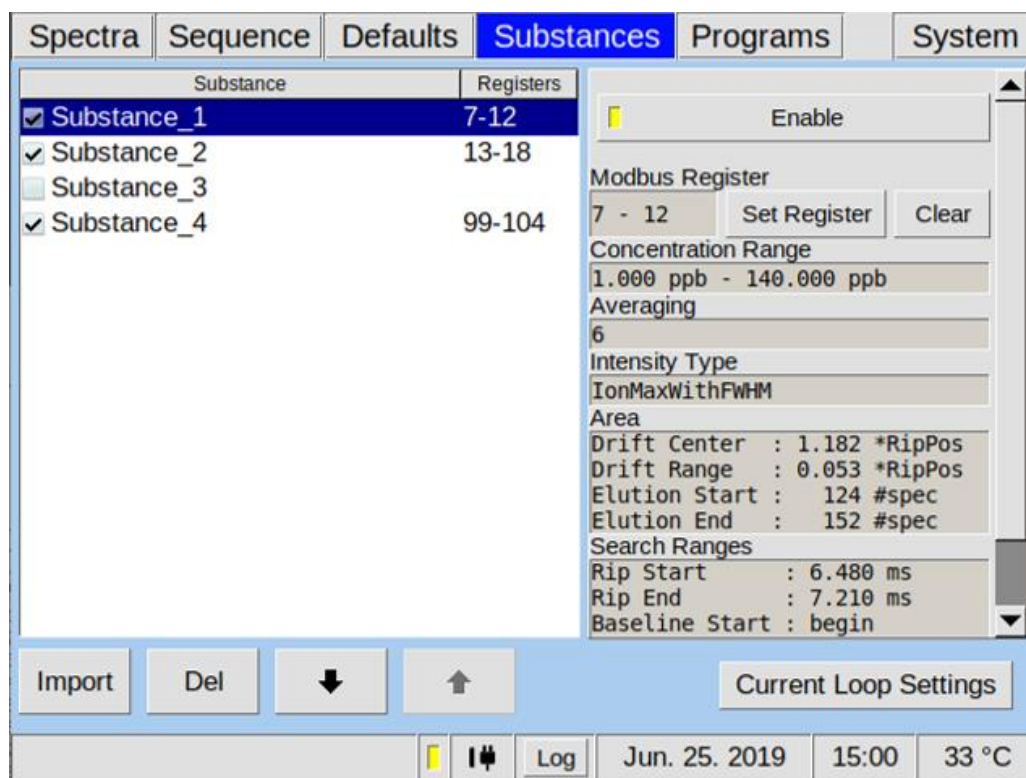


Figure 34: Substances Window

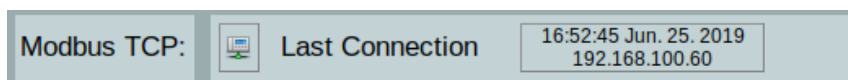


Figure 35: Information about the last Modbus TCP Connection

The results are put into the holding registers (40001-40250 function code FC03). These **250 registers** are **divided** into **two 125 register** long arrays which contain the current results in the first 125 and the results from before that in the latter 125 registers. At the beginning of each of these register blocks is the information header, which is 6 registers in size. See Chapter **9.6 Modbus TCP Specification**.

BreathSpec® – User Manual

Since the size of a register is 16 bit, 32bit Integers will have to be split up into two separate registers with each containing a half of the bits. In figure 37 you can see in what order the 32bit are split up.

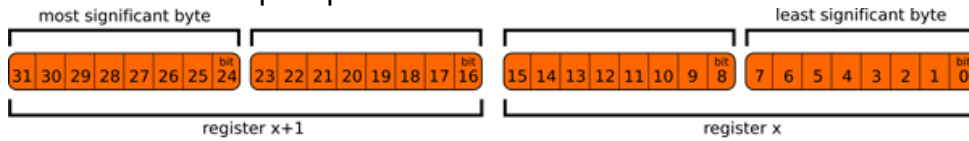


Figure 36:32 bit split up into 16 bit registers

In Figure 40 an example Modbus result is shown. The **Header** tells us in register 1 that we have 3 results available and in register 2 that an error with error code 4 occurred (target temperature not reached). Registers 3 and 4 contain the timestamp, which is 1561475754 seconds since January 1st 1970, corresponding to Tuesday, June 25th 2019 15:15:54. Of the 3 results you can only see 2, because they have been mapped to 7-12 and 13-18. The third result has been mapped into the range not shown. The concentration of **substance 1** was not within the calibrated range which can be identified by looking at register 10. This contains the value 2, which means, that the concentration is below the calibrated range. The concentration put into registers 7 and 8 is thus an invalid arbitrary value. The 1 in register 9 means, that the substance has been selected for evaluation. If **substance 1** wouldn't have been selected for evaluation, the other 5 registers would be empty and register 9 would contain a 2. **Substance 2** is mapped into the registers 13-18. The calculated concentration is 0.559 (559/1000 three decimal point precision) and mapped into registers 13 and 14. Whether or not this is within the calibrated precision can be seen in the calibration protocol you have been supplied with. Register 15 contains a 1 meaning the substance had been selected for evaluation. The concentration was within the calibration range, so the status code in register 16 is a 1.

Offset	Standard address	Hex	uint16	uint32
1	40001	0x0003	3	
2	40002	0x0004	4	
3	40003	0x3A...	15018	
4	40004	0x5D12	23826	1561475754
5	40005	0x0000	0	
6	40006	0x0000	0	
7	40007	0xFC18	64536	
8	40008	0xFFFF	65535	4294966296
9	40009	0x0001	1	
10	40010	0x0002	2	
11	40011	0x0000	0	
12	40012	0x0000	0	
13	40013	0x022F	559	
14	40014	0x0000	0	559
15	40015	0x0001	1	
16	40016	0x0000	1	
17	40017	0x0000	0	
18	40018	0x0000	0	
19	40019	0x0000	0	
20	40020	0x0000	0	
21	40021	0x0000	0	
22	40022	0x0000	0	
23	40023	0x0000	0	
24	(...) ↓	0x0000	0	
25	40025	0x0000	0	

Figure 37: First 25 registers of an example Modbus result.

6.5.4 Substance Calibration Information Area

Substance specific calibration information such as used Average, Intensity type, Area, Ranges and the Quantification model name of the selected Substance in the substance window are shown.

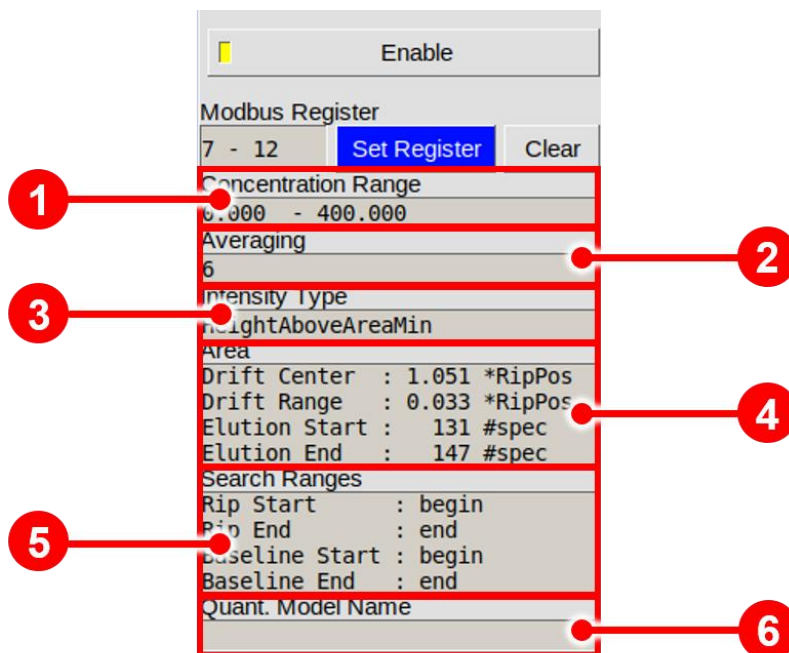
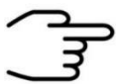


Figure 38: Substance Calibration Information Area

1	Concentration Range	Displays the used calibration range of the actual substance calibration file.
2	Averaging	Displays the used average of the actual substance calibration file.
3	Intensity Type	Displays the used intensity type of the actual substance calibration file.
4	Area	Displays the used area parameter of the actual substance calibration file.
5	Search Ranges	Displays the used search ranges of RIP and baseline of the actual substance calibration file.

6	Quant Model Name	Displays the quantification model name of the actual substance calibration file.
---	-------------------------	--



INFORMATION!

All substance calibration information are part of the calibration file set in the G.A.S. software VOCAL.

For detailed Information refer to the [VOCAL Tutorials](#).



INFORMATION!

The calibration file must be named as **calibration.gsd**

6.5.5 Recognised substances window

When substances are enabled in the substance window the recognised substances window appears at the end of every measurement. This screen displays a list with the results in a concentration unit which is defined in the valid calibration curve. When a current loop is available the last result of this list will be overwritten. By starting the next measurement this window disappears until the next measurement will be finished.

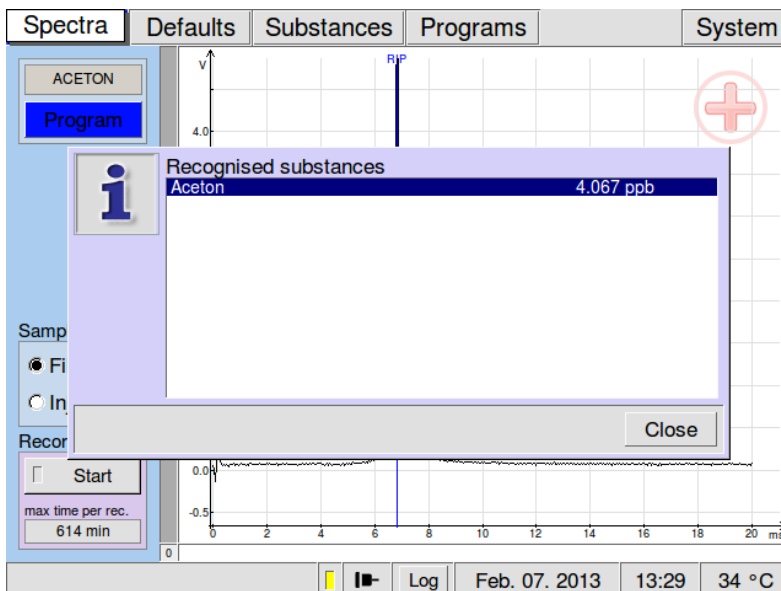


Figure 39: Recognized Substances Window

6.6 Programs Window

6.6.1 Overview

In Programs Window user-defined measurement programs can be set and managed.

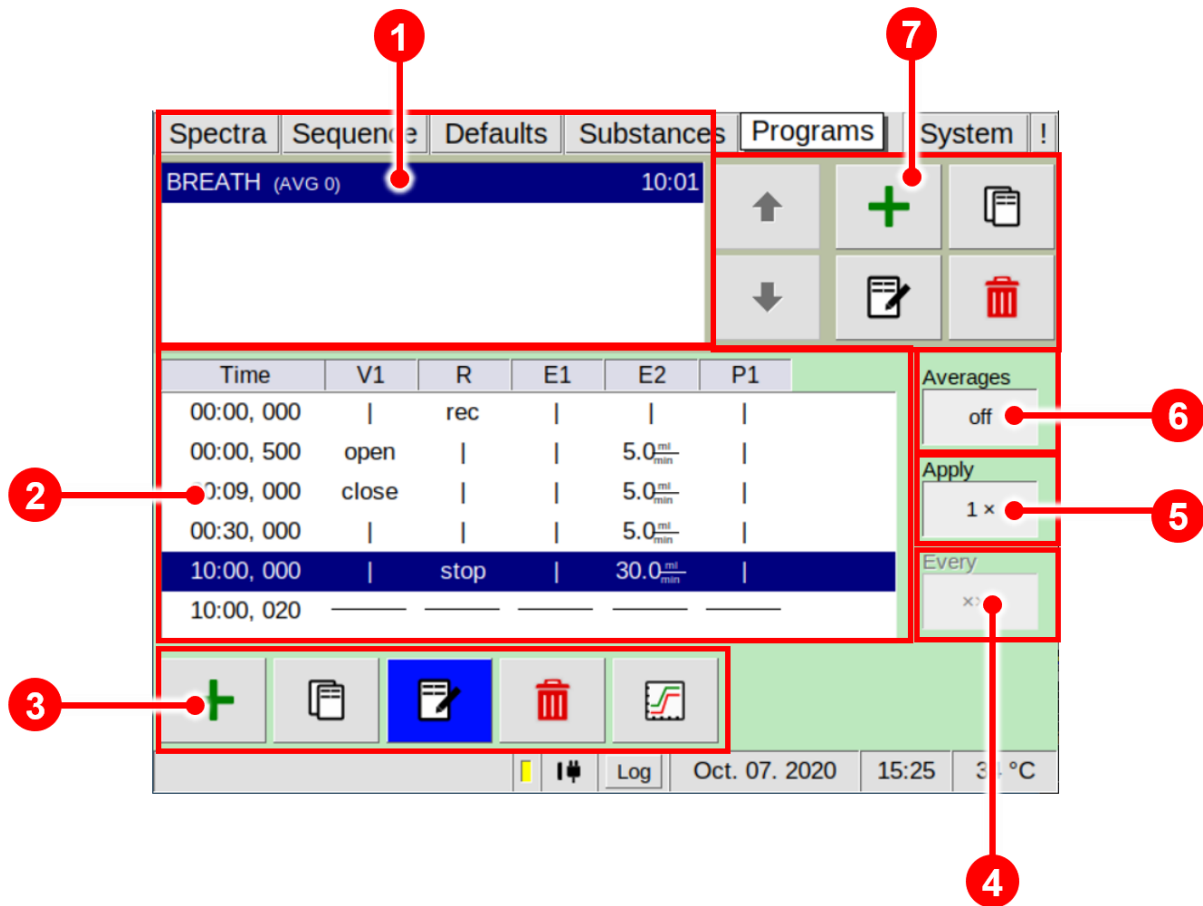










Figure 40: Operating Interface - Programs Window

1	Measurement Program List area	All created programs are listed in this box by name. The highlighted program is selected for execution or modification.
2	Selected Program area	All instructions of a selected program are listed here in a chronological order. For every device component that can be controlled by a program a separate column is displayed.
3	Program Action Control Panel	Buttons for creating, changing or deleting actions of the selected program <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> New</div> <div style="text-align: center;"> Edit</div> <div style="text-align: center;"> Copy</div> <div style="text-align: center;"> Del</div> </div>







4	Program Repetition Time	The time interval for program repetitions can be set.
5	Program Repetition Rate	The number of program repetitions can be set.
6	Average Settings	Average of the current selected program can be set. The current average is appended to the name of the measurement program.
7	Program Control Panel	Buttons for creating, changing or deleting actions of the selected program  New  Edit  Copy  Del

6.6.2 Create Measurement Programs

The Measurement Program List window displays all measurement programs currently existing. The measurement programs list can contain **up to 100 entries**. The current average value is part of the program name. The selected program can be edited.



Figure 41: Measurement Control Panel

 Up	The list order of the selected program can be changed stepwise upwards
 Down	The list order of the selected can be changed stepwise downwards.
 New	The New button which will open a keyboard window for entering the program name.
 Edit	By pressing the Edit button the program name for the selected entry can be edited into a keyboard window.
 Copy	By pressing the Copy button the program of the selected program will be copied.
 Delete	By pressing the Delete button the program of the selected program will be deleted.

Measurement programs can be set for repeated execution. Execution rules can be defined for each program in the **Apply** and **Every** fields.

Valid values for the Apply field range from 1x (once, the default) **up to 9,999 repetitions** or infinite, which means the program will be repeated endlessly. In the Average field the average of the current selected program can be set. It is appended to the name of the measurement program.

BreathSpec® – User Manual

The time span (hours, minutes, and seconds) between two program runs - more exactly between two program starts - is set in the “every” field. Hence the minimum time span to be entered here is the duration of the currently selected measurement program as displayed in the programs list. Depending on the used average the acquisition of spectra produces a large amount of data. The processing of this data can cause latency between program end and program restart of up to about 1 second.

6.6.3 Edit Measurement Programs

Each program consists of a list of chronological ordered steps, so called actions. The Selected Program Window displays the list of actions for the currently selected program. Each row in this list represents a step in the measurement program in which various changes to the device components are made.

Time	V1	R	E1	E2	P1
00:00, 000		rec	150.0 ^{ml} / _{min}	50.0 ^{ml} / _{min}	25%
00:02, 000	open				
00:05, 000	close				
30:00, 000		stop	150.0 ^{ml} / _{min}	50.0 ^{ml} / _{min}	
30:00, 020	_____	_____	_____	_____	_____

Figure 42: Selected Program Window

1	Time: Time point of action start
2	V1: Switch the Valve Position (open / close)
3	R: Start / Stop recording spectra (rec / stop)
4	E1: Flow rate control for EPC1 drift gas (0- 500 ml/min)
5	E2: Flow rate control for EPC2 carrier gas (0- 150* ml/min)

6	P1: The sample flow can be set in percent of the pump power (0- 100 %)
7	Selected program action line
8	End of Program line

**INFORMATION!**

The EPC2 maximum flow (carrier gas) of 150 ml/min is restricted by the installed column dimensions. It only can be attained with an installed column of the following diameter: 15 m length, 0.53 mm inner diameter. **Using the standard Column for BreathSpec the EPC2 maximum flow is limited to 80 ml/min.**

A value here determines the new state of the respective device component. A vertical line “|” indicates that the respective device component is not involved in this action.

The last row in this action list contains horizontal lines only. It indicates the end-of-program. The point of time of this end-of-program marker can be increased. This determines the duration of the program run.

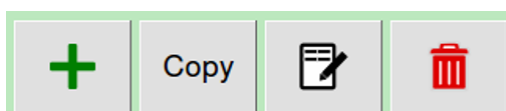


Figure 43: Selected Program Window Control Panel

With the buttons in the Selected Program Window Control Panel the currently displayed program can be created, modified, or deleted. A newly created action is positioned after the currently selected action. Pressing the **Copy** button copies the selected action and orders the copy behind the selected action. To maintain the chronological order of the actions the system may rearrange the actions by ordering them according to their numbers later. By pressing the **Del** button, the currently selected action is deleted. Pressing the **Edit** button or the **New** button opens the Edit Action dialogue.

6.6.4 Flow Ramps

The flow rate set points in a measurement program determine the target flow rates at the specified time index. If set points differ from the default flow rate or varying flow rate set points are specified in a program, the course of the actual flows will be conducted as a linear ramp of the flow. Starting point of the ramp is the latest set point. If no earlier set point is given the ramp starts with program initialization using the default set point.

An exemplary program using a dynamic flow rates is visualized in the following figure:

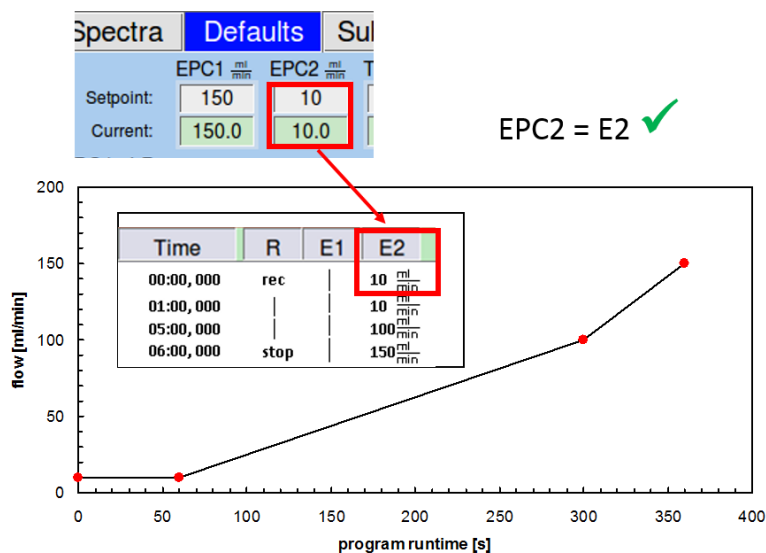


Figure 44: Flow Ramps

The E2 (carrier gas flow) value is initially set to 10ml/min. The flow is kept constant for one minute. Between runtime 1min – 5min the flow is linearly increased to the target value 100ml/min. In the following the flow is increased linearly to 150ml/min in one minute.



INFORMATION!

Before starting a measurement make sure that the highest flow set points can be achieved. Note that large changes in the flow set points will need finite time.



INFORMATION!

Please make sure that default values of EPC1 and EPC2 (Default window) corresponds with the start value of E1 and E2 in the program, otherwise the reproducibility of the measurement cannot be guaranteed.



INFORMATION!

Make sure that the EPC2 start pressure is reached again at the beginning of the next program run.

RECOMMENDATION:

Make sure that the initial flow at EPC2 is kept constant during the first 60 seconds after injection before starting a flow ramp, especially when a low flowrate is chosen.

6.7 System Window

In the System Window system specific information are displayed and can be set.

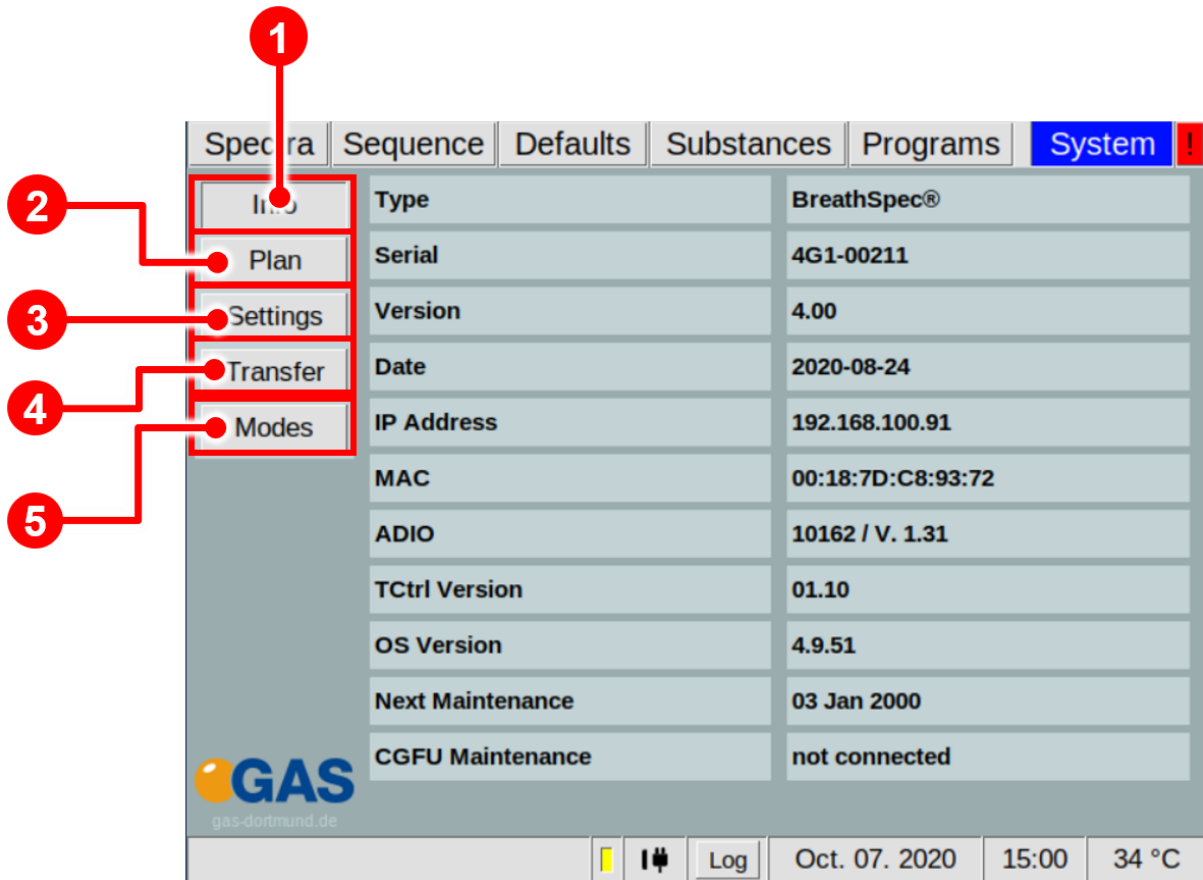


Figure 45: Operating Interface - System Window

1	Info Button	Displays the System Information Window
2	Plan Button	Displays the Device Plan Window
3	Settings Button	Displays the Settings Window. Various device parameter like Export Setting, Livedata output, Device attributes can be set.
4	Transfer Button	Displays the current data transfer settings. Data transfer settings can be set.
5	Modes Button	Special application modes can be set.

6.7.1 System Info Window

Tab	Field	Value
System	Type	BreathSpec®
System	Serial	4G1-00211
System	Version	4.00
System	Date	2020-08-24
System	IP Address	192.168.100.91
System	MAC	00:18:7D:C8:93:72
System	ADIO	10162 / V. 1.31
System	TCtrl Version	01.10
System	OS Version	4.9.51
System	Next Maintenance	03 Jan 2000
System	CGFU Maintenance	03 Jan 2000

Info | Plan | Settings | Transfer | Modes

Log | Oct. 07. 2020 | 15:00 | 34 °C

Figure 46: Operating Interface - System Info Window

1	Type	Device type.
2	Serial	Device Serial Number.
3	Version	Current Firmware Version.
4	Date	Date of current Firmware Version.
5	IP-address	Displays the current IPv4-Address.
6	Next Maintenance	Displays the next maintenance date.

7	CGFU Maintenance	Displays the next maintenance date (only if available!)
----------	-------------------------	--

6.7.2 System Plan Window

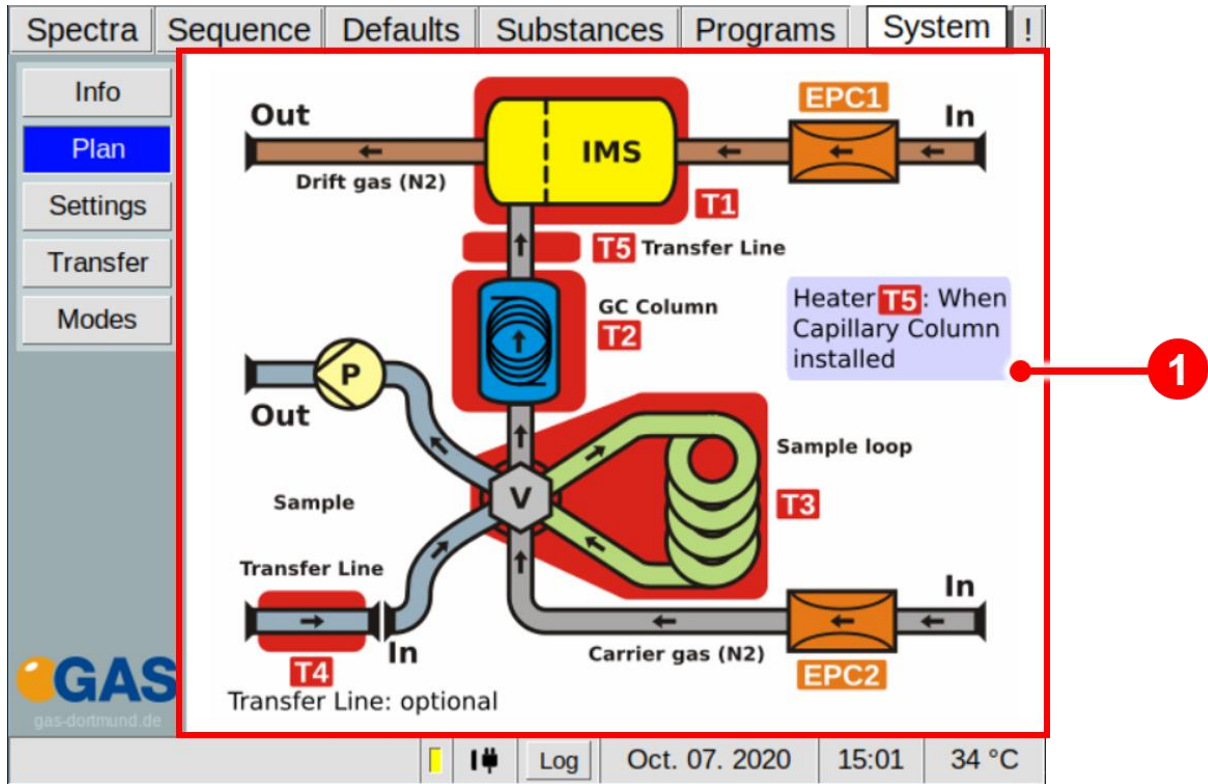


Figure 47: Operating Interface - System Plan Window

1	Plan	Displays an overview plan of the device
----------	-------------	---

6.7.3 System Settings Window

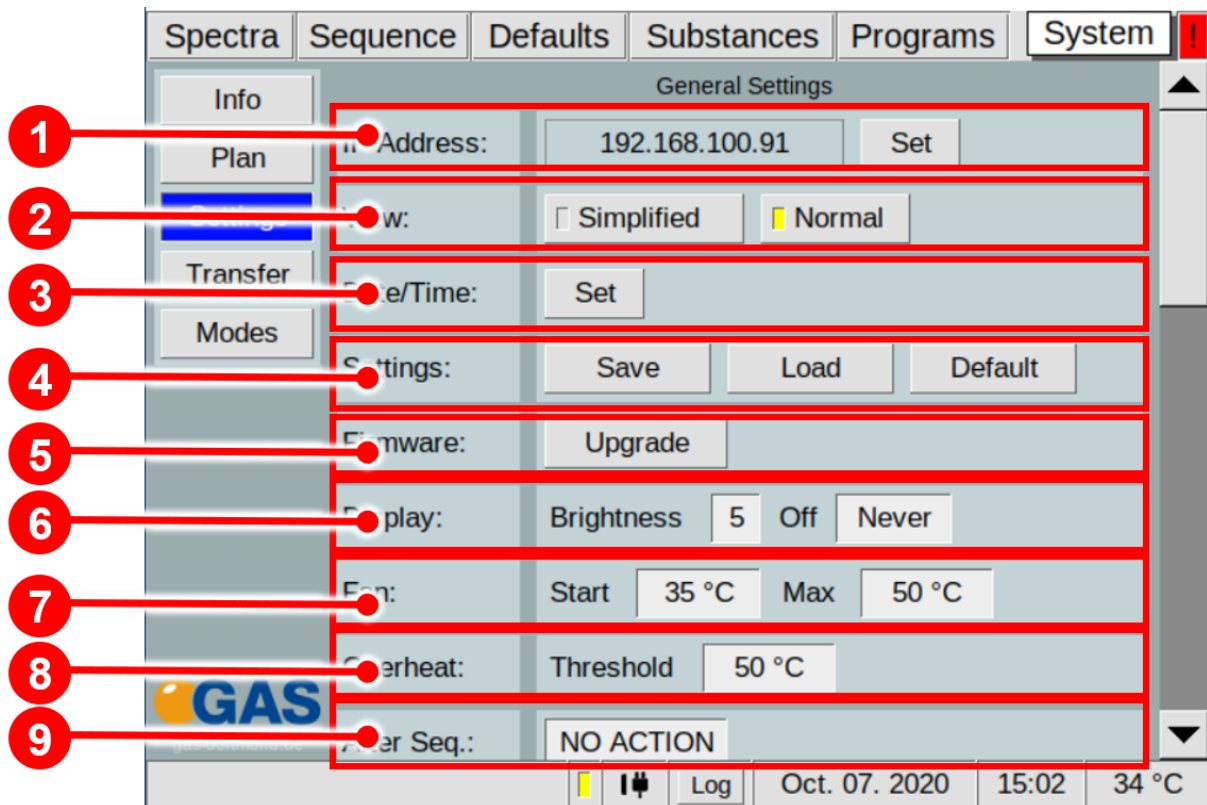


Figure 48: Operating Interface - System Settings Windows 1

1	IP Adress	Displays the current set IPv4-Adress of the device. With Set-Button the IPv4-adress can be set
2	View	Toggles between simplified and normal view.
3	Date/Time	With Set-Button the Date and Time can be set
4	Settings	<p>Save Button: The system settings can be saved to a connected USB volume.</p> <p>Load Button: The system settings can be loaded from a connected USB volume.</p> <p>Default Button: Resets all system settings to factory default values. All measurement-programs and substance-entries set by user will be deleted.</p>

5	Firmware	With Upgrade-Button a firmware upgrade can be performed from a connected USB volume.
6	Display	The display brightness and screen-saver time-out can be set.
7	Fan	The behaviour of the cooling fan can be set. When the temperature inside the device reaches the temperature in the field Start the cooler fan starts working. The power of the cooler fan is increased up to the desired temperature of the value in the field Max.
8	Overheat	The threshold temperature for the overheat alarm can be set.
9	After Seq.:	The After Sequence Action can be set. The following options are available: No Action, Cleaning, Standby, Custom.

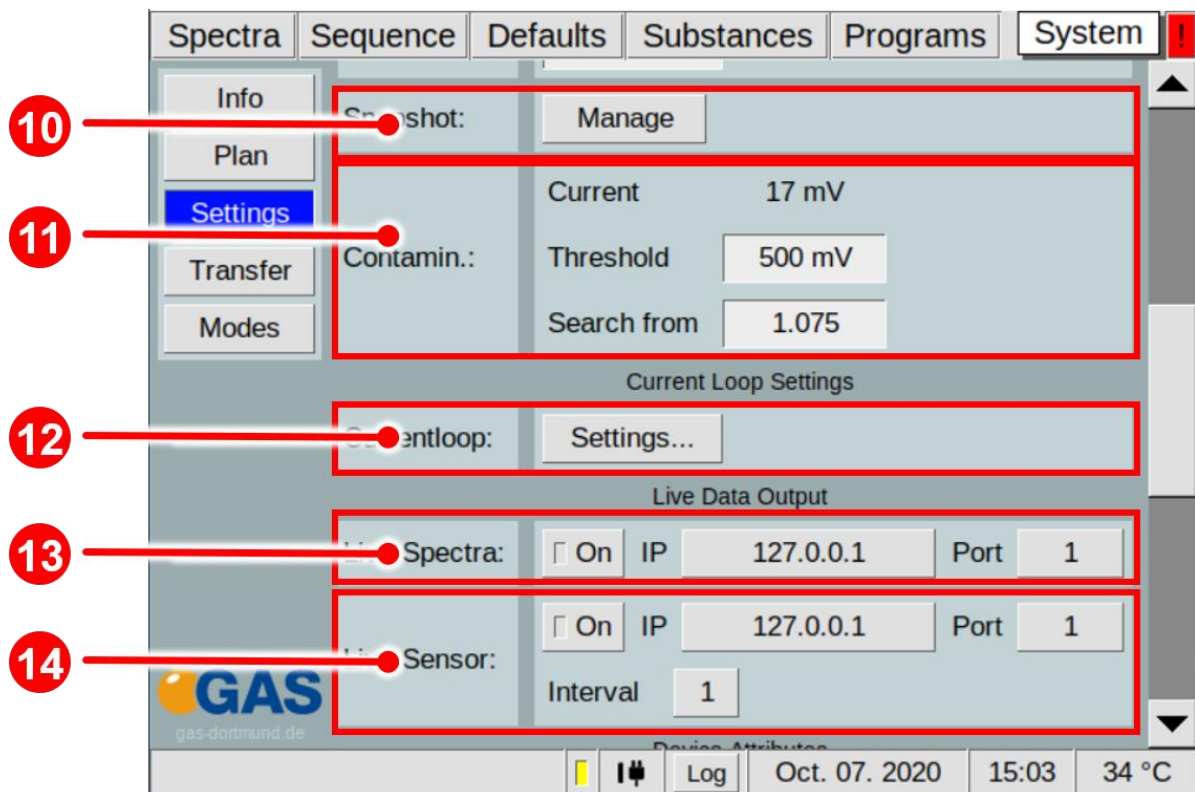


Figure 49: Operating Interface - System Settings Window 2

10	Snapshot	<p>The Manage Button opens <u>the</u> snapshot window. User-specific target values can be set. A new snapshot can be recorded or can be imported</p> <p>Snapshot is a new function to allow automatic instrument performance checking</p>
11	Contamin	<p>Define the automatic search area for contamination. The search window can be defined by setting the Threshold (signal level in mV which is recognised as a contamination) and the Start of the search in the drift-time spectrum given as RIP relative proportional factor.</p> <ul style="list-style-type: none"> • Current: Shows the currently detected contamination Shows the currently detected contamination. • Threshold: The set value from which an error is triggered. <p>Search from: The RIP-relative starting position of the search.</p>
12	Current Loops (optional)	<p>Activating the Settings Button opens a current loop setup dialog (only visible if available)</p>
13	Live Spectra:	<p>Prepared for further use! Currently not in function!</p>
14	Live Sensor:	<p>The settings for Live Data communication with G.A.S. Sequence Designer Software can be set. For detailed Information refer to the G.A.S. Sequence Designer Software Manual.</p>

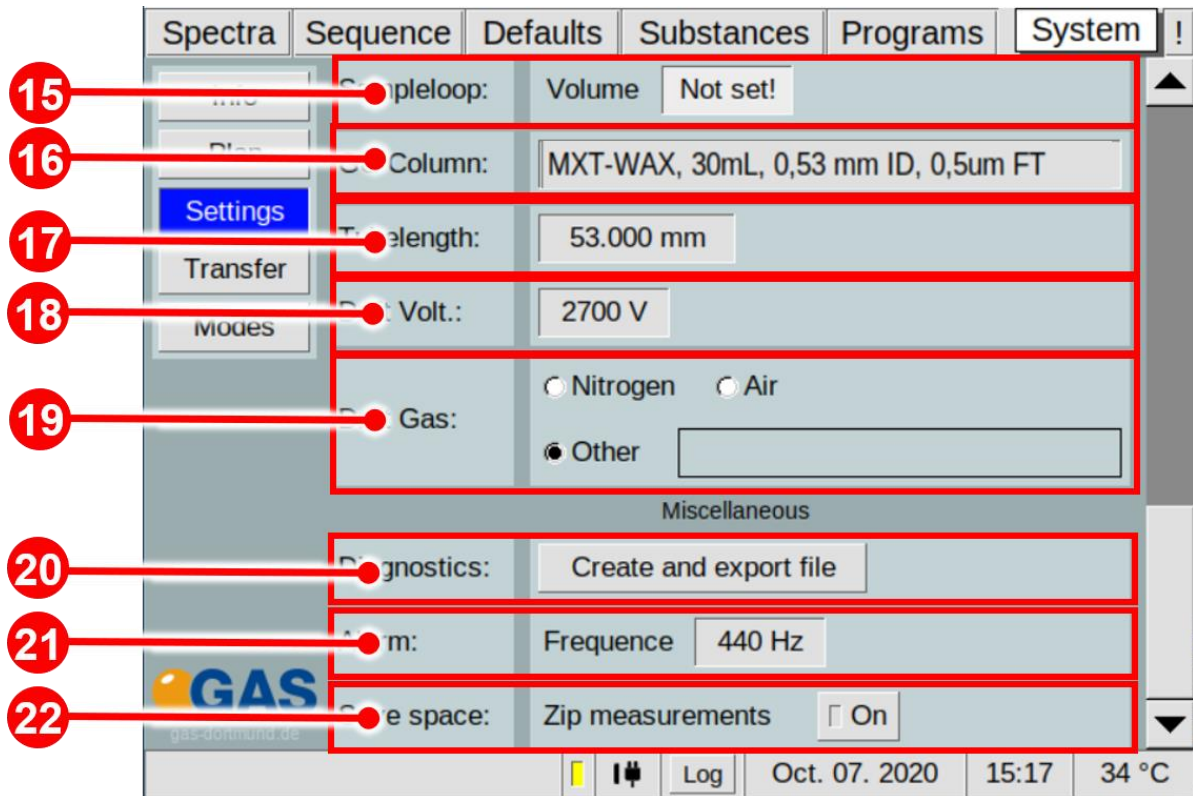


Figure 50: Operating Interface - System Settings Windows 3

15	Sampleloop:	The Sample Loop Volume can be set. This data is stored in the metadata of the measurement. The standard value is 1000 µl.
16	GC Column:	Input filed for Column ID. The value is stored with measurement file. This data is stored in the metadata of the measurement.
17	Tubelength:	Prepared for further use! Currently not in function!
18	Drift Volt.:	Prepared for further use! Currently not in function!
19	Drift Gas:	Selection field for operating gas type. The value is stored with measurement file.
20	Diagnostics:	With Create and export file-Button an encrypted diagnostic file is created for diagnostic purposes by G.A.S..

21	Sound:	The frequency of the warning sound can be set.
22	Compression:	Compresses the measurement data to zip

6.7.3.1 Snapshot Window

The instrument performance and status can be monitored using recorded snapshots. It is an automatic comparison of current instrument settings versus the operator defined target settings which helps the operator to assess the readiness of the system for starting a measurement. This automatic monitoring can recognize among other a System contamination, insufficient gas quality or system leaking. For this purpose, the following parameters are constantly cross-checked against the target-settings:

- The carriergas pressure - EPC2 pressure (kPa)
- The height of the Reaction-Ion-Peak (RIP) - Rip-height (V)
- The position of the Reaction-Ion-Peak (RIP) normalized to normal pressure – Rip Pos at 101.33 kPa (ms)
- The full width at half maximum of the Reaction-Ion-Peak - FWHM (ms)
- The temperature values T1-T6
- The gasflow and pressure of Driftgas (EPC1) and Carriergas (EPC2)

The user can change the default factory settings for his needs. Error messages are displayed in the Error Information Window.

The screenshot shows the 'Snapshot' window interface. It is divided into several sections:

- Checked Values:** A table comparing snapshot values with current values and their percentage deviation.

Name	Snapshot Value	Current Value	%
EPC2 Pressure [kPa]	120.096	120.096	100.00%
Rip Height [V]	6.746	6.737	99.87%
Rip Pos at 101.33 kPa [ms]	4.522	4.522	100.00%
FWHM [ms]	0.106	0.106	100.00%
- Edit Thresholds:** A section for editing setpoints.
- Setpoints:** A table for defining target values.

Name	Setpoint	Snapshot
T1 [°C]	45	45
T2 [°C]	40	40
T3 [°C]	80	80
T4 [°C]	80	80
T5 [°C]	45	45
- Buttons:** 'Take new Snapshot', 'Import Snapshot', and 'Done' buttons are located at the bottom.

Numbered callouts (1-6) point to specific elements: 1 points to the 'Checked Values' table; 2 points to the 'Edit Thresholds' section; 3 points to the 'Setpoints' table; 4 points to the 'Take new Snapshot' button; 5 points to the 'Import Snapshot' button; 6 points to the 'Done' button.

Figure 51: Operating Interface – Snapshot Window

1	Checked values Area	The checked Snapshot values (EPC2 Pressure; Rip Height, Rip-Position at 101,33 kPa, Rip-half-value width FWHM are displayed.
2	Edit Threshold	The selected Snapshot values (EPC2 Pressure; Rip Height, Rip-Position at 101,33 kPa, Rip-half-value width FWHM can be edited.
3	Setpoints Area	Display of the current setpoints and the corresponding snapshot values.
4	Take new Snapshot Button	Take a new snapshot of the current system status.
5	Import Snapshot Button	Import a Snapshot-file with prepared values by G-A.S.
6	Done Button	Closes the snapshot window

6.7.3.1.1 Snapshot window in detail

The system is delivered with standard limits for EPC2-Pressure, RIP-Height, RIP Position at 101.33 kPa and FWHM. The upper and lower limits of these parameters r can be adjusted by the customer.

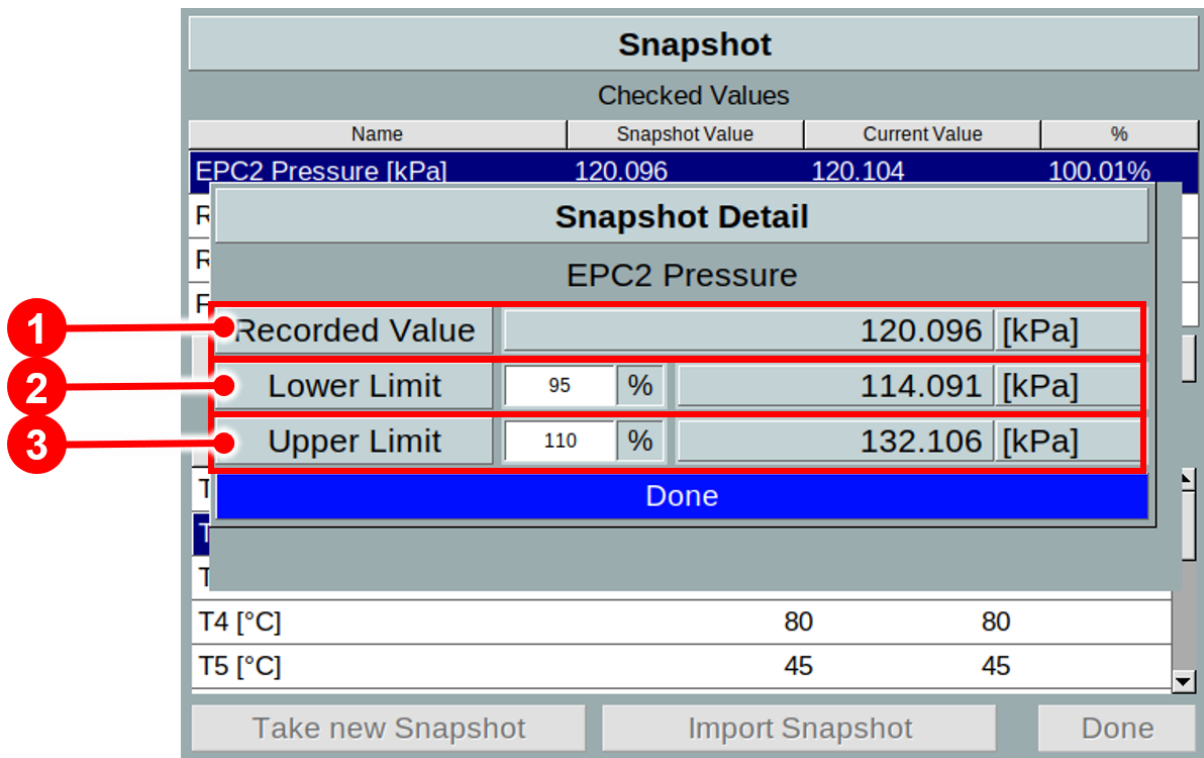


Figure 52: Operating Interface – Snapshot Window in detail (example EPC2 pressure)

1	Recorded Value	Displays the current recorded snapshot value (Example EPC2 pressure).
2	Lower Limit	The lower limit of the current recorded snapshot value (Example EPC2 pressure) is displayed. This limit can be specified by the user.
3	Upper Limit	The upper limit of the current recorded snapshot value (Example EPC2 pressure) is displayed. This limit can be specified by the user.

Factory default limits

Name	Lower limit (%)	Upper limit (%)
EPC2-Pressure (kPa)	95	110
RIP Height (V)	80	150
RIP Position at 101.33 kPa (ms)	95	105
FWHM (ms)	80	120

**INFORMATION!**

The device is delivered with an acceptance snapshot. This snapshot defines the system performance during device acceptance and is used to assess the readiness for measurement. Any deviations from this are displayed in the Error Information Window. **The default values can be adjusted by the customer.**

6.7.3.2 Simplified View Window

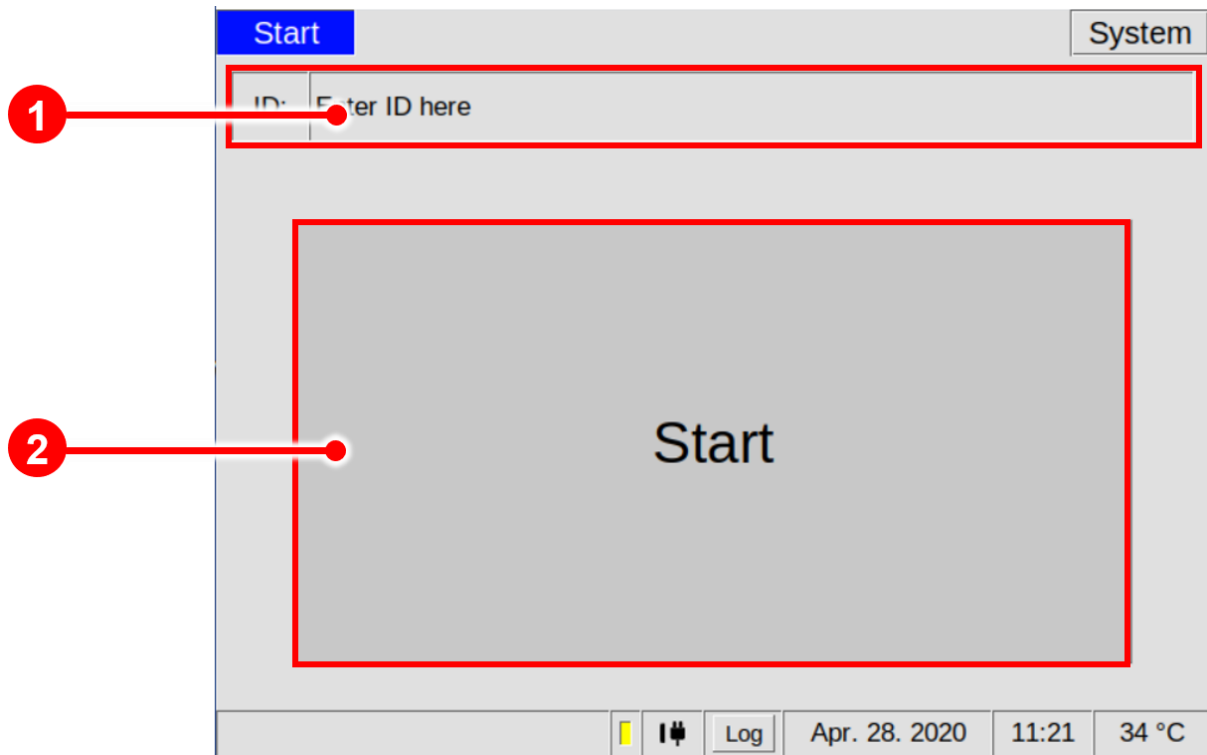


Figure 53: Operating Interface - Simplified View Window

1	ID	A measurement identification can be specified by the customer.
2	Start Button	By selecting this button, the current program is initialized.

6.7.4 System Transfer Window

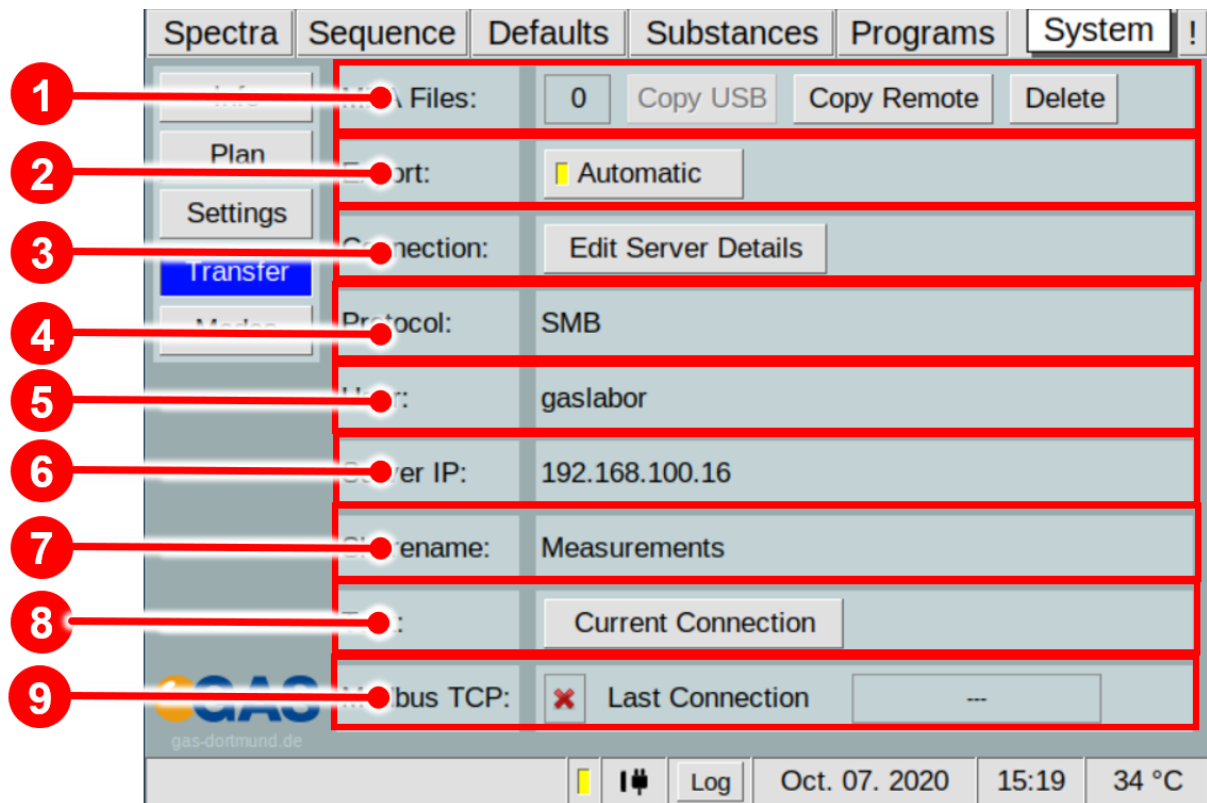


Figure 54: Operating Interface - System Transfer Window

1	MEA Files:	The current number of internal stored measurement files and the following measurement file managing options are displayed and available: Copy to USB: Copy all internal stored measurements to a connected USB device. Copy to remote: All internal stored measurement files will be copied to the connected shared folder. Delete: Deleting all internal stored measurement files.
2	Export:	Activating the automatic storage to a connected shared folder on a network as storage location for measurements.
3	Connection:	With Edit Server Details Button the Export settings (transfer protocol, IPv4-adress, shared folder name) can be set.

4	Protocol:	Displays the current used transfer protocol (smb , sftp or fttp).
5	User:	Displays the current used username.
6	Export:	Displays the current used IPv4-address.
7	Sharename:	Displays the current used sharename of the storage folder.
8	Test:	With Current Connection button the device tries to establish to the shared folder using the current export settings. A message will appear to indicate if the connection was successful.
9	Modbus TCP	The last Modbus TCP connection can be checked. It will give you information on when and from which IP the last connection was made and whether it is still active.

6.7.5 System Modes Window

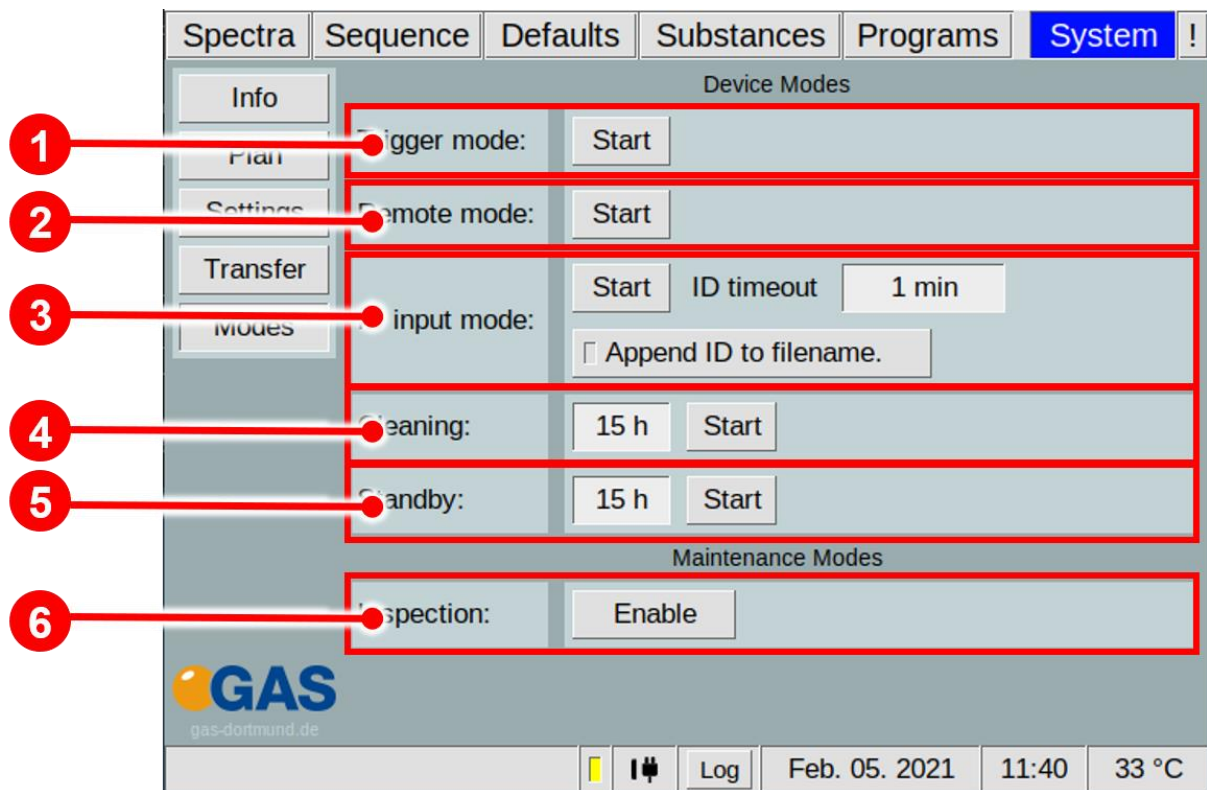


Figure 55: Operating Interface - System Modes Window

1	Trigger mode: (only System 4G2)	Activate trigger mode with Start .
2	Remote mode:	Activate remote mode with Start .
3	ID Input mode: (only System 4G2)	<p>Sets the system to trigger mode to control the system via a μTD:</p> <ul style="list-style-type: none"> • Activate the ID Input mode with Start. The ID Input Mode window appears. • In ID Timeout, the validity period for the ID can be entered. The measurement must be started within this time. • To append the ID to the filename activate Append ID to filename

<p>4</p>	<p>Cleaning:</p>	<p>Setup and activate of cleaning mode. With Start-Button the cleaning process is activated and the Cleaning Mode Window appears. Possible Values: (1-96 hours or infinity) Activate Cleaning Mode with Start.</p>
<p>5</p>	<p>Standby:</p>	<p>Setup and activate of standby mode. With Start-Button the standby process is activated and the Standby Mode Window appears. Possible Values: (1-96 hours or infinity). Activate Standby Mode with Start.</p>
<p>6</p>	<p>Inspection</p>	<p>With Enable-Button the access to the inspection and diagnostic functions of the device is allowed.</p>

6.7.5.1 Trigger Mode Window (only System 4G2)

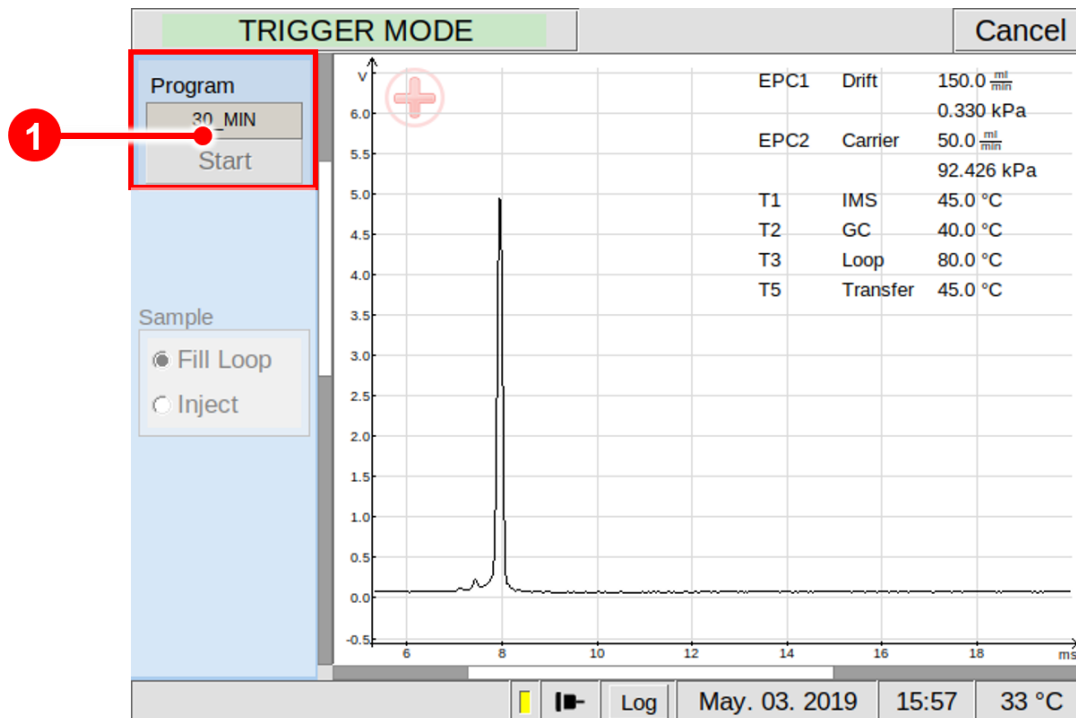


Figure 56: Operating Interface - Trigger Mode Window

<p>1</p>	<p>Program Start Area</p>	<p>In Trigger mode the displayed program is started by a connected device (e.g. μTD) that operates as master device.</p>
-----------------	----------------------------------	---

6.7.5.2 Remote Mode Window

By activating the Remote Mode, the **Remote Mode Window** appears. The window is initially empty. The device is waiting for a sequence file to import.



INFORMATION!

The sequence file must be created with the **G.A.S. Sequence Designer Software**. For detailed Information refer to the **G.A.S. Sequence Designer Software Manual**.

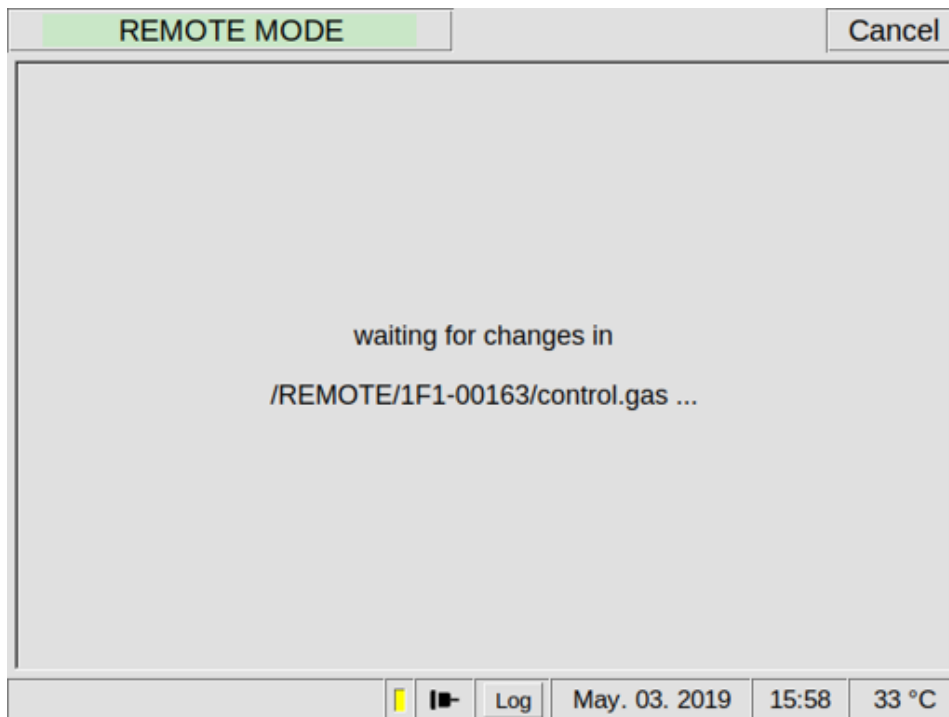


Figure 57: Operating Interface - Remote Mode Window

6.7.5.3 ID Input Mode Window (only System 4G2)

By activating the ID Input Mode, the **Remote Mode Window** appears. A measurement identification must be set. The device is waiting for an external trigger signal (e.g. from μ TD).

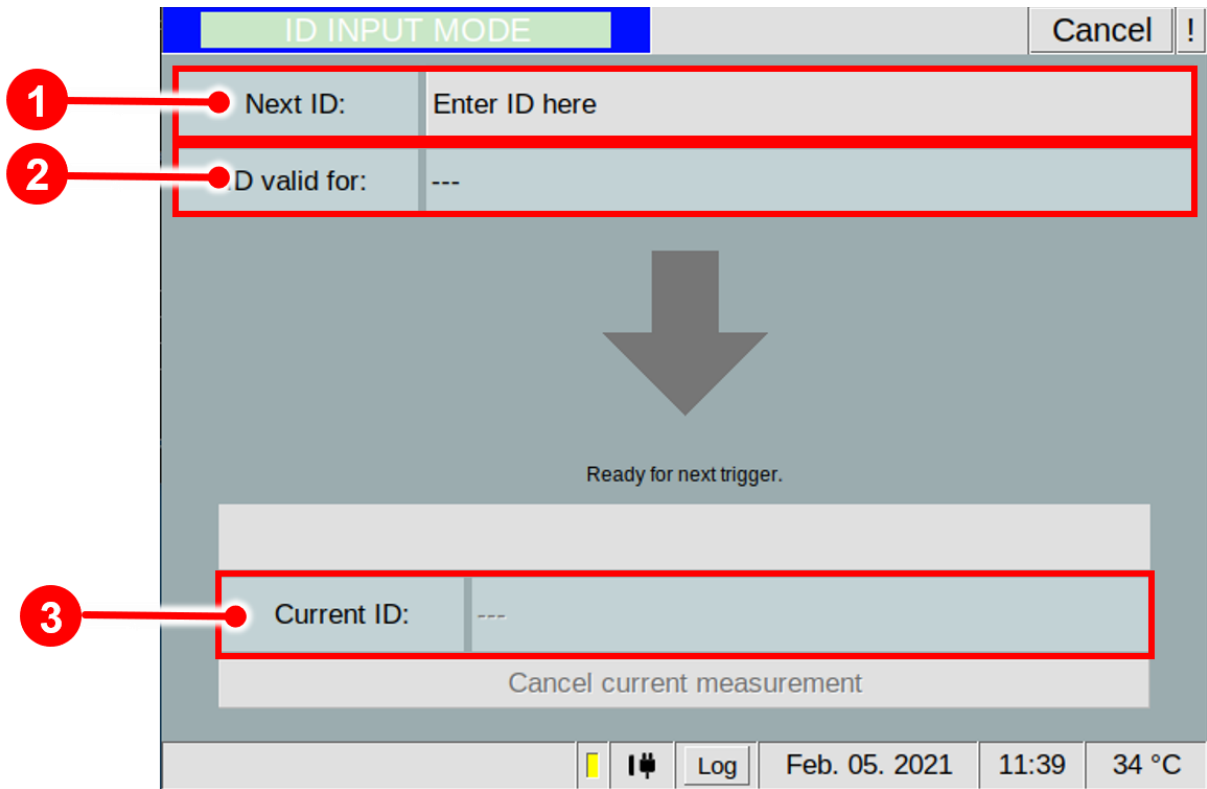


Figure 58: Operating Interface - Simplified View Window

1	Next ID:	A measurement identification must be set.
2	ID valid for:	The set validity period is displayed
3	Current ID:	The current ID is displayed for the current measurement.

6.7.5.4 Cleaning Mode Window

By activating the Cleaning Mode, the **Cleaning Mode Window** appears. During the cleaning process the available system temperatures (T1-T6) are heated up to their maxima. The user default flow rates settings for Driftgas (EPC1) and Carriergas (EPC 2) setup in Defaults window are used. After the setup time has expired the cleaning process is terminated.

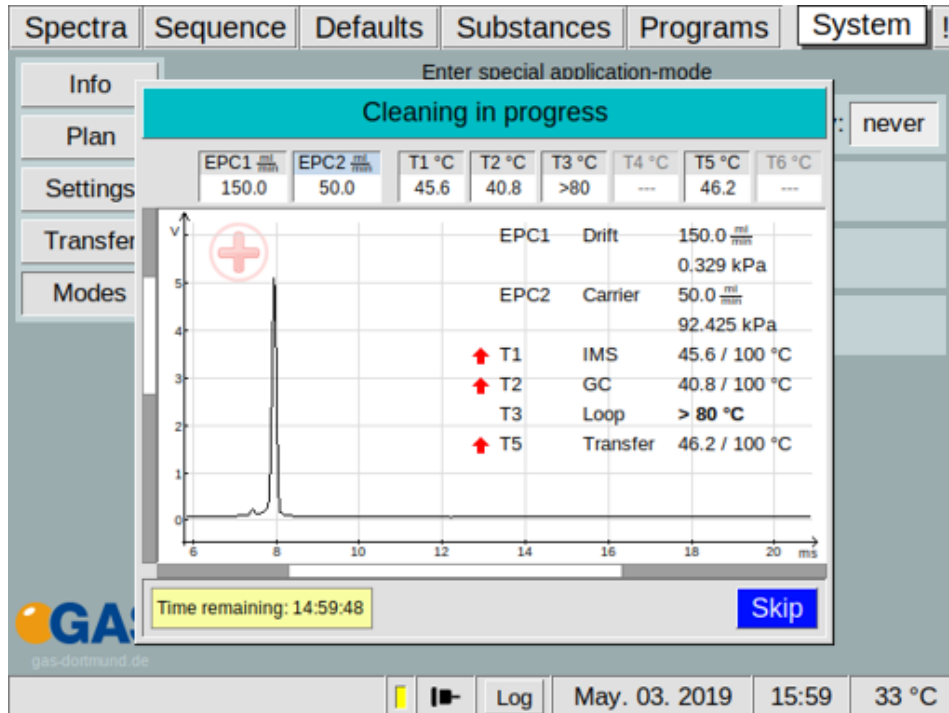


Figure 59: Operating Interface - Cleaning Mode Window



INFORMATION!

During the cleaning process the available heating module temperature (T1-T6) are set to their maxima. Values of more than 80 °C are displayed as >80°C.

6.7.5.5 Standby Mode Window

By activating the Standby Mode, the **Standby Mode Window** appears. The flowrate of the Drift gas (EPC1) and the carrier gas (EPC2) will be decrease to reduce gas consumption. The **standby mode flowrate** for drift gas (EPC1) is 10 ml/min and for carrier gas (EPC2) is 5 ml/min.

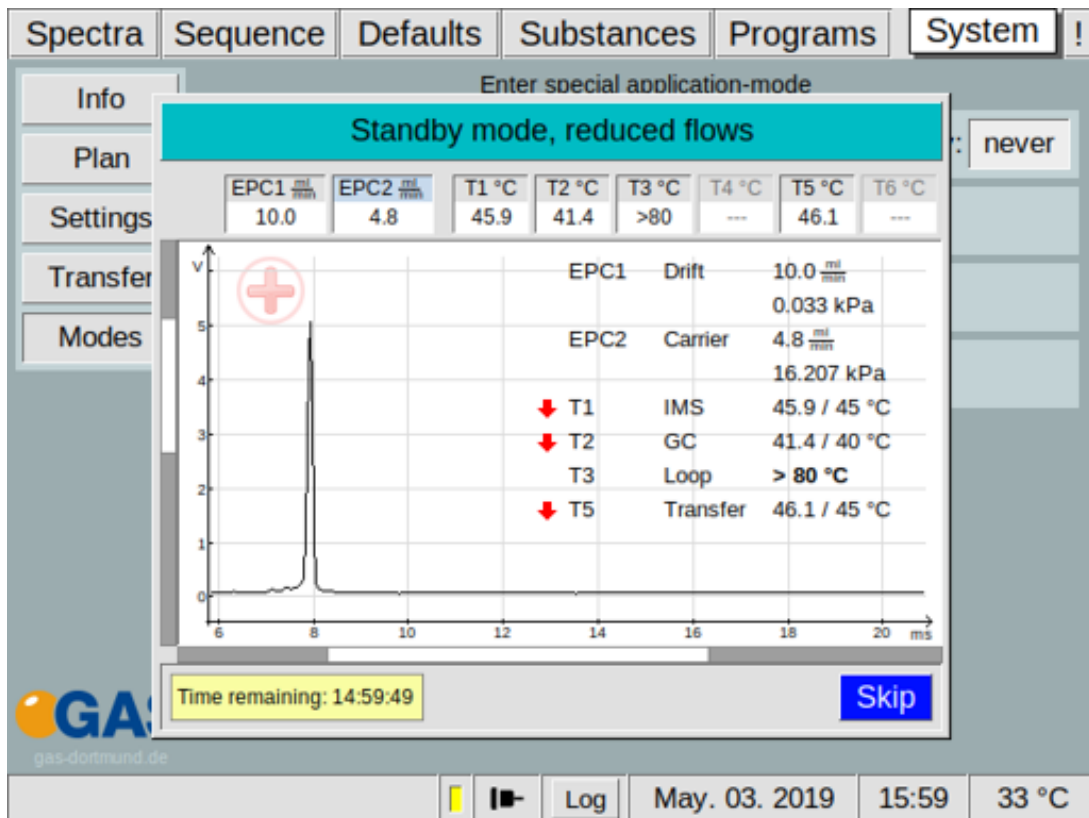


Figure 60: Operating Interface - Standby Mode Window

6.8 Error Information Window

In case if an Error the **I-Tab** is blinking red. The error window shows an overview of the current error events. When the device is restarted, the error events are deleted.

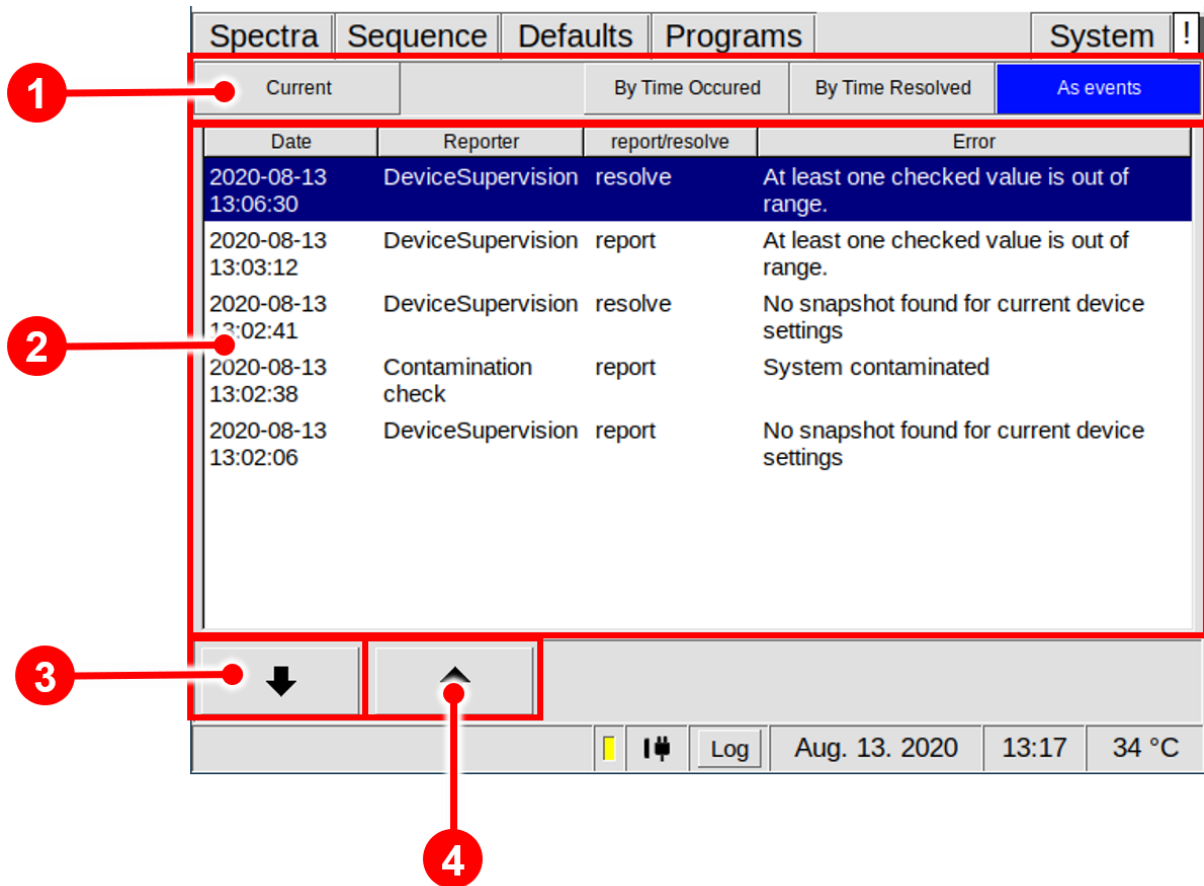


Figure 61: Error Information Window

1	Selection Sort Order Bar	Selects the following sort order: Current ; By Time Occurred ; By Time Resolved ; As Event
2	Entry List	A list of system event messages. The display depends on the selected sort order
3	Down Button	Scrolls one message down.
4	Up Button	Scrolls one message up.

6.9 Additional Dialog Windows

6.9.1 Log Messages Dialog Window

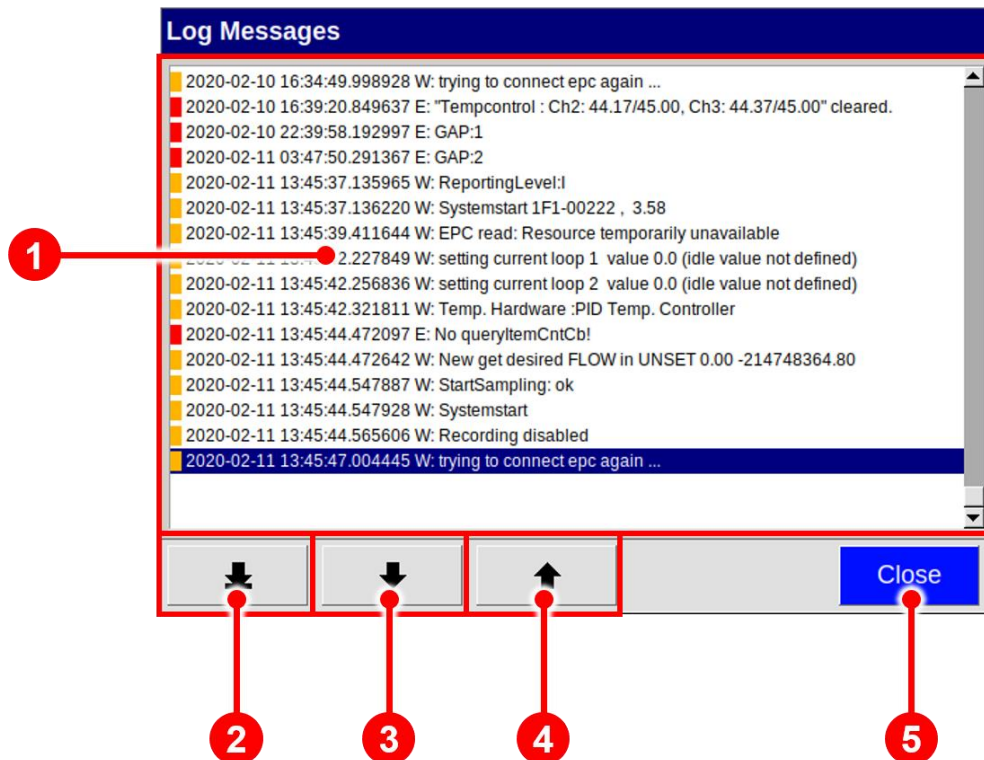


Figure 62: Log Messages Dialog Window

1	Entry List	A chronological list of system event messages. Warnings are marked orange, error messages are marked red.
2	To Last Entry Button	Scrolls down to the latest entry.
3	Page Down Button	Scrolls one page down.
4	Page Up Button	Scrolls one page up.
5	Close Button	Closes the dialog.

6.9.2 IP Address Input Dialog Windows

The IP Address Input Dialog is used to edit the static IP address of the device and the IP address of a remote server. This is necessary when configuring the LAN file transfer.

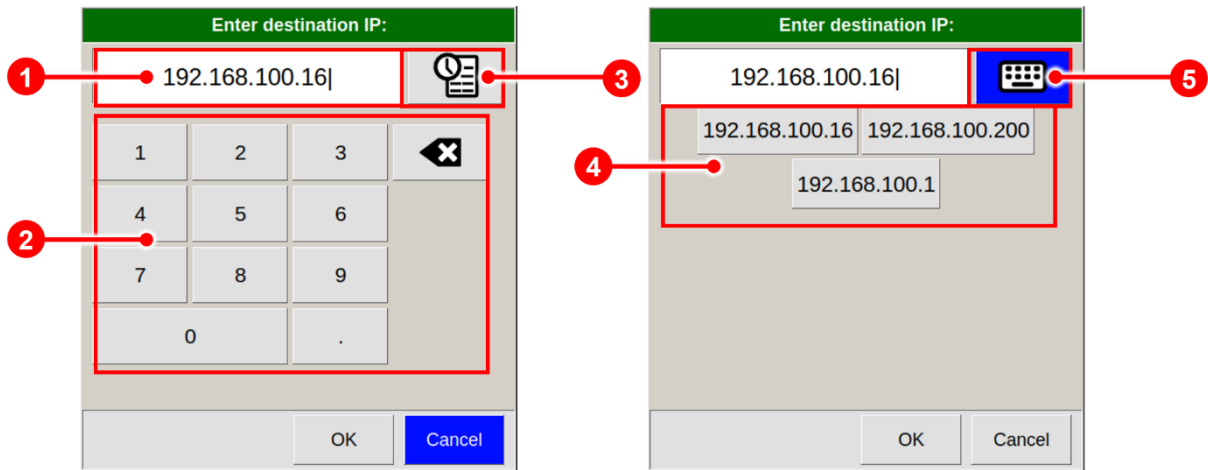


Figure 63: IP Address Input Dialog Windows

1	IP Address Field	The current IP address.
2	Digit and Dot Buttons / Backspace Button	Use these buttons to enter an IP address.
3	History Button	Displays a menu of previously used IP addresses to choose from.
4	History Entry Buttons	Buttons for entering previously used IP addresses.
5	Keyboard Button	Displays the keyboard.

6.9.3 Date and Time Input Dialog Window

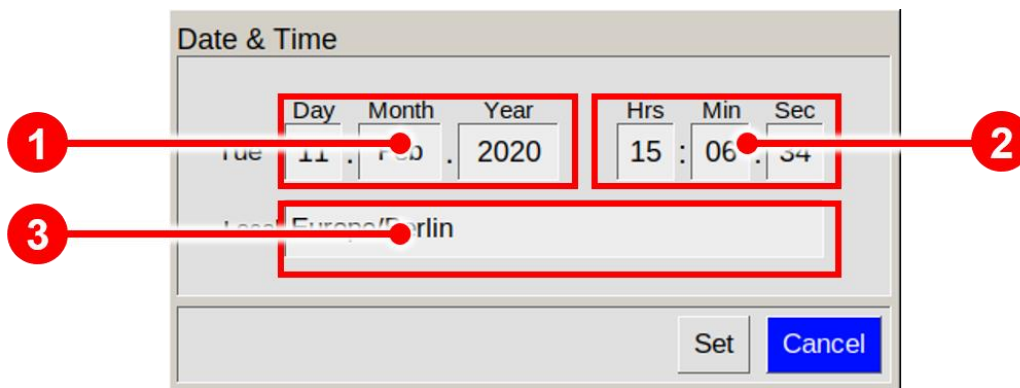


Figure 64: Date and Time Input Dialog Window

1	Date Fields	Fields displaying and modifying day, month and year.
2	Time Fields	Fields displaying and modifying hours, minutes and seconds.
3	Timezone	Field for selection of timezone.

6.9.4 Text Input Dialog Window

The Text Input Dialog is used to enter identifiers, e.g. shared folder name.

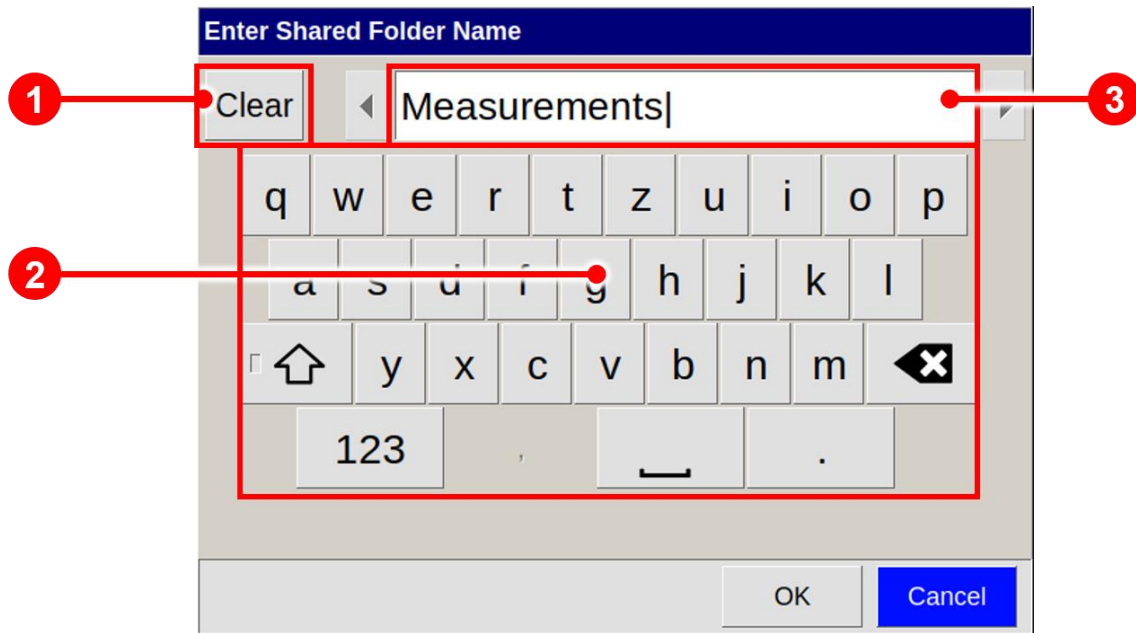


Figure 65: Text Input Dialog Window

1	Clear Button	Deletes the text in the current text field
2	Keyboard Buttons	Character and control buttons for entering a text. Depending on the context some buttons are disabled.
3	Current Text Field	The editable text.

6.9.5 Number Input Dialog Window

The Number Input Dialog is used in Program Window to enter number values, e.g. Start time, Flow Rates and Pump Power setpoints in Program Actions.

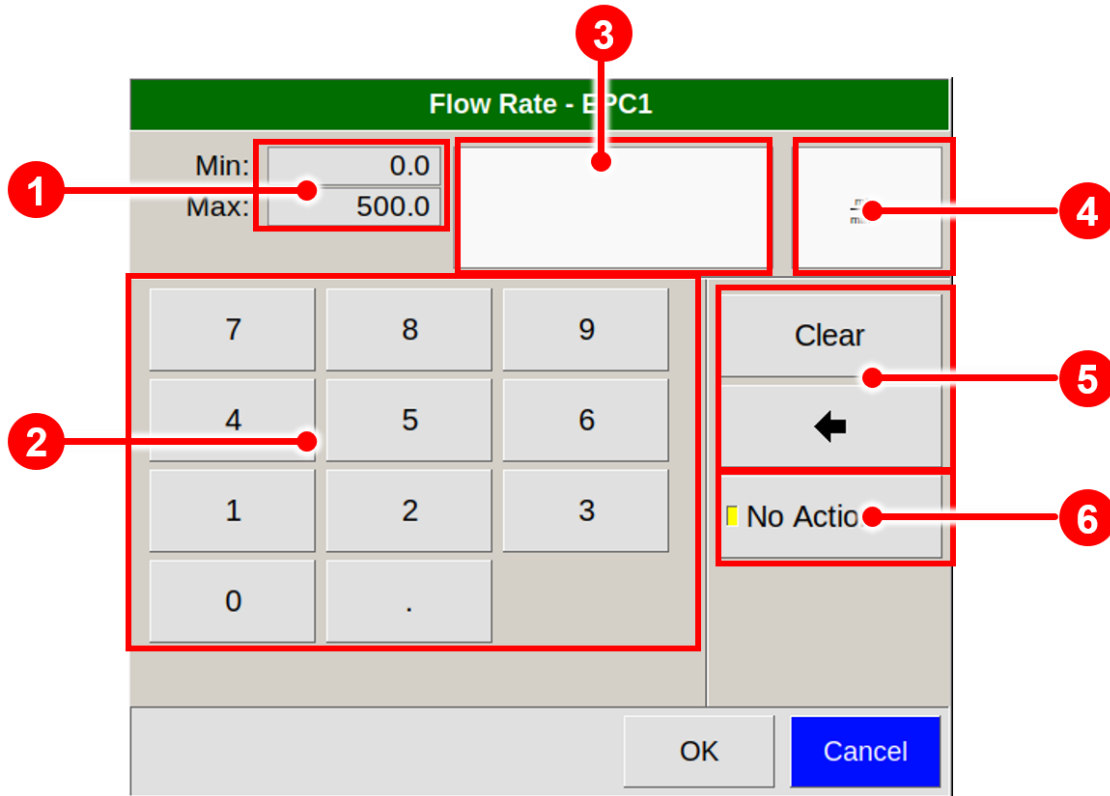


Figure 66: Number Input Dialog Window (Example)

1	Range / Raster Info	Displays the valid value range.
2	Keyboard Buttons	Buttons for entering a number.
3	Value Field	The entered numerical or selected special value.
4	Unit	Value unit name.
5	Clear and Backspace Button	Buttons for clearing the input field or deleting the last digit.
6	Dedicated Values Buttons	Dedicated value like No Action (only if available)

7 Installation BreathSpec® Device (Version 4G1) with Ciruclar Gas Flow Unit (CGFU)

7.1 Installation Requirements

The following requirements must be fulfilled by the customer:

Location of Installation

- Available space of 600 x 700 x 300 mm (W x D x H)
- Ambient temperature of 5 – 40 °C
- Humidity: 0-90 % RH, non-condensating

Electricity

- Electricity supply free of interferences
- Power Supply of 230 V \pm 10%, 50- 60 Hz \pm 1%

Safety

- Availability of exhaust system for device exhaust gas tube (Sample Gas out)

Computer

- Computer with current Microsoft Windows operating system
- Administrator right to install G.A.S. software



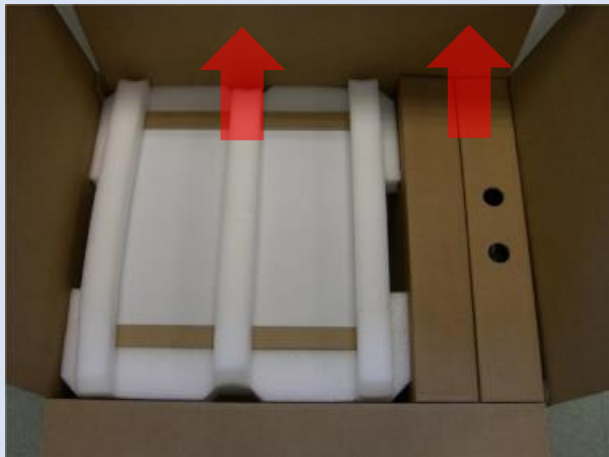
INFORMATION!

To ensure correct measurements it is necessary to **connect the supplied exhaust tube** (Sample gas out).

The exhaust system must **not generate any negative pressure.**

7.2 Installing the device

1



Unpack the device.

Remove the foam spacers.

Remove the accessories boxes.

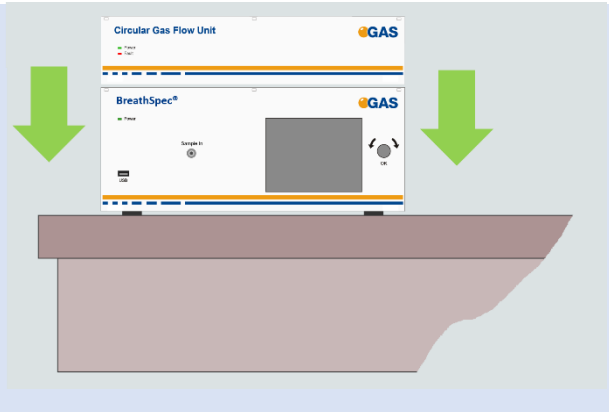
Lift the device from the transport box.



WARNING!

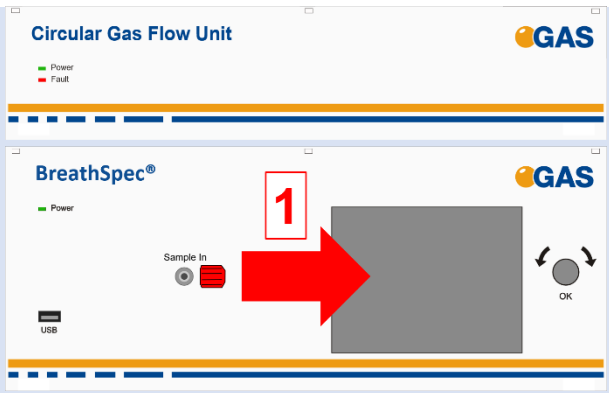
Do not deploy the device in areas exposed to explosive substances or mixtures!

2



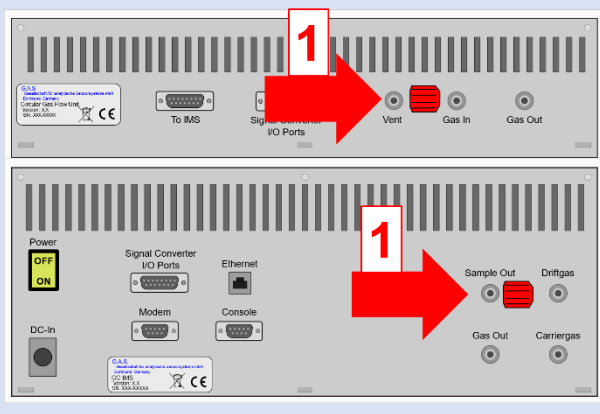
Place it on a robust tabletop of minimum footprint size of 60 cm x 70 cm. Ensure that there is enough working space at the rear side of the device.

3



Remove red protective cap from gas sockets at front of housing. Retain for future use.

4



Remove red protective caps from gas socket at rear of housing. Retain for future use.



INFORMATION!

Protective caps should be put on gas sockets in case the device is stored or transported.



WARNING!

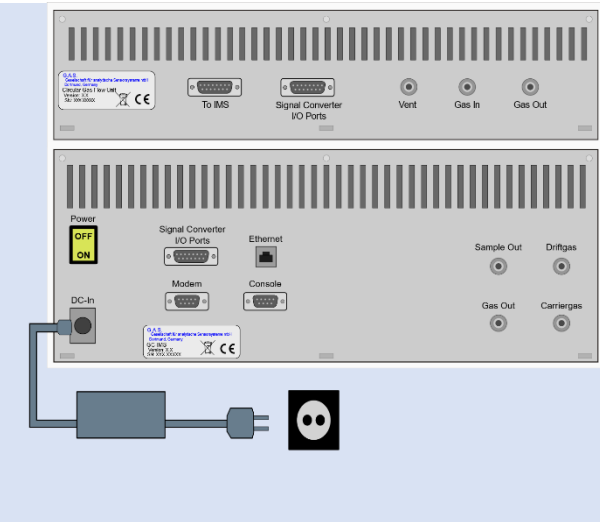
It is absolutely necessary to remove all protective caps before the system is switched on.



INFORMATION!

Gas tubes and GCFU Connection Cable are preinstalled.

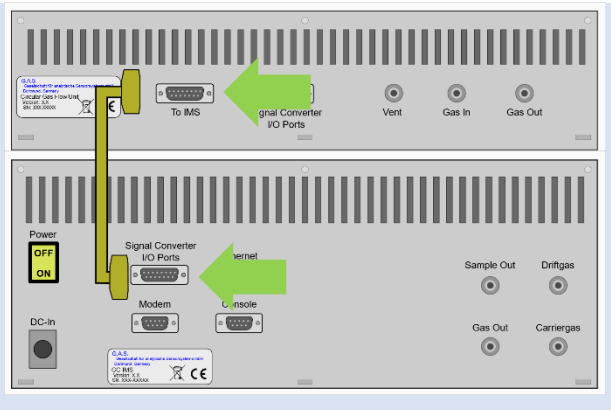
5



Connect device to power supply.

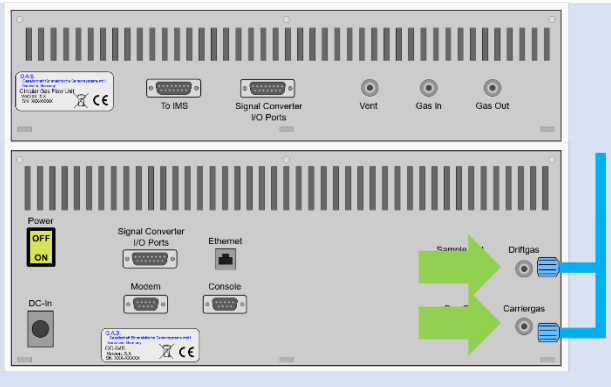
Connect power supply to power socket.

6



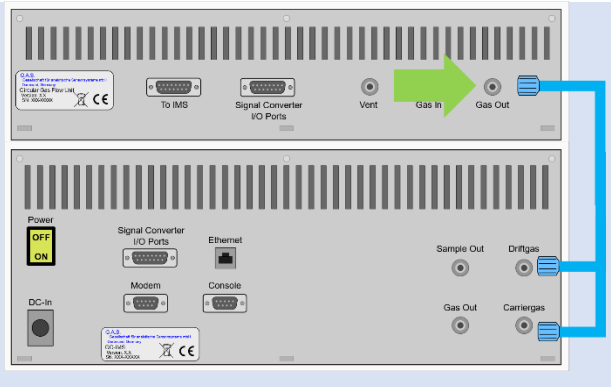
Connect CGFU-Connection-Cable.
(normally pre-installed!)

7



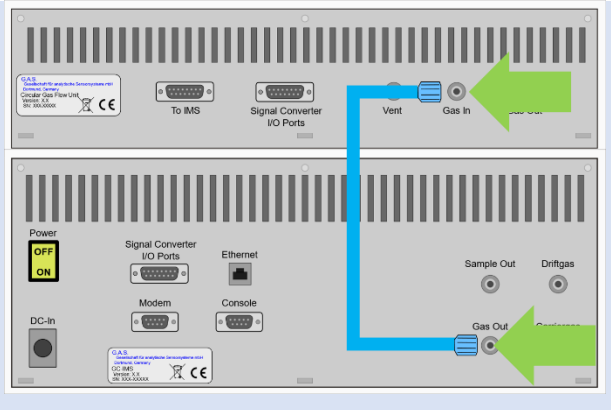
Connect the **Driftgas-/Carriergas-Adapter** to the **Driftgas-** and the **Carriergas-Connector**.
(normally pre-installed!)

8



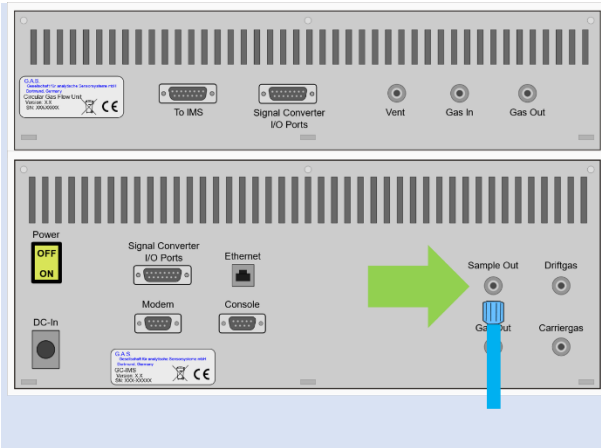
Connect CGFU **Gas Out** outlet to **Driftgas-/Carriergas-Adapter** using a PFA tube.
(normally pre-installed!)

9

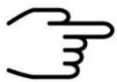


Connect CGFU **Gas In** inlet to GC-IMS **Gas Out** outlet using a PFA tube.
(normally pre-installed!)

10



Connect **Sample Out** to an appropriate waste gas ventilation system.



INFORMATION!

To ensure correct measurements it is absolutely necessary to **connect the supplied exhaust tube** (Sample out).

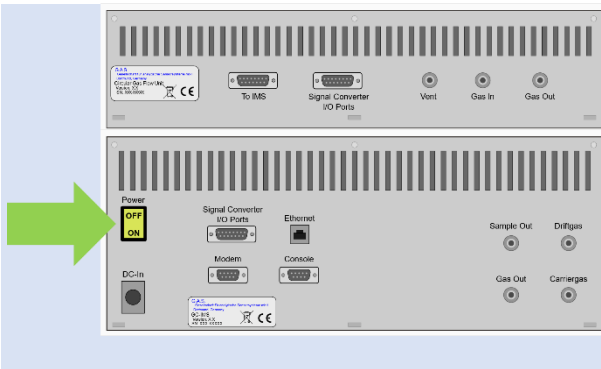
The exhaust system must **not generate any negative pressure.**

11

Connect the Sampling System:

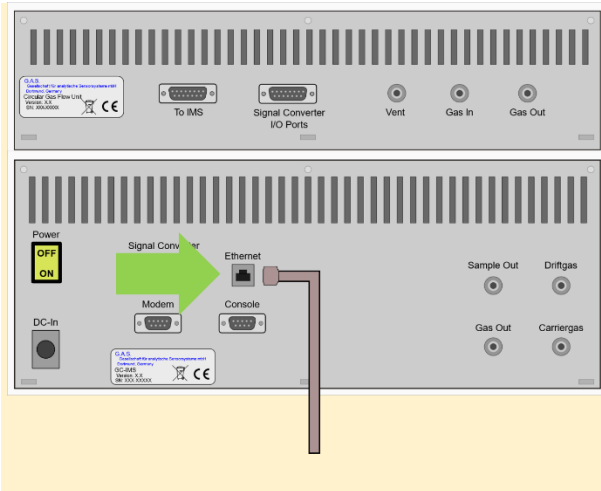
- Mouthpiece tube with heated transferline **see chapter 7.4**
- Heated Luer-Lock-Adapter **see chapter 7.5**

12

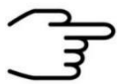


Switch on device.

13
Option



For file transfer via LAN:
Connect the **Ethernet** socket with an appropriate Ethernet cable to a LAN.



INFORMATION!

When using a CGFU unit the total flow (EPC1 and EPC2) is limited to 400ml/min.

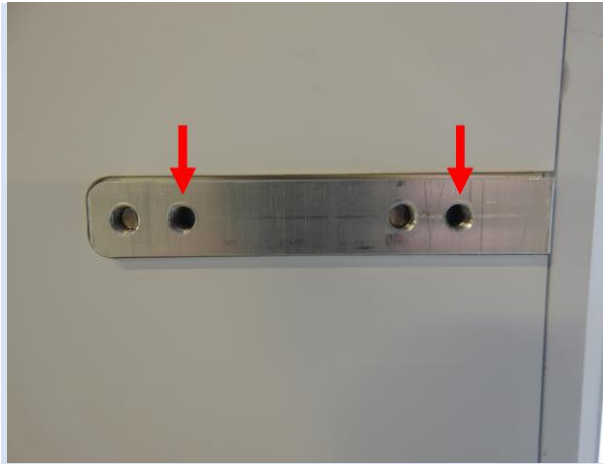
7.3 Mounting the Mouthpiece holder

1



Mouthpiece-Handheld holder arm with screws

2



For mounting the arm use the marked holes.

3



Mount the arm with a Torx screwdriver T30.

7.4 Connecting the Mouthpiece tube

1



Mouthpiece Handheld with heatable Transfer-line

2



Pull the screw upwards.

3



Remove the handling screw.

4



Connect the transferline to the sample-in connector.

5



Tighten the screw with a spanner.

6



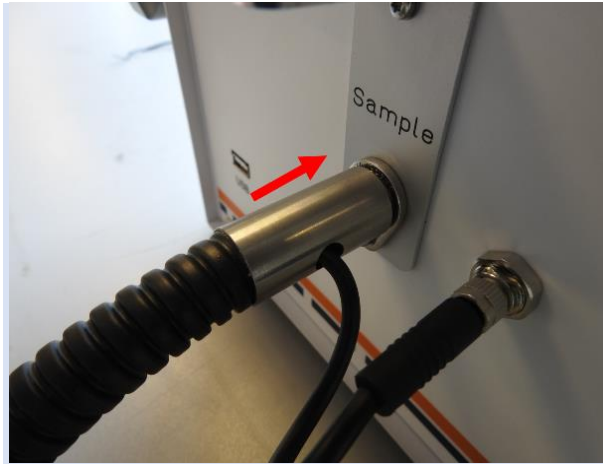
Connect the current supply cable.

7



Tighten the current supply cable.

8



Push the Transfer-line connector onto the **Sample in connector**.

9



Place the Mouthpiece handheld into the handheld holder.

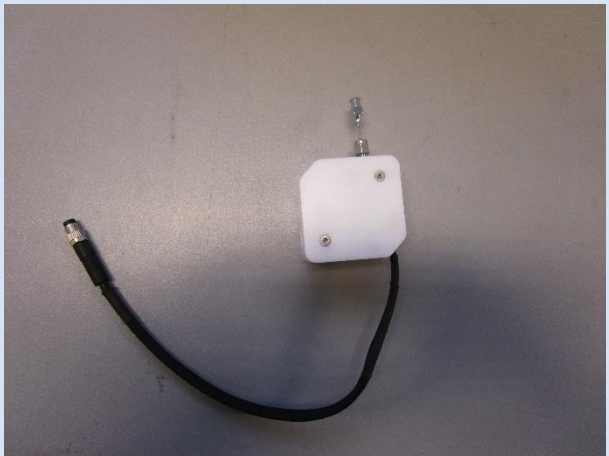
10



Switch on the BreathSpec.

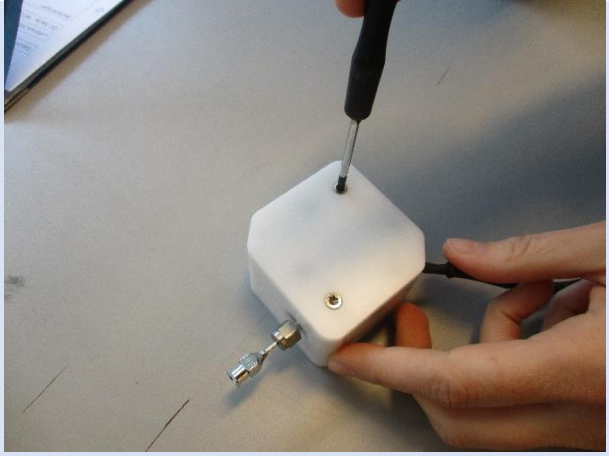
7.5 Installation of Luer-Lock adapter [optional]

1



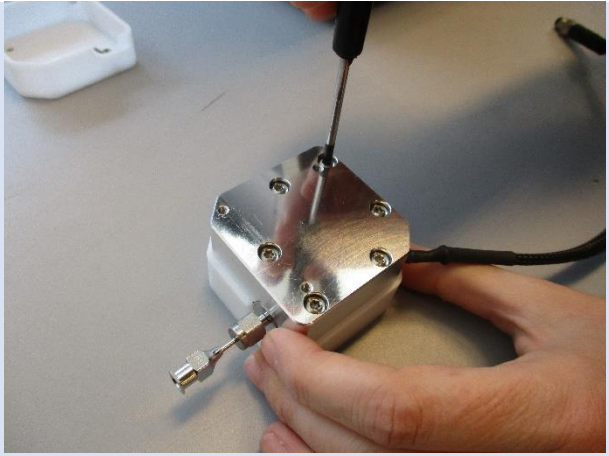
Luer-Lock-Adapter with heater

2



Loosen both screws and remove the plastic cover.

3



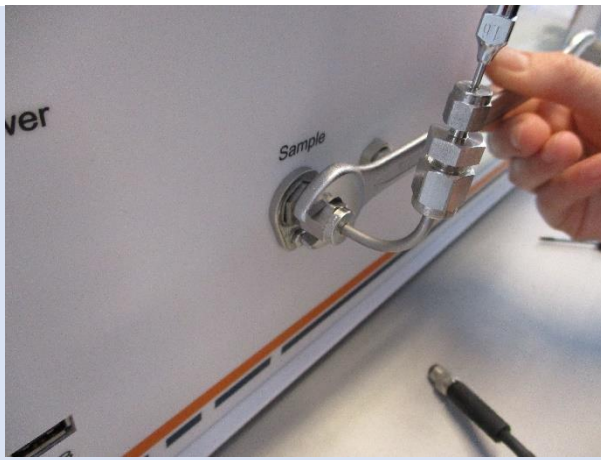
Loosen all screws and remove the heating block.

4



View of Luer-Lock-Adapter with opened heating block.

5



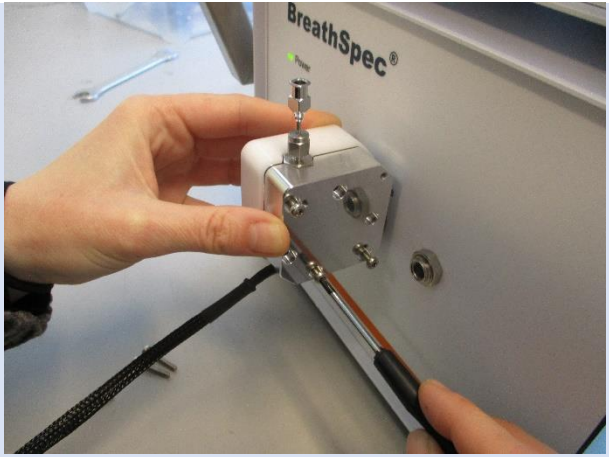
Connect the Luer-Lock-Adapter to the Sample In connector and tighten the screw with a spanner.

6



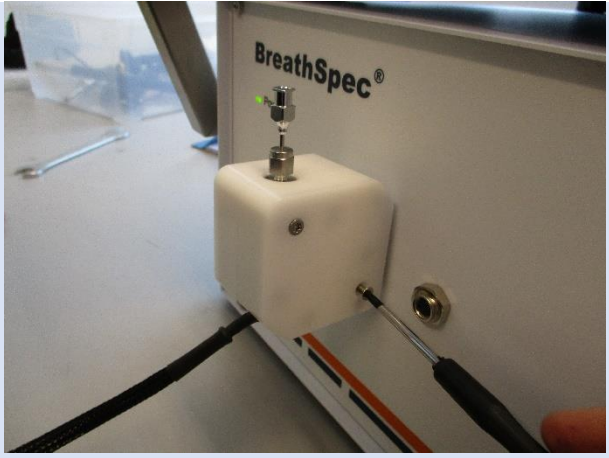
Attach one side of the heating block.

7



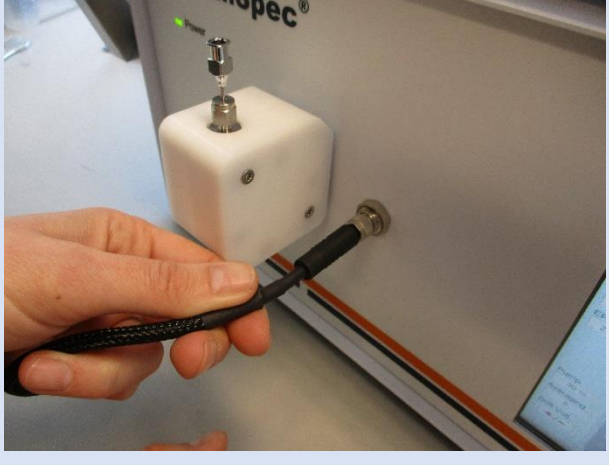
Attach the other side of the heating block and tighten all screws.

8



Attach the plastic cover and tighten all screws.

9



Connect the current supply cable and tighten it.

10

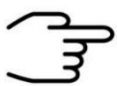


Switch on the
BreathSpec.

7.6 Prepare the device for operation

Before using the device for the first time or after being disconnected from the nitrogen source for some time it must be cleaned to ensure proper operating conditions. In this case start the **cleaning mode**.

An appropriate cleaning period duration must be chosen depending on how long the device was switched off and on the extent of contamination. It is recommended to clean the device for at least **15 hours** before operating it for the first time. If the Spectrum is not clean repeat the process. A **reference spectrum** for the evaluation can be found in the supplied **Analytical Approval**.

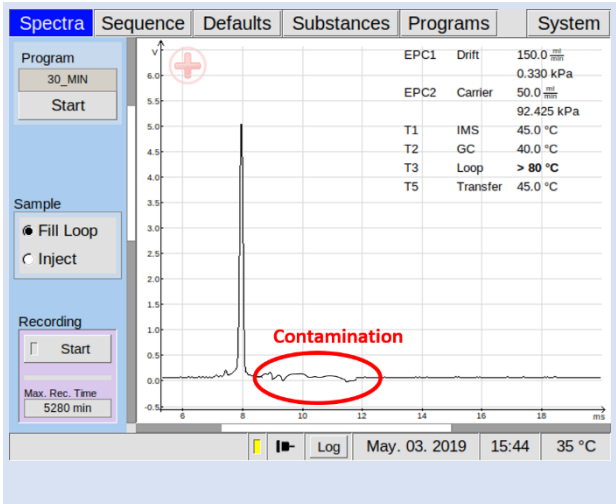


INFORMATION!

After the cleaning process the device needs at least **2 hours** to cool down the internal components to their required temperatures.

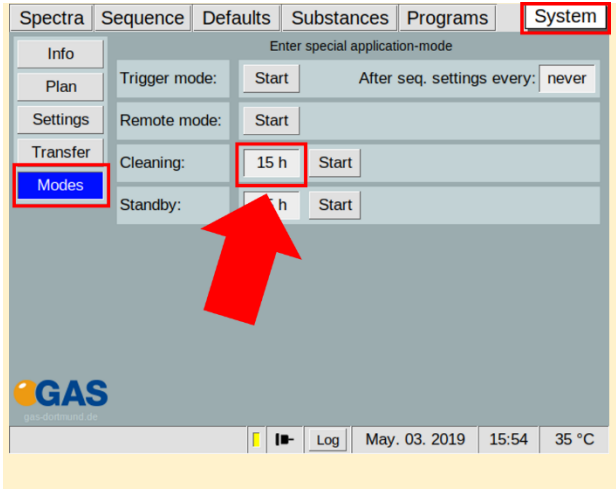
The duration of the cool down process is depending on the temperature default settings.

1



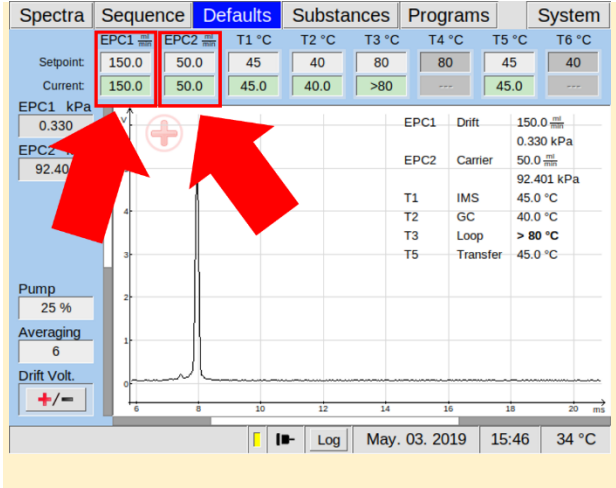
Inspect spectrum for contamination. Control the baseline. Start cleaning when contaminated. Contamination is indicated by peaks or the disappearing of the RIP.

2
Option



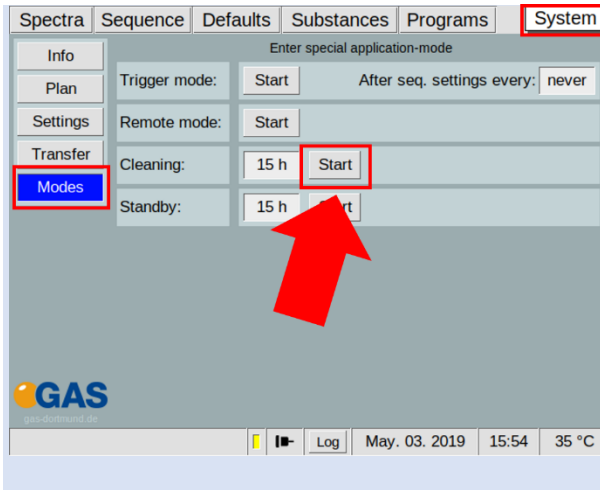
Select duration in hours:
System > **Modes** > **Cleaning Mode** > **x h**

3
Option



To speed up this process, increase flow rate of EPC1 and EPC2 to their maximum values (e.g 500/150 ml/min):
Defaults > **EPC1** > **EPC2**

4

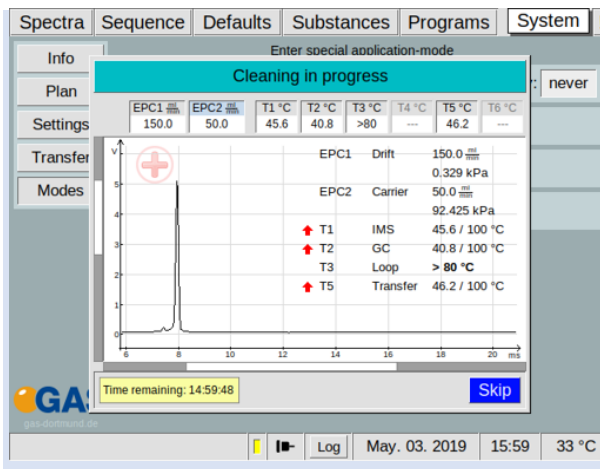


Start cleaning:

System > **Modes** >

Cleaning Mode > **Start**

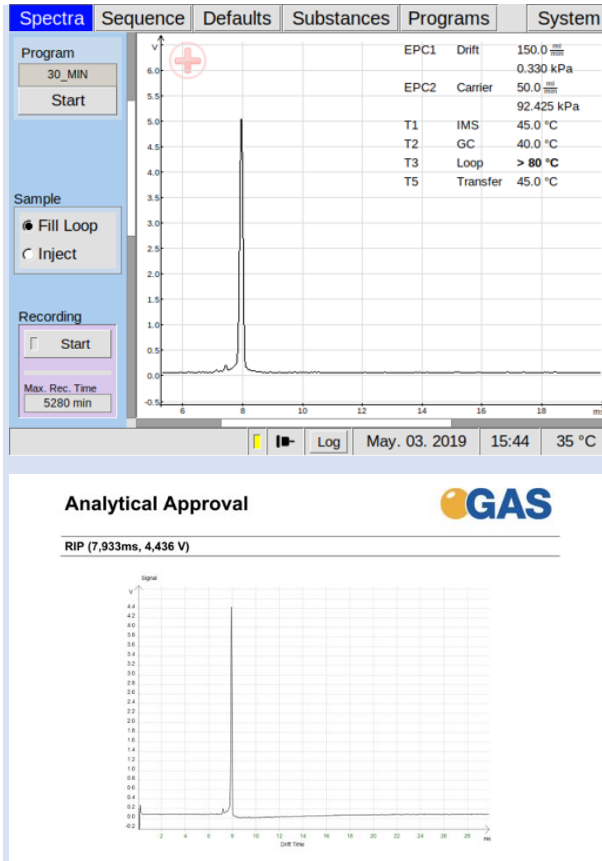
5



Wait until cleaning process is completed.

The process can be stopped with **Skip**.

6



After all temperatures reached the default values inspect visually the current spectrum and compare it with the reference spectrum of the analytical approval. **The RIP should reach ~80% of the RIP height displayed in the delivered Analytical Approval of the device under same measurement conditions of G.A.S.** The assessment of the readiness to measure is additionally supported by the system.

If not check the gas quality and/or install additional purification cartridges and start the cleaning procedure again.



INFORMATION!

The device is delivered with an acceptance snapshot. This snapshot defines the system performance during device acceptance and is used to assess the readiness for measurement. Any deviations from this are displayed in the Error Information Window. **The default values can be adjusted by the customer.**

8 Installation BreathSpec® Device (Version 4G2) with Airsense μ TD

8.1 Installation Requirements

The following requirements must be fulfilled by the customer:

Location of Installation

- Available space of 600 x 700 x 300 mm (W x D x H)
- Ambient temperature of 5 – 40 °C
- Humidity: 0-90 % RH, non-condensating

Electricity

- Electricity supply free of interferences
- Power Supply of 230 V \pm 10%, 50- 60 Hz \pm 1%

Gas supply

- Nitrogen (Quality 5.0 (99,999%) or Synthetic Air (Quality 5.0 (99,999%))
- Stainless steel pressure reducer adjustable adjustable pressure range of 3 – 6 bar and 3 mm Swagelok connector

Safety

- Availability of exhaust system for device exhaust gas tubes (Gas out and Sample Gas out)

Computer

- Computer with current Microsoft Windows operating system
- Administrator right to install G.A.S. software



INFORMATION!

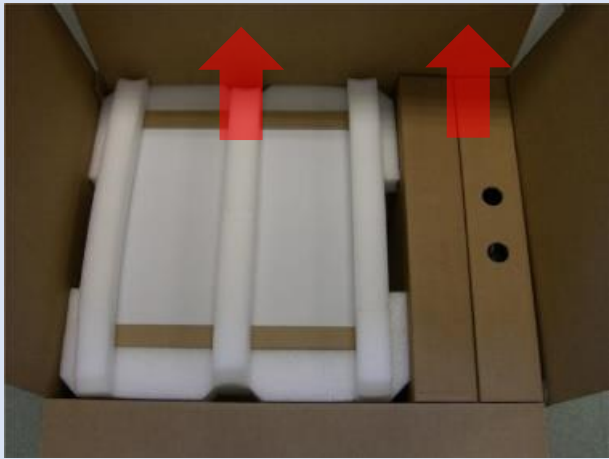
To ensure correct measurements it is absolutely necessary to **connect the supplied exhaust tubes** (Gas out and Sample gas out).

The exhaust tubes (Gas out and Sample gas out) **must be led separately into the exhaust system and must not be connected.**

The exhaust system must **not generate any negative pressure.**

8.2 Installing the device

1



Unpack the device.

Remove the foam spacers.

Remove the accessories boxes.

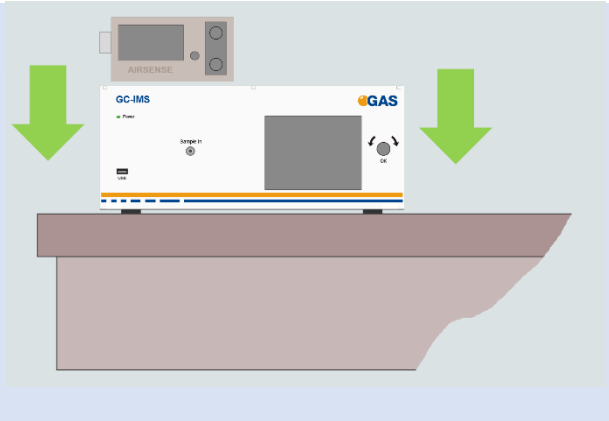
Lift the device from the transport box.



WARNING!

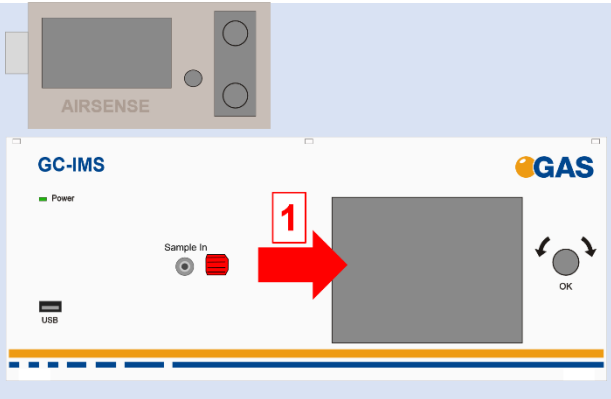
Do not deploy the device in areas exposed to explosive substances or mixtures!

2



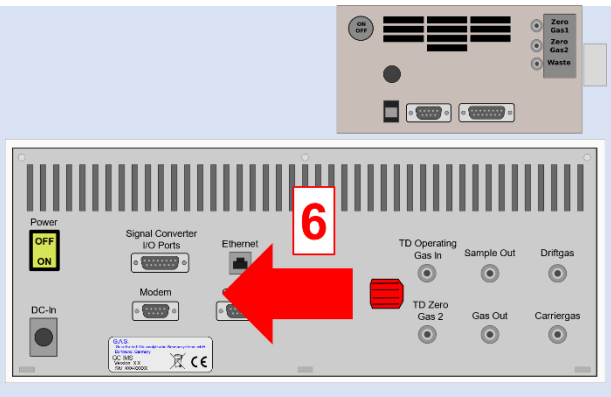
Place it on a robust table top of minimum footprint size of 60 cm x 70 cm. Ensure that there is enough working space at the rear side of the device.

3



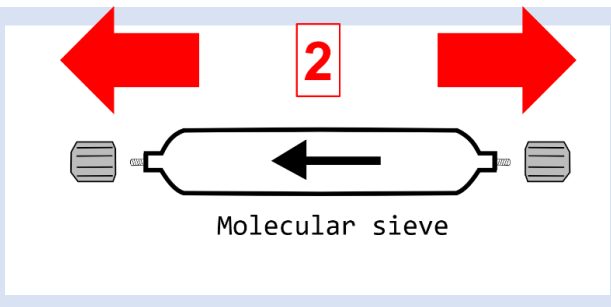
Remove red protective caps from gas sockets at front of housing. Retain for future use.

4

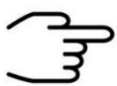


Remove red protective caps from gas socket at rear of housing. Retain for future use.

5



Remove protective caps from molecular sieve. Retain for future use.



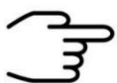
INFORMATION!

Protective caps should be put on gas sockets in case the device is stored or transported.



WARNING!

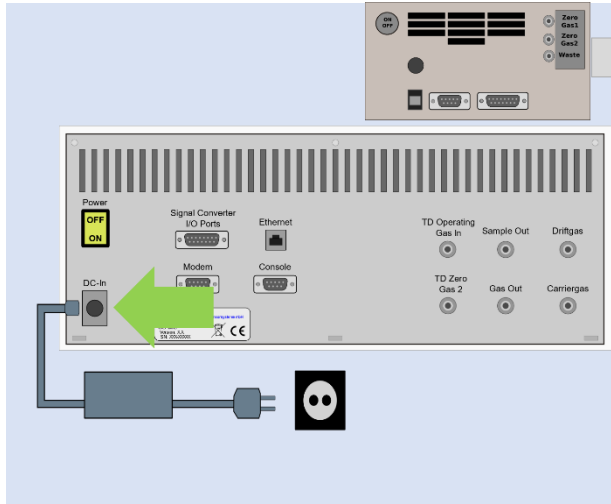
It is absolutely necessary to **remove all protective caps before the system is switched on.**



INFORMATION!

Make sure that the power switch is set to OFF before connecting the power supply.

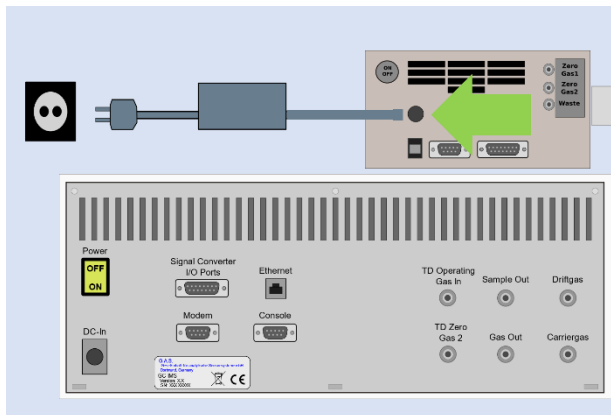
6



Connect BreathSpec device to power supply.

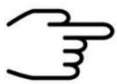
Connect power supply to power socket.

7



Connect µTD device to power supply.

Connect power supply to power socket.



INFORMATION!

Only use **stainless steel pressure reducers**, **PFA tubes** with 3 mm outer diameter and **3 mm Swagelok** connectors.

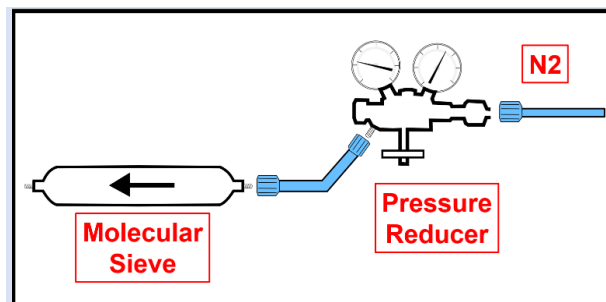
Screw on the Swagelok caps manually and fix them by screwing a further half-turn using a 12 mm open-end wrench.



WARNING!

Do not introduce aggressive gases or liquids into the device.

8



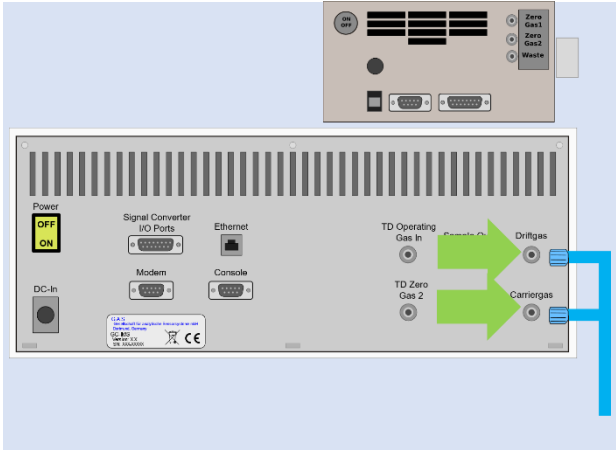
Connect nitrogen gas (Purity 5.0 or better) source to input of supplied molecular sieve using a PFA tube.



INFORMATION!

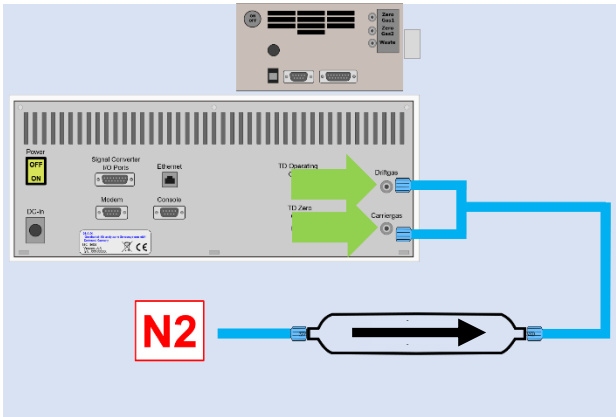
Recommended pressure of **Operation Gas** (Driftgas / Carriergas) is **3 bar (300 kPa)**. 6 bar (600 kPa) must not be exceeded.

8



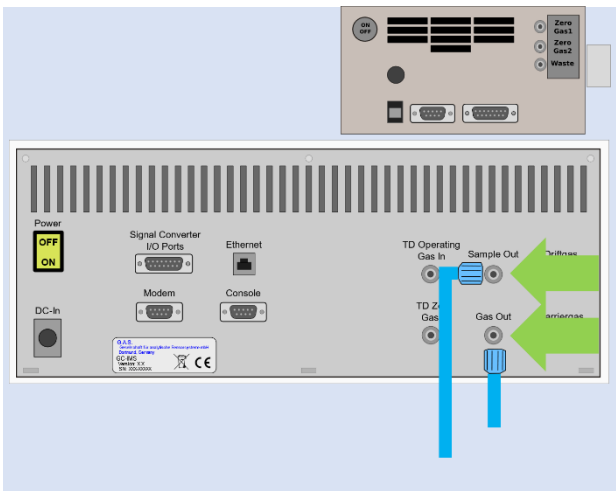
Connect the Driftgas-/Carriergas-Adapter to the Driftgas- and the Carriergas-Connector.

9



Connect molecular sieve outlet to **Driftgas-/Carriergas-Adapter** using a PFA tube.

10



Separately connect sockets **Sample Out** and **Gas Out** to appropriate waste gas ventilation system.



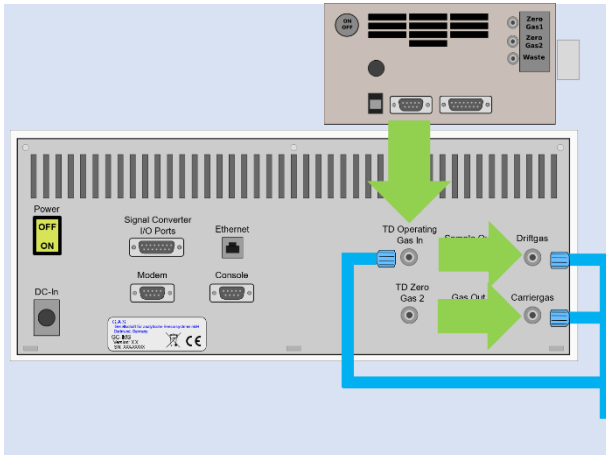
INFORMATION!

To ensure correct measurements it is necessary to **connect the supplied exhaust tubes** (Gas out and Sample gas out).

The exhaust tubes (Gas out and Sample gas out) **must be led separately into the exhaust system and must not be connected.**

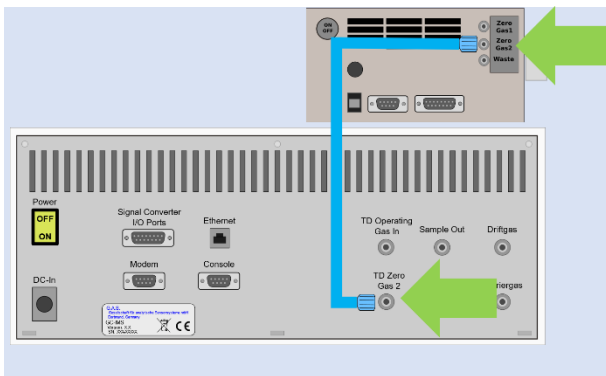
The exhaust system must **not generate any negative pressure.**

11



Connect TD operating gas in socket to **Driftgas- / Carriergas-Adapter** using a 3 mm Swagelok PFA tube.

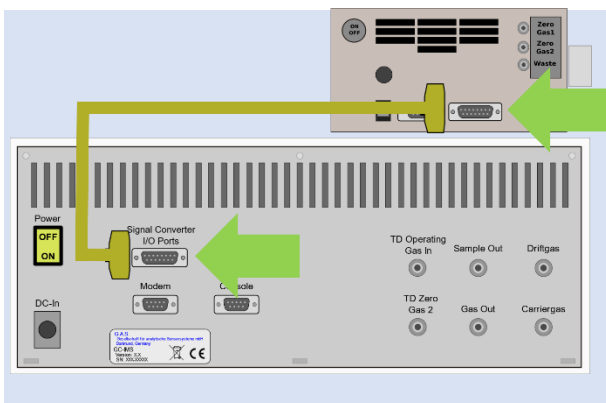
12



Also connect Outlet **ZeroGas 2** and **TDZero Gas 2** using a 3 mm Swagelok PFA tube.

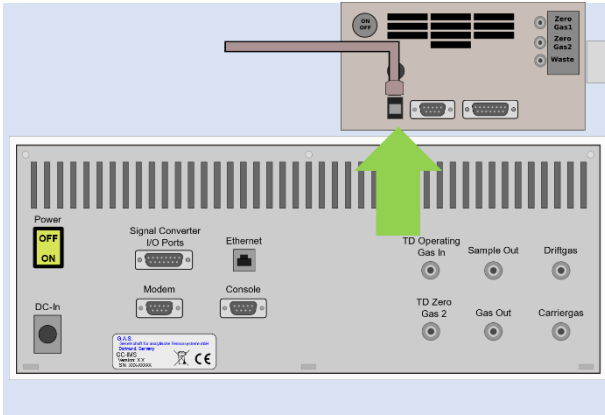
For further information see: Airsense μ TD manual

13



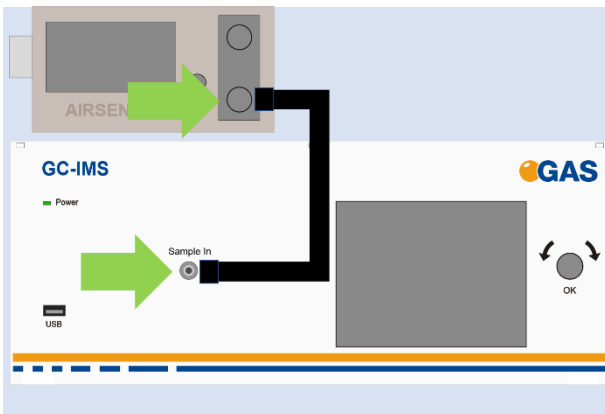
Connect BreathSpec **Signal Converter I/O-Port** to **μ TD Digital Port** with appropriate Connection-Cable.

14



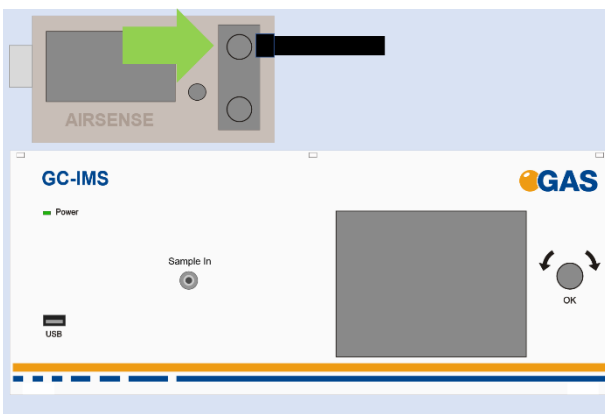
Connect the μ TD with a computer via USB cable.

15



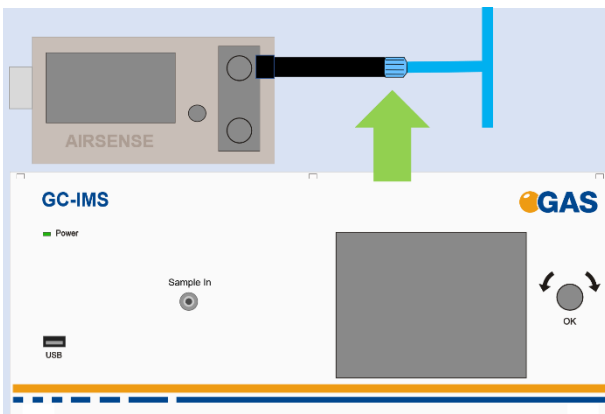
Connect the μ TD detector transfer line to sample in socket of BreathSpec.

16



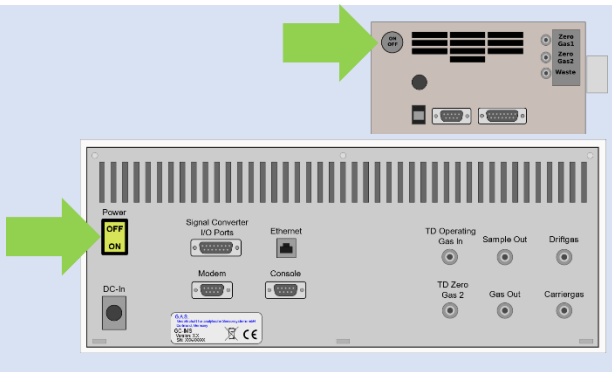
Connect the μ TD sampling transfer line to μ TD.

17



Connect a sample gas source to sampling transferline with the delivered bypass adapter.

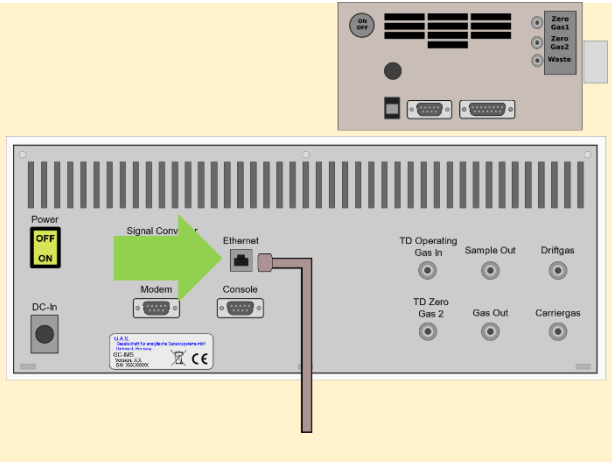
18



Switch on both devices.

19

Option



For file transfer via LAN:
Connect the **Ethernet** socket with an appropriate Ethernet cable to a LAN.



INFORMATION!

For detailed information about the installation and operation of the μ TD please refer the **[\$\mu\$ TD-BreathSpec Quickstart Manual](#)** and the **[Airsense \$\mu\$ TD Manual](#)**.



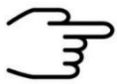
INFORMATION!

When the μ TD unit is connected to BreathSpec®, the current loop data output cannot be used.

8.3 Prepare the device for operation

Before using the device for the first time or after being disconnected from the nitrogen source for some time it must be cleaned to ensure proper operating conditions. In this case start the **cleaning mode**.

An appropriate cleaning period duration must be chosen depending on how long the device was switched off and on the extent of contamination. It is recommended to clean the device for at least **15 hours** before operating it for the first time. If the Spectrum is not clean repeat the process. A **reference spectrum** for the evaluation can be found in the supplied **Analytical Approval**.

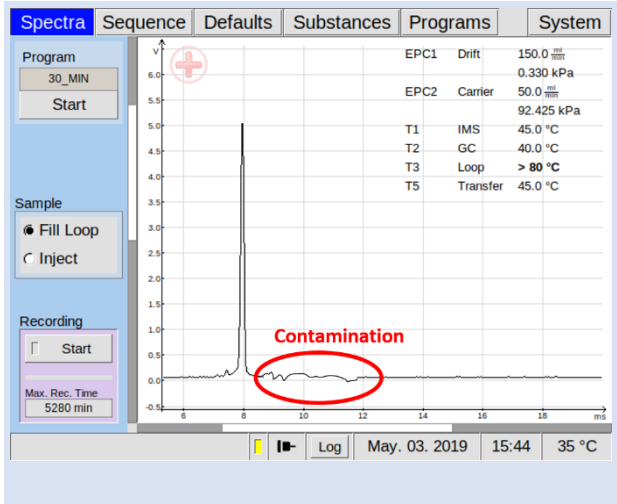


INFORMATION!

After the cleaning process the device needs at least **2 hours** to cool down the internal components to their required temperatures.

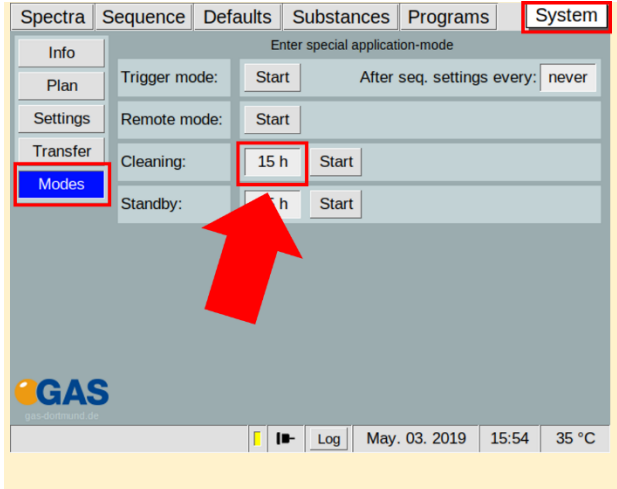
The duration of the cool down process is depending on the temperature default settings.

1



Inspect spectrum for contamination. Control the baseline. Start cleaning when contaminated. Contamination is indicated by peaks or the disappearing of the RIP.

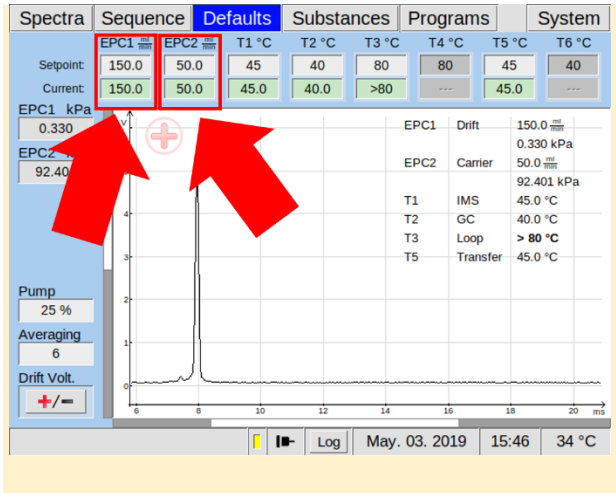
2
Option



Select duration in hours:

System > **Modes** >
Cleaning Mode > **x h**

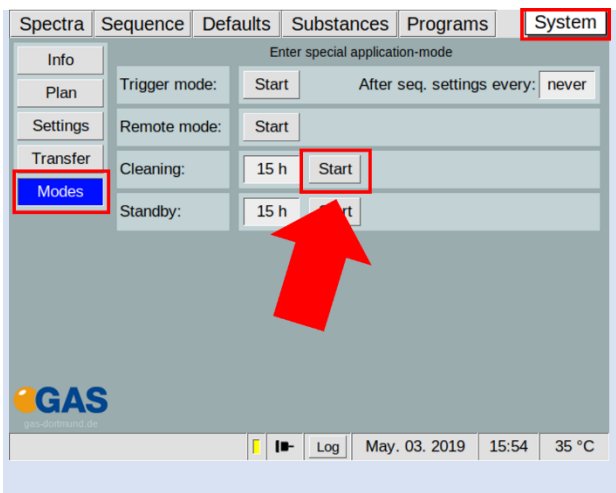
3
Option



To speed up this process, increase flow rate of EPC1 and EPC2 to their maximum values (e.g 500/150 ml/min):

Defaults > **EPC1** > **EPC2**

4

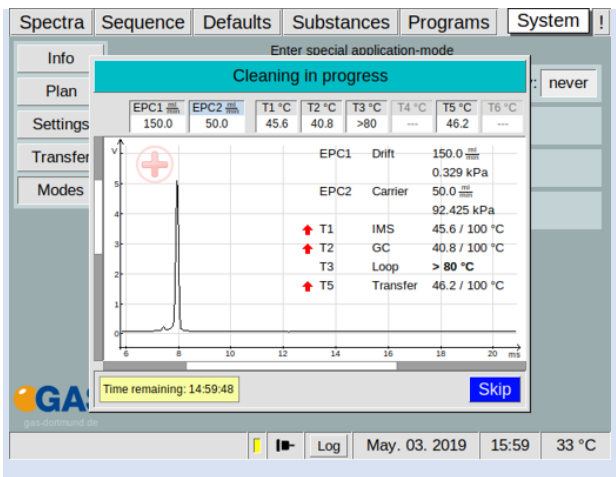


Start cleaning:

System > **Modes** >

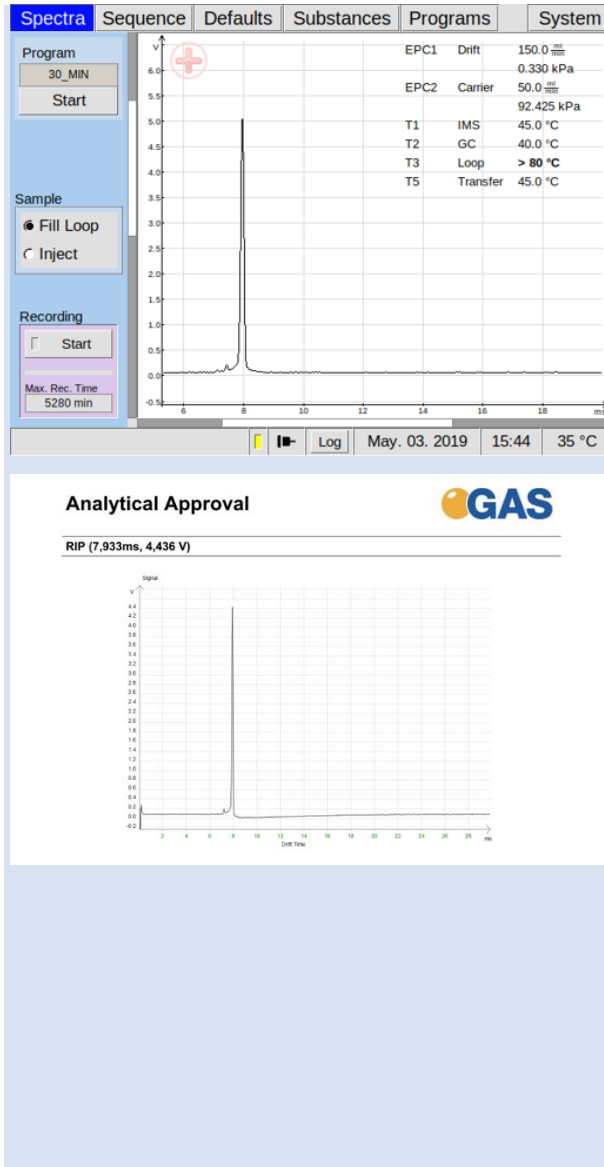
Cleaning Mode > **Start**

5



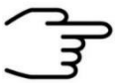
Wait until cleaning process is completed. The process can be stopped with **Skip**.

6



After all temperatures reached the default values inspect visually the current spectrum and compare it with the reference spectrum of the analytical approval. **The RIP should reach ~80% of the RIP height displayed in the delivered Analytical Approval of the device under same measurement conditions of G.A.S.** The assessment of the readiness to measure is additionally supported by the system.

If not check the gas quality and/or install additional purification cartridges and start the cleaning procedure again.



INFORMATION!

The device is delivered with an acceptance snapshot. This snapshot defines the system performance during device acceptance and is used to assess the readiness for measurement. Any deviations from this are displayed in the Error Information Window. **The default values can be adjusted by the customer.**

9 System Operation

9.1 Measurement Requirements



INFORMATION!

Only use the original accessories supplied with the device.



INFORMATION!

Make sure that the gas quality is 5.0 (99,999%) or better.



INFORMATION!

Only use stainless steel pressure reducer.



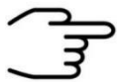
INFORMATION!

Make sure that the spectrum is clean a without contamination.



WARNING!

Do not introduce any liquids. This can destroy the device.



INFORMATION!

Make sure that that all temperature-, flow- and pressure values have reached their default value and are stabilized.

9.2 Measurement Program

The BreathSpec will **by default** be equipped with a general measurement program called **'BREATH'**. This program may need to be subject for method optimization **see chapter 6.6**. Please be aware that editing the program may require changes in the timeline of sampling in order to sample the exhaled breath.

The following workflows describe the analysis of human breath exemplarily using the 'BREATH' program.

9.3 Workflow: Breath Sampling via Handheld Breath Sampler

9.3.1 Workflow: Installation of Disposable Reservoir Tube and Mouthpiece



INFORMATION!

In order to sample via the handheld breath sampler, the respective tube port has to be installed [see chapter 7.4](#).



DANGER

- Biohazard: wear appropriate gloves at all handling steps
- Take measures to prevent contamination from one subject/patient to other



WARNING

- Pinching possible

1



The image shows the parts necessary to set up the device for a breath analysis.

2



Insert new reservoir tube.

Check matching of Luer tip and reservoir's drilled hole.

BreathSpec® – User Manual

3



Plug in the mouthpiece into narrow end of the reservoir tube. Screwing the mouthpiece may ease plugging in.

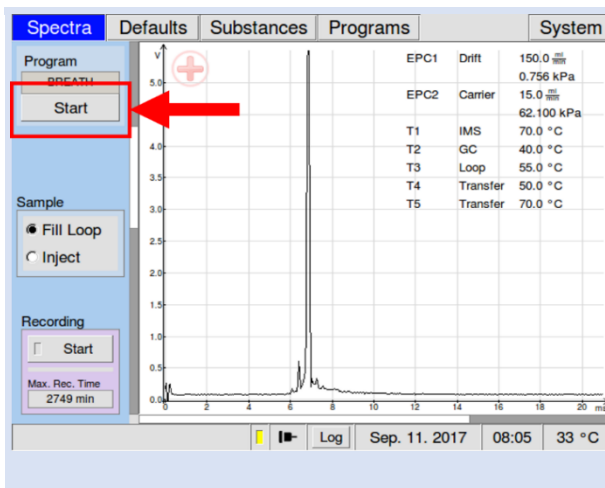
4



The image shows installed reservoir tube kit.

9.3.2 Workflow: Execute a breath measurement using the Handheld

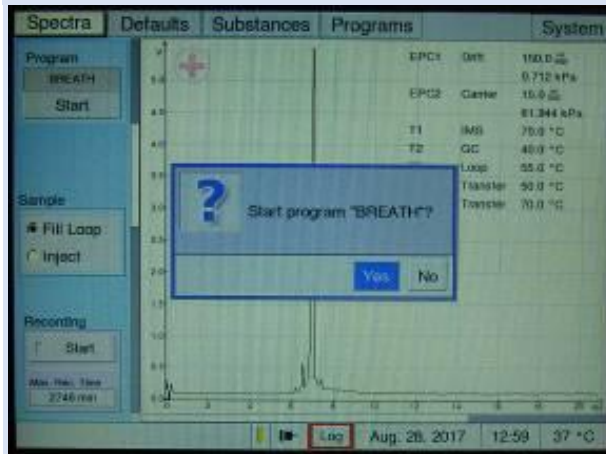
1



Select the Start button.

The **dialog** 'Start program' appears.

2



Select the <Yes>button with the pushable rotary knob (focus - background is blue), but do not start.

3



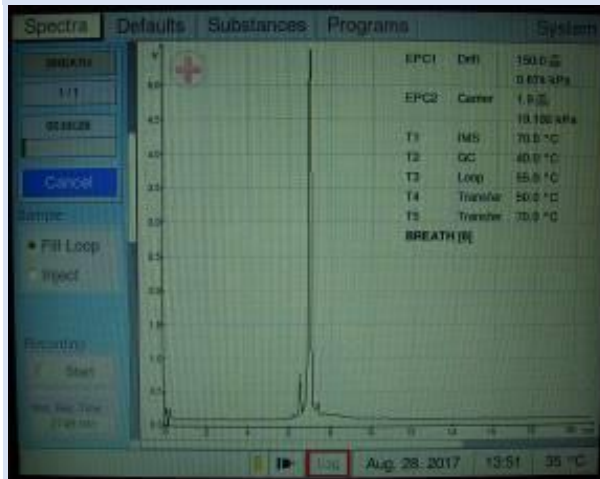
Ask the subject/patient to exhale smoothly into the mouthpiece mounted on the handheld.

[in case of a mistrial (cough etc.) the subject/patient can repeat exhalation]



{best practice is letting the subject/patient exhale into the handheld still attached to the device without touching it. If touched, the handheld can be wiped clean with an alcohol free tissue}

4



Upon ending of exhalation, the operator presses the pushable rotary knob to start the selected program.

[Arranging a sign with the patient to indicate ending of exhalation may be of benefit to match the right starting point]

> subject/patient can stop exhaling

> analysis is initiated (progress bar indicates runtime)

5



Pull out the used disposable reservoir tube.

The analysis will continue as defined in the program (approx. 10min for the 'BREATH' program)

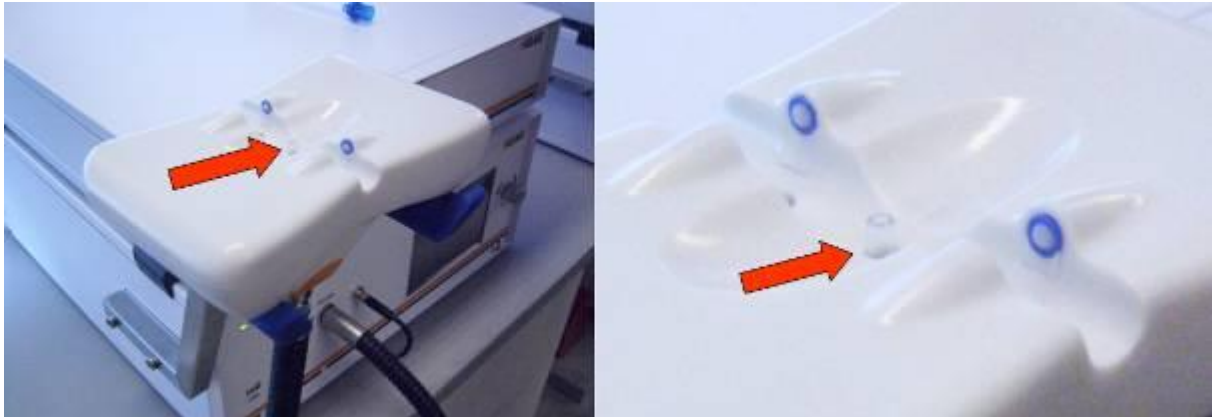


INFORMATION!

Dispose the syringe, reservoir tube and mouthpiece.

9.3.3 Workflow: Exchanging the inner syringe body

The sampling tube is capped by a disposable syringe body to allow exchanging of all parts that are in direct contact to breath. The syringe's Luer tip protrudes from the handheld sampler (see images below).



The procedure steps are described as follows:



DANGER

- Biohazard: wear appropriate gloves at all handling steps
- Take measures to prevent contamination from one subject/patient to other



WARNING

- Pinching possible

1



- move click located at the bottom of the handheld to disconnect handheld and tube and pull out the tube.

BreathSpec® – User Manual

2



- pull syringe body from tube

3



- remove piston from a new, clean syringe and impose syringe body on tube

4



- re-insert tube equipped with new syringe body into handheld

9.3.4 Workflow: Execution of an ambient air measurement using the Handheld

The analysis of the ambient air may indicate volatile compounds that do not originate from the subject/patients breath but are present in the air.

To analyze the ambient air follow the steps described in 9.3.2. A Reservoir tube and Mouthpiece must not be installed.

9.4 Workflow: Breath Sampling via Disposable Breath Sampler

9.4.1 Start a breath measurement using disposable breath sampler



INFORMATION!

To sample via the Luer-Lock-Adapter the respective tube port has to be installed [see chapter 7.5](#).



DANGER

- Biohazard: wear appropriate gloves at all handling steps
- Take measures to prevent contamination from one subject/patient to other



WARNING

- Pinching possible

1

The screenshot shows the software interface with the following elements:

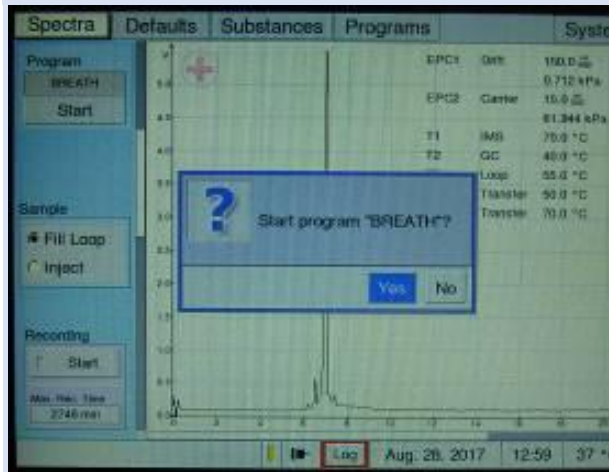
- Program List:**

EPC1	Drift	150.0 $\frac{mV}{min}$
		0.756 kPa
EPC2	Carrier	15.0 $\frac{mV}{min}$
		62,100 kPa
T1	IMS	70.0 °C
T2	GC	40.0 °C
T3	Loop	55.0 °C
T4	Transfer	50.0 °C
T5	Transfer	70.0 °C
- Recording Section:**
 - Start (checkbox)
 - Max. Rec. Time: 2749 min
- Bottom Bar:** Log | Sep. 11, 2017 | 08:05 | 33 °C

Press Start Button to initialize the selected program.

The **dialog** 'Start program' appears.

2



Select the <Yes>button with the pushable rotary knob (focus - background is blue), **but do not start.**

3



Plug in the mouthpiece into the narrow end of the reservoir tube. Screwing the mouthpiece may ease plugging in.

4



Connect the 5ml Syringe with the reservoir tube. Screwing the mouthpiece may ease plugging in.

5



Ask the subject/patient to exhale smoothly into the mouthpiece mounted on the handheld.

During the exhalation sample breathing air into the syringe.

[in case of a mistrial (cough etc.) the subject/patient can repeat exhalation]

[Note that the breath sample may alter with time in the syringe]

6



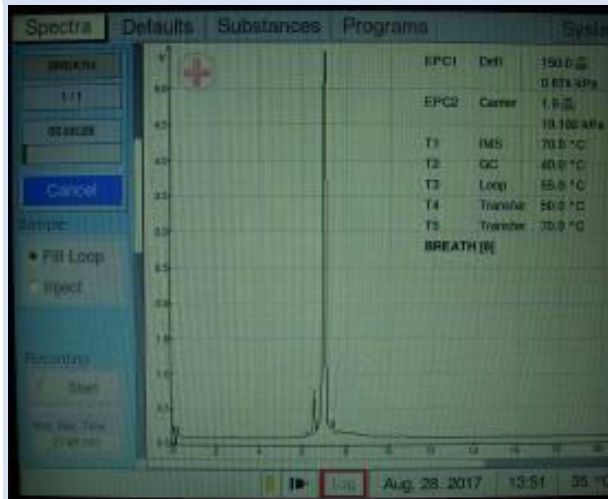
Disconnect the syringe from the reservoir tube.

Insert the syringe into the Luer lock adapter.

Smoothly inject the breathing air into the sampling Luer port.

Towards the ending of injection press the pushable rotary knob to trigger the selected program.

7

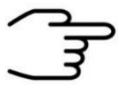


> analysis is initiated (progress bar indicates runtime)



INFORMATION!

THE DESCRIBED MODE OF OPERATION ONLY WORKS WITH THE DEFAULT BREATH PROGRAM. PROGRAM ADJUSTMENTS BY THE USER MAY REQUIRE ADJUSTMENTS IN THE SAMPLING.



INFORMATION!

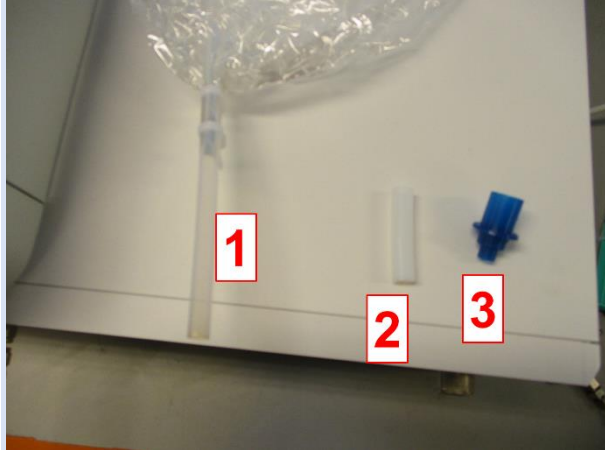


Dispose the syringe, reservoir tube and mouthpiece.

9.4.2 Execution of an ambient air measurement using syringes

The analysis of the ambient air may indicate volatile compounds that do not originate from the subject/patient's breath but are present in the air.

To analyze the ambient air follow the steps described in chapter 9.4.1. The ambient air can be sampled directly into a syringe.

9.5 Workflow: Exemplary Breath sampling with a sample bag

1		<p>The components for breathing air sampling with the gas bag:</p> <ul style="list-style-type: none">1: Sampling bag2: Sampling bag adapter3: Mouthpiece
2		<p>Put all components together</p>
3		<p>Fill the sample bag with breathing air.</p>

4



Connect the sampling bag to μ TD sampling transferline.

5



Set BreathSpec to Triggemode and start the μ TD.



INFORMATION!

- For detailed Information refer to the [Airsense uTD Handbook](#) and the [\$\mu\$ TD GC-IMS Additional Information Quickstart](#)

9.6 Workflow: Measurement in Normal mode

1



Select Normal Mode:

System > **Settings** >
Normal

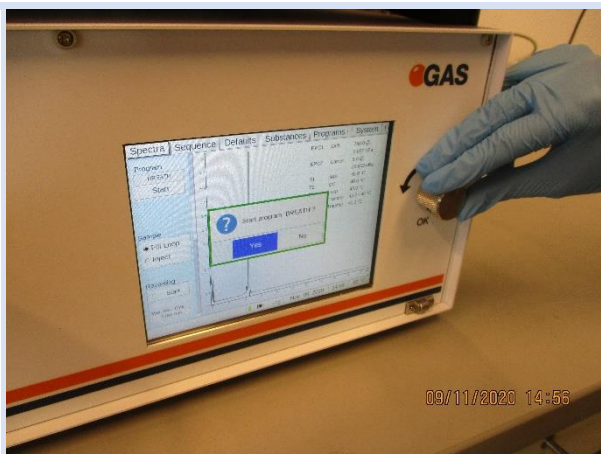
2



Select Start:

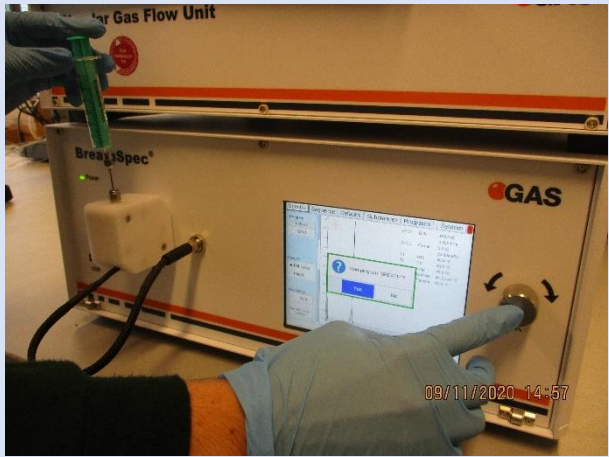
Spectra > **Start**

3



Preselect **OK** in the dialog box, but do not start.

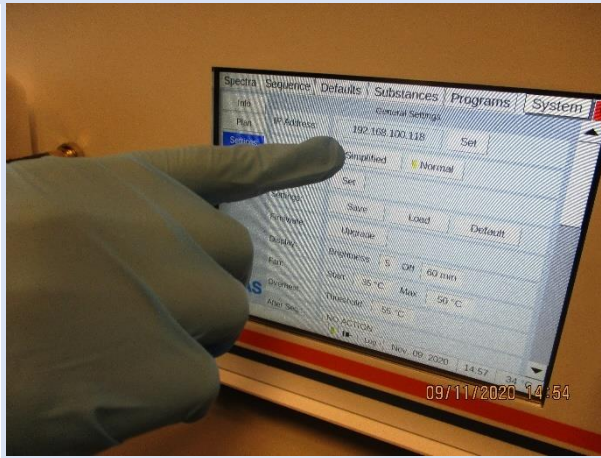
4



Insert the sample (here exemplary with syringe and Luer-Adapter) and start the program by pressing the rotary knob.

9.7 Workflow: Measurement in Simplified mode

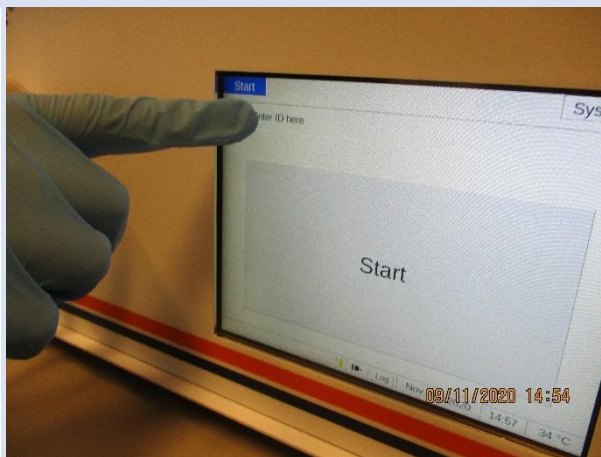
1



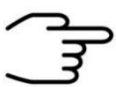
Select Normal Mode:

System > **Settings** >
Simplified

2



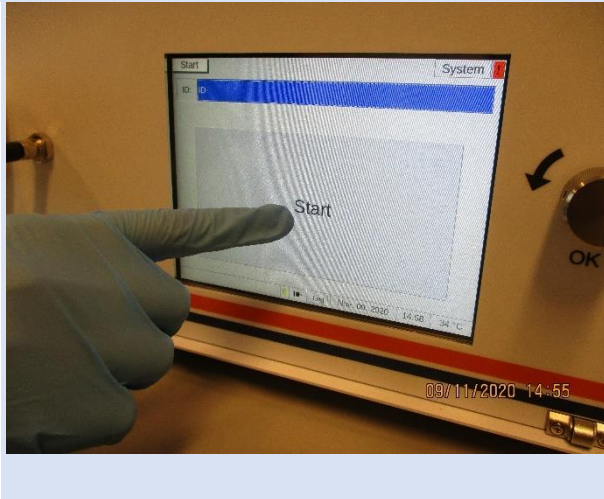
In simplified window select the ID field and enter an ID.



INFORMATION

The entry of an ID is only possible in Simplified Mode and is mandatory.

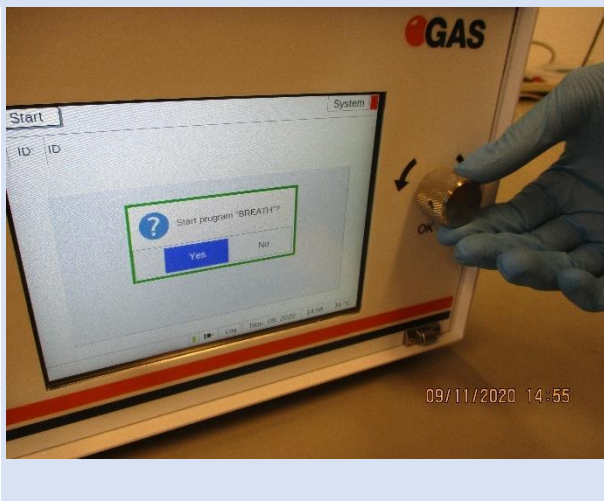
3



Select Start:

Start > **Start**

3



Preselect **OK** in the dialog box, **but do not start.**

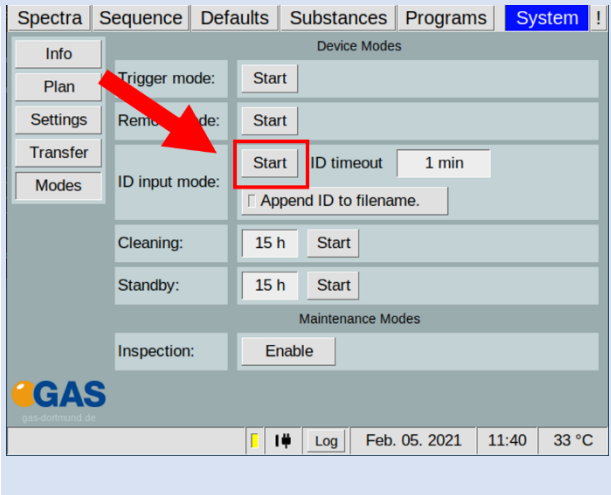
4



Insert the sample (here exemplary with syringe and Luer-Adapter) and start the program by pressing the rotary knob.

9.8 Workflow: Measurement in ID Input Mode

1

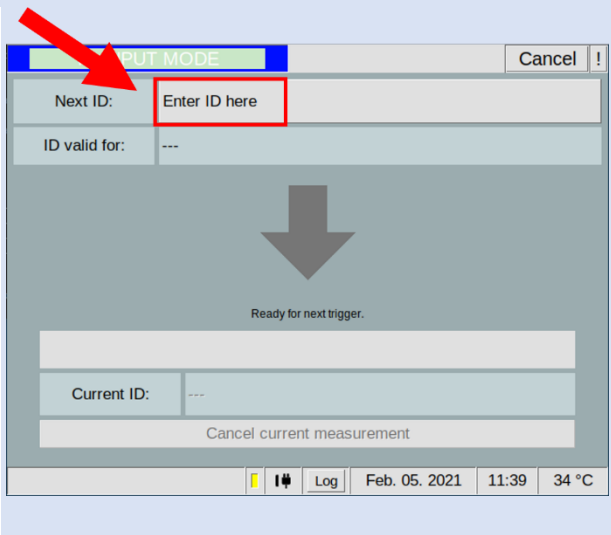


Select ID Input Mode:

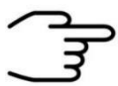
System > **Modes** > **ID**

Input Mode > **Start**

2



In ID Input Mode window select the ID field and enter an ID.



INFORMATION

The entry of an ID is mandatory.

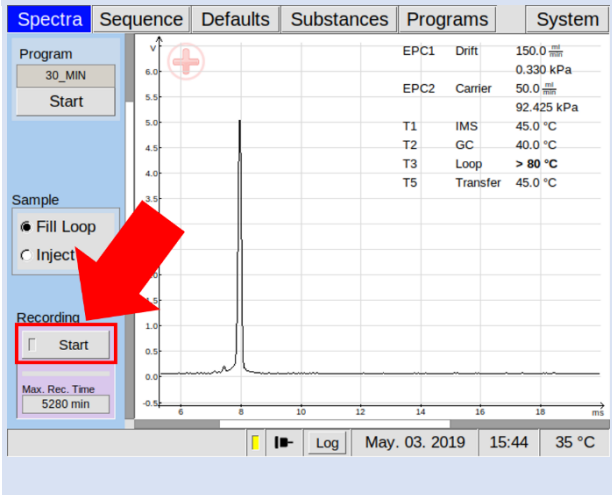
3



Start measurement with μ TD-start button.

9.9 Workflow: Manual Measurement Recording

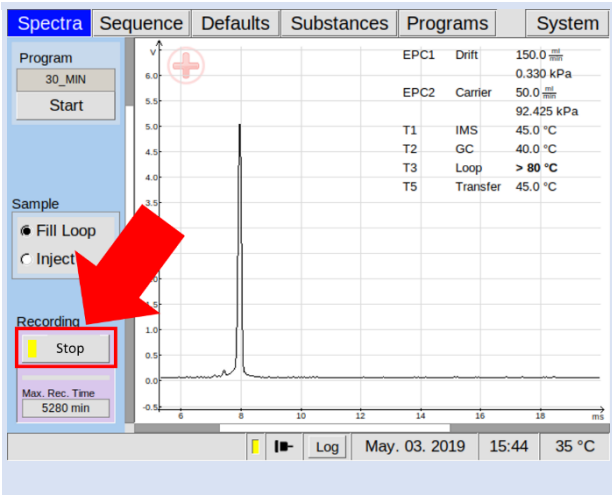
1



To record a measurement manually select:

Spectra > **Recording-**
Start

2



To stop the measurement select:

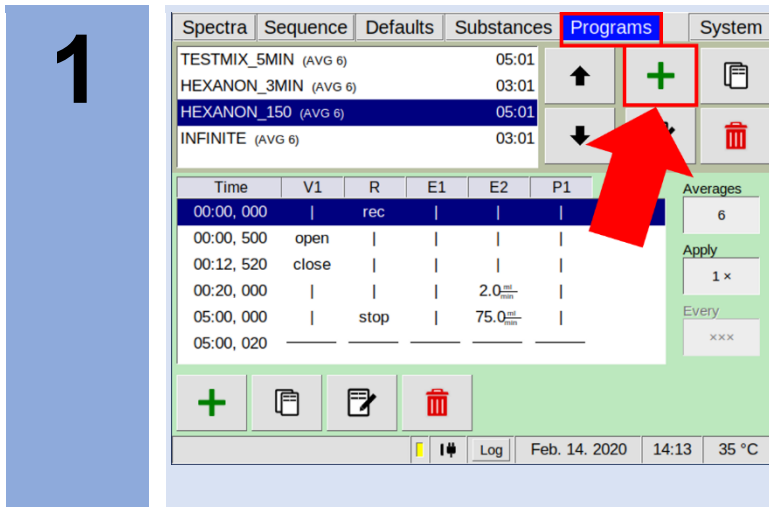
Spectra > **Recording-**
Stop




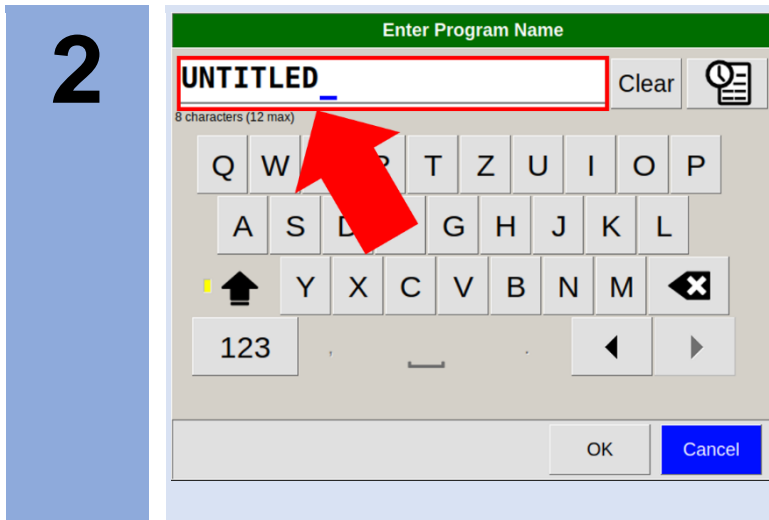
INFORMATION!

The maximum measuring time is limited to **59 minutes 59 seconds and 980 milliseconds.**

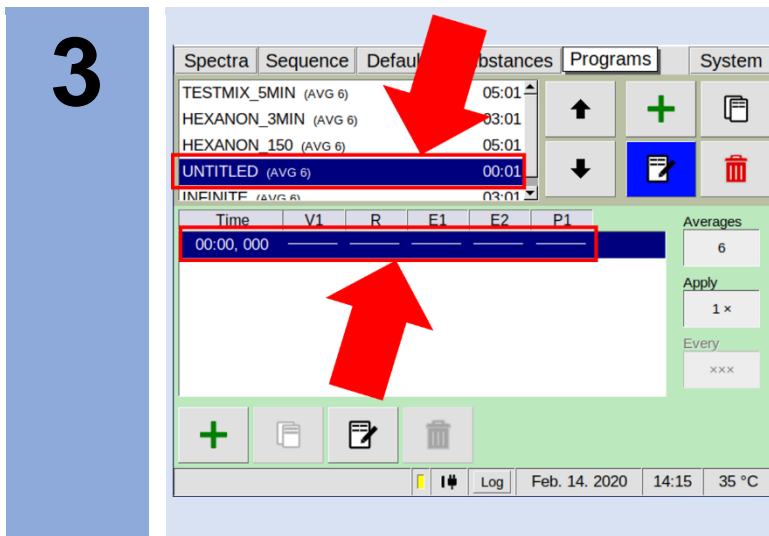
9.10 Workflow: Create a Measurement Program



Select:
Programs
 To create a new program select the Button 

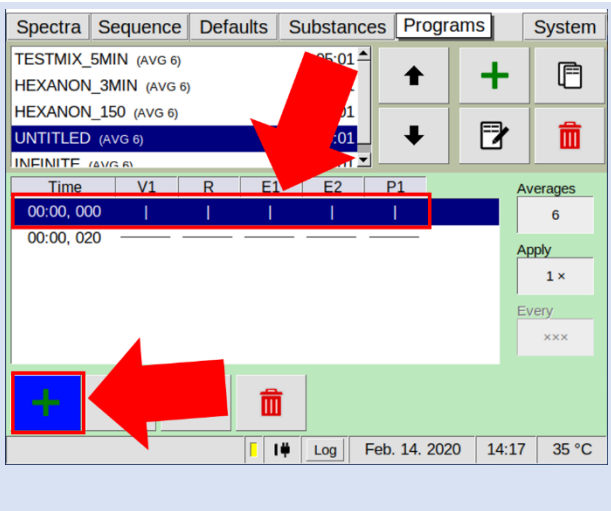


Enter a new program name or use the default name.



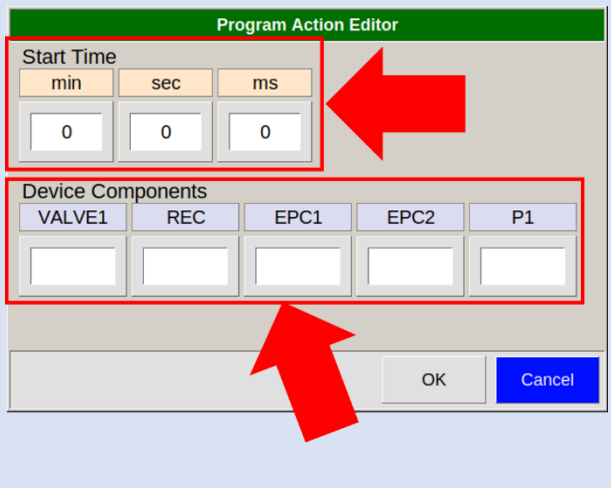
The program end time is displayed as the final line

4



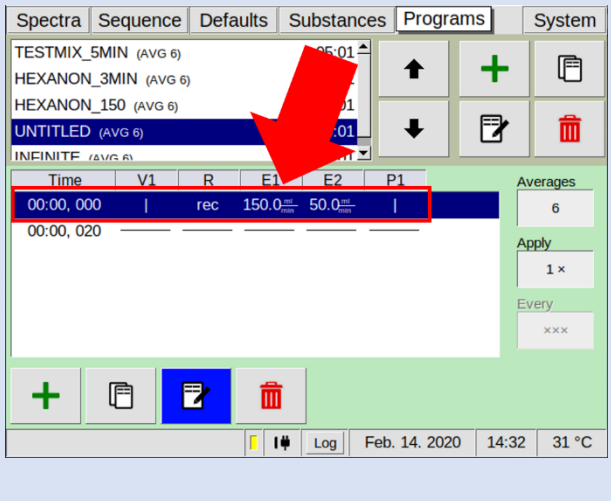
To create a new program action line select the '+' Button

5



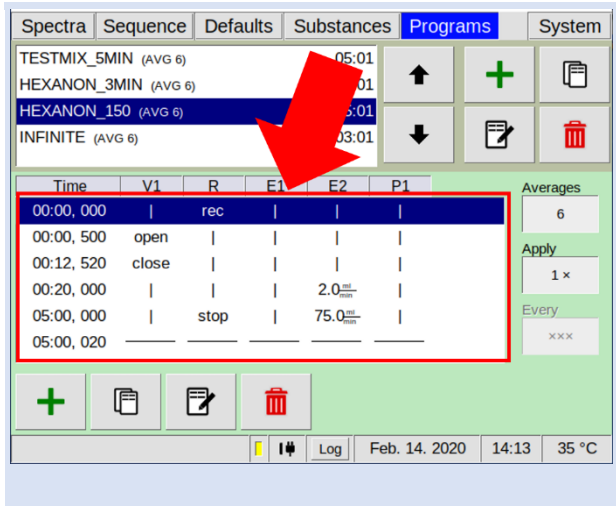
This line can be filled with values. For more information see also [Chapter 6.6.3 Edit Measurement Programs](#)

6

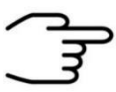


After the necessary values have been entered, repeat step 4 and 5 to create the next program action line.

7



A complete program sequence can be created line by line.



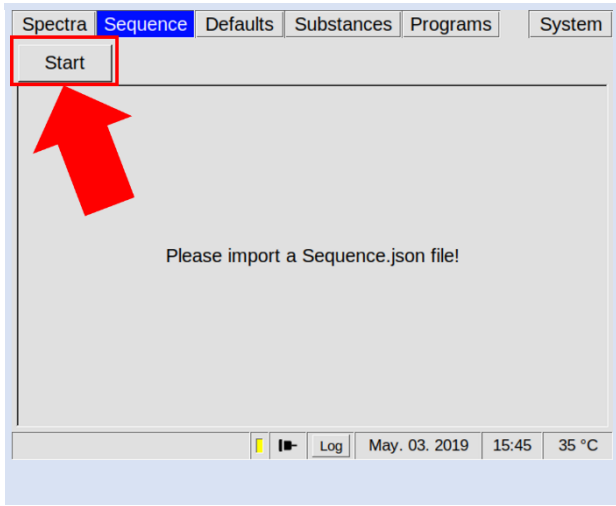
INFORMATION!
 The device is delivered with standard programs that can be adapted to your needs.
 Customer-specific programs can also be created optionally.

9.11 Workflow: Start Sequence



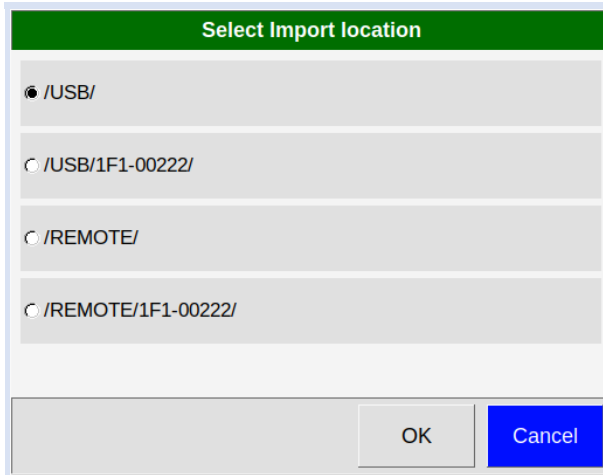
INFORMATION!
 The sequence file must be created with the **G.A.S. Sequence Designer Software**. For detailed Information refer to the **G.A.S. Sequence Designer Software Manual**.

1



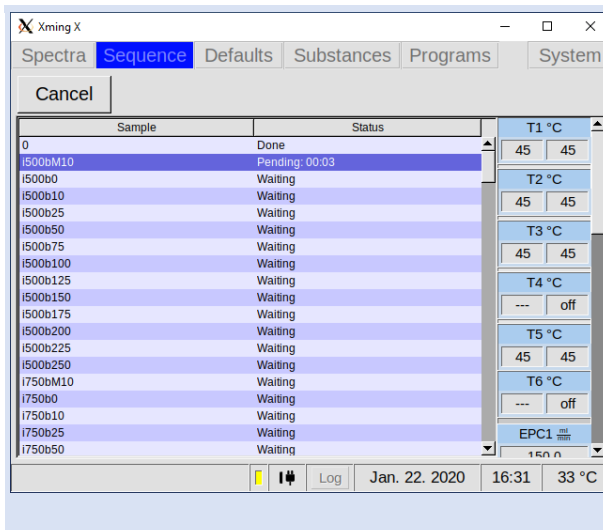
To start a sequence select:
Spectra > **Start**

2



Select the import location of the sequence file named **Sequence.json**

3



The Sequence will be executed.



INFORMATION!

The file must be named **Sequence.json** for the software to recognize it. Make sure, that the parameters specified in the programs and after-run settings are within your devices permitted regions.



WARNING!

Careful when changing device critical parameters by applying After Run Settings. A device can become inoperable with faulty IMS parameters. After Run settings are also applied if the Sequence is cancelled by the user. In case of cancellation, the devices default parameters will be the same as if the sequence had successfully finished, taking all previous After Run Settings into consideration.

9.12 Workflows: File Transfer Setup

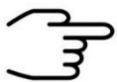
9.12.1 Overview

Files can be transferred to and from the device by LAN connection and by USB device connected to the USB port at the front of the housing.



INFORMATION!

A connected USB device is always preferred to a LAN connection when exporting or importing files manually.



INFORMATION!

The USB device must be formatted to FAT32. Consult your system administrator on formatting USB devices.

Generated measurement files and measurement result files are stored on the internal storage volume of the device.

The following file types are generated from measurements:

File Type	Description
MEA Measurement Files	Contains the complete data of one single measurement including the raw sampling data.

When a connection to a server is established and the export is activated these files are copied to this server when created in the workflow. Measurement files once copied to one of these locations are marked and will be overwritten in case the internal storage is full.

By default, the **Service Message Block Protocol (SMB)** also known as Common Internet File System (CIFS) is used. The **Secure File Transfer Protocol (SFTP)** or a modified version of the **Trivial File Transfer Protocol (TFTP)** can also be used. LAN file transfer settings can be modified in **System** > **Transfer** > **Connection** > **Edit Server Details**.

Manual transfer of measurement files stored on the device can be done **System** > **Transfer** > **Mea Files** > **Copy to Remote**.

Manual transfer of measurement files stored on the device can be done **System** > **Transfer** > **Mea Files** > **Delete**.

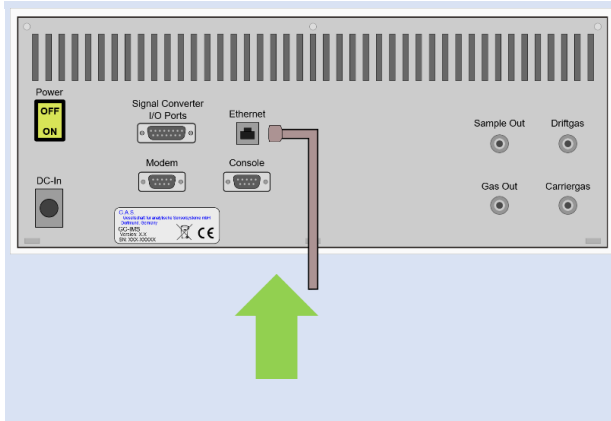
9.12.2 Connecting to a Server in a LAN



INFORMATION!

Some PC Ethernet interfaces may not be suited for a direct connection to the device. In that case consider using an Ethernet switch to connect both devices.

1a

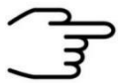


Connect the device with a standard Ethernet cable (LAN cable) to the LAN or directly to a computer.

1b



In the status bar the connection icon is displayed.



INFORMATION!

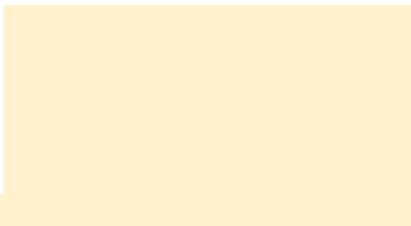
Make sure that any firewall present in the network does not block necessary traffic. Consult your system administrator on how to configure your firewall.



INFORMATION!

Consult your system administrator on how to set up a server with one of the protocols **SMB** and **SFTP**. The **TFTP** protocol requires the G.A.S. TFTP Server software to run on a Microsoft® Windows® computer.

2a
Option



For **SMB** set up a SMB share on a server. Consult your system administrator on how to do that.

2b

Option



For **SFTP** set up a SFTP server. Consult your system administrator on how to do that.

For an example SFTP server for Microsoft® Windows® PCs see:

<http://www.coreftp.com/server>

2c

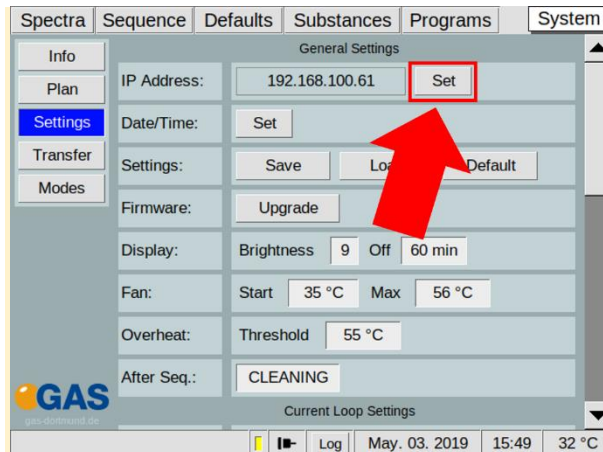
Option



For **TFTP** install the G.A.S. IMS-Control TFTP-Server on the PC. For detailed information see the **IMS Software Suite IMScontrol TFTP-Server manual**.

3a

Option



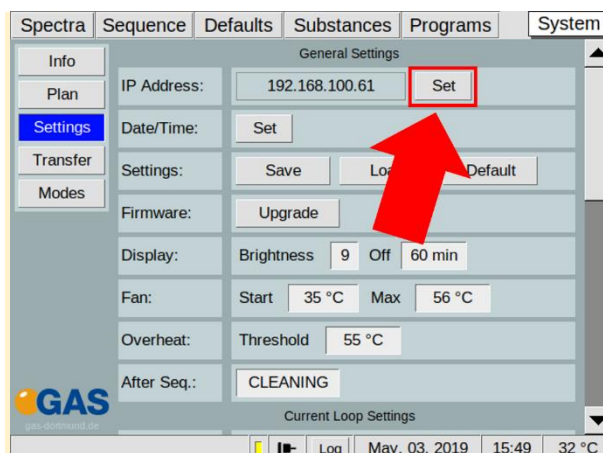
Set a static device IP
(Recommended for direct connection of PC and device):

Use System > **Settings** > **Set**

In the next dialogbox select: **Yes**

3b

Option



Get device IP From DHCP Server

(Recommended for LAN integration of the device):

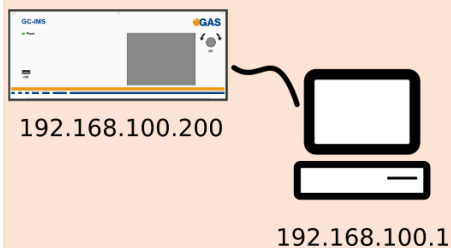
Use System > **Settings** > **Set**

In the next dialogbox select: **No**

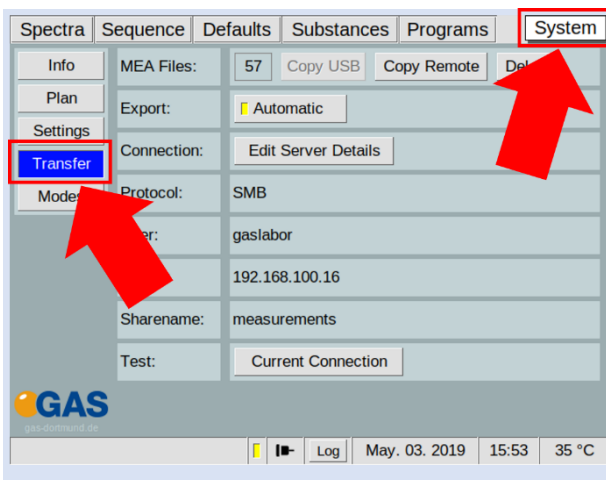


INFORMATION!

Note that both devices must be in the same subnet mask area of **255.255.255.0** i.e. only differ in the fourth number of the four-part IPv4 address.

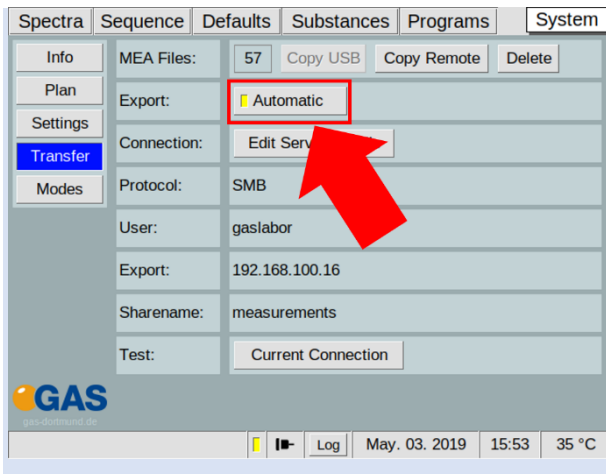


4



Open **System** > **Transfer**

5



Activate or deactivate automatic file transfer to the server with **Automatic Export**.

6

Server Settings

Protocol: SMB SFTP TFTP

User: gaslabor

Password: ●●●●●●

Server IP: 192.168.100.16

Folder: Measurements

Select the desired protocol **SMB**, **SFTP** or **TFTP**.

7a

Option

Server Settings

Protocol: SMB SFTP TFTP

User: gaslabor

Password: ●●●●●●

Server IP: 192.168.100.16

Folder: Measurements

For **SMB** enter **Server IP Address**, **Folder** name, **User** name and **Password** for the SMB share on the server.

7b
Option

Server Settings

Protocol: SMB SFTP TFTP

User: gaslabor Edit

Password: ●●●●●● Edit

Server IP: 192.168.100.16 Edit

Port: 22 Edit

Test connection Cancel

For **SFTP** enter **Server IP Address**, **IP Port**, **User name** and **Password** for the SFTP server.

7c
Option

Server Settings

Protocol: SMB SFTP TFTP

Server IP: 192.168.100.16 Edit

Test connection Ok Cancel

For **TFTP** enter the **Server IP Address**.

8

Server Settings

Protocol: SMB SFTP TFTP

Server IP: 192.168.100.16 Edit

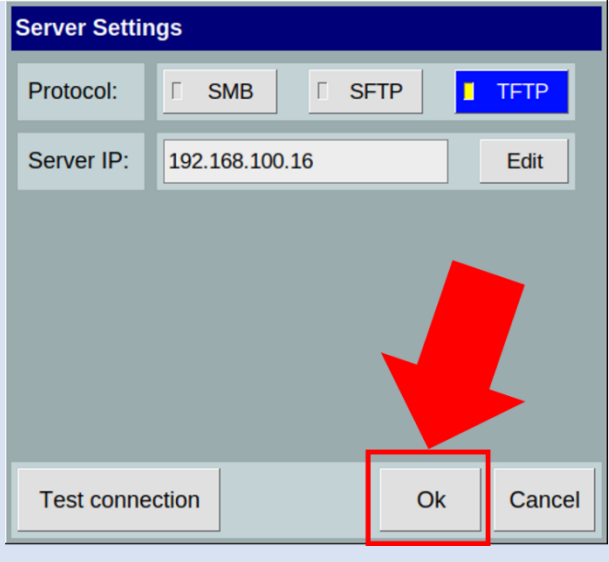
Test connection Ok Cancel

Test the connection with **Test Connection**.



INFORMATION!
When the connection cannot be established check the Ethernet cable connection. Main the network IP address of the server, the used protocol, the name of the shared folder (**SMB**) on the server and the server account login data (**SMB**, **SFTP**). Consult the manuals of your server operating system and your system administrator.

9



Close Dialog with **OK**.

9.12.3 Workflow: Manual Transfer of measurement files to USB-Stick



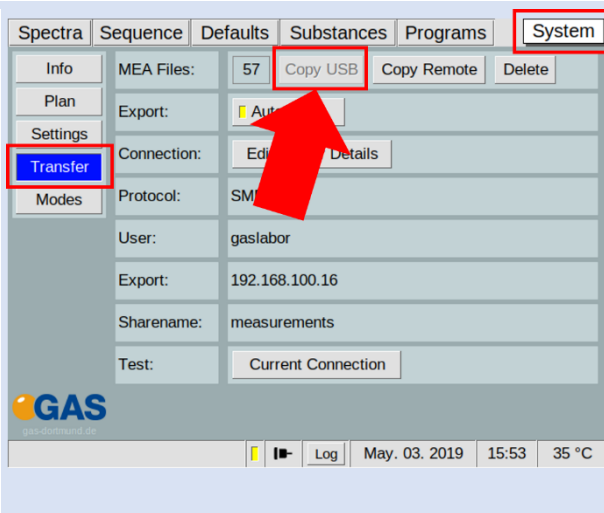
INFORMATION!
Do not turn off the device during the download process!

1



Connect the USB device (FAT32-formatted) to the USB socket at the front side of the housing.

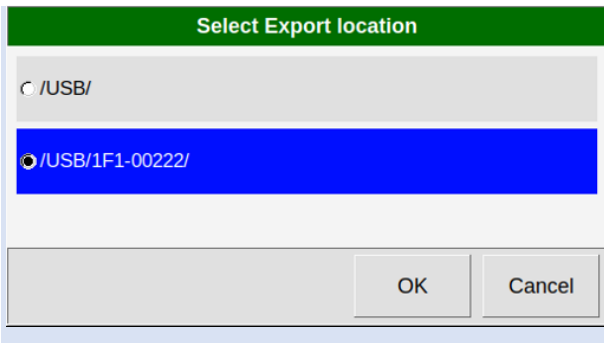
2



Open page: **System** > **Transfer**.

Press: **Copy USB**.

3



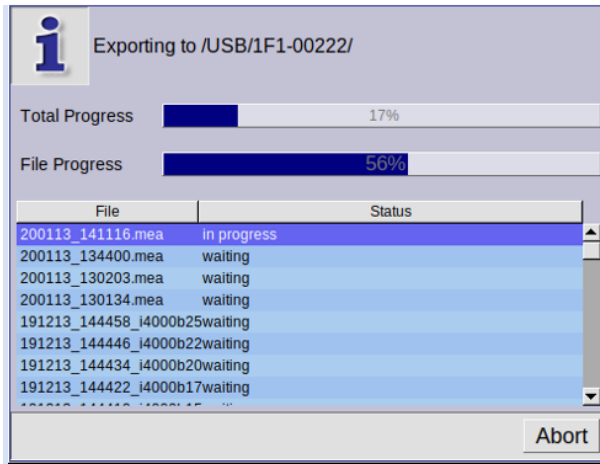
A confirmation dialog opens. Select the storage location.

Press **OK** to start the process.



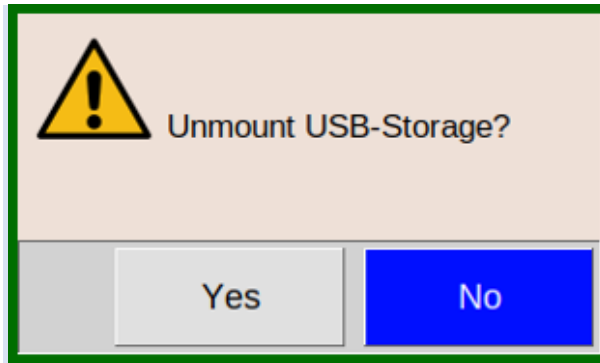
INFORMATION!
All internally stored measurements are transferred.
The process can be stopped at any time

4



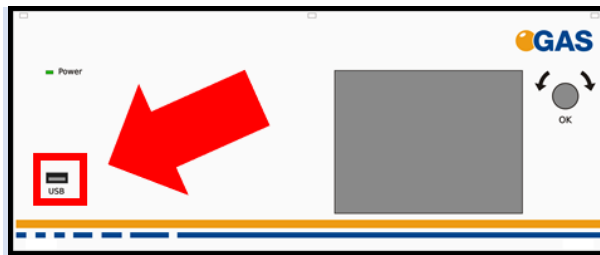
Wait until the exporting process is completed.

5



A confirmation dialog opens. Press **OK** to unmount the USB-Stick

6



Remove the connected USB device from the **USB** socket at the front side of the housing.



The measurement files has been downloaded.

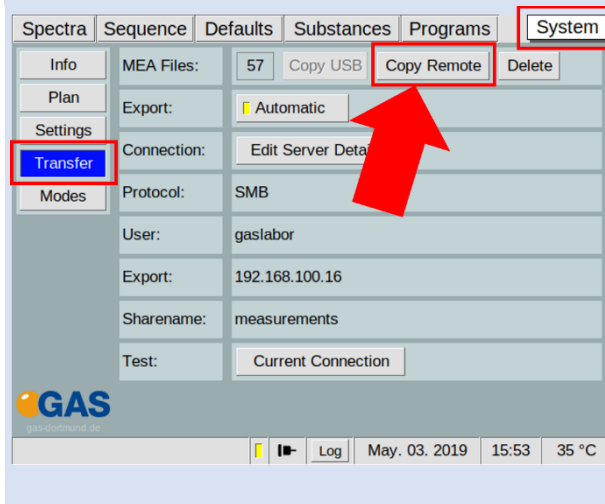
9.12.4 Workflow: Manual Transfer of measurement files to connected server



INFORMATION!

Do not turn off the device during the download process!

1



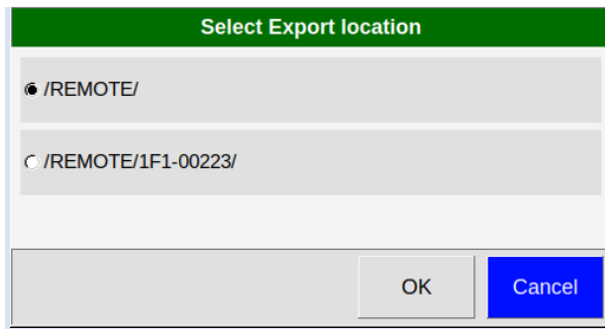
Open page:

System > **Transfer**.

Press:

Copy Remote.

2



A confirmation dialog opens. Select the storage location.

Press **OK** to start the process.



INFORMATION!

All internally stored measurements are transferred.

The process can be stopped at any time

3

File	Status
190112_154137.me	done
190112_132324.me	in progress
190112_125958.me	waiting
190112_122802.me	waiting
190112_095523.me	waiting
190111_162300.me	waiting
190111_135805.me	waiting
190111_124921.me	waiting

Wait until the exporting process is completed.



The measurement files have been exported.

9.13 Workflow: Current Loop Setup (only available in Version 4G2)

9.13.1 Introduction

The device writes the measured concentration of the main substance as electrical current to the 0-20 mA-current loop interface.

The concentration range of the output substance is mapped to a sub-interval within 0-20 mA.

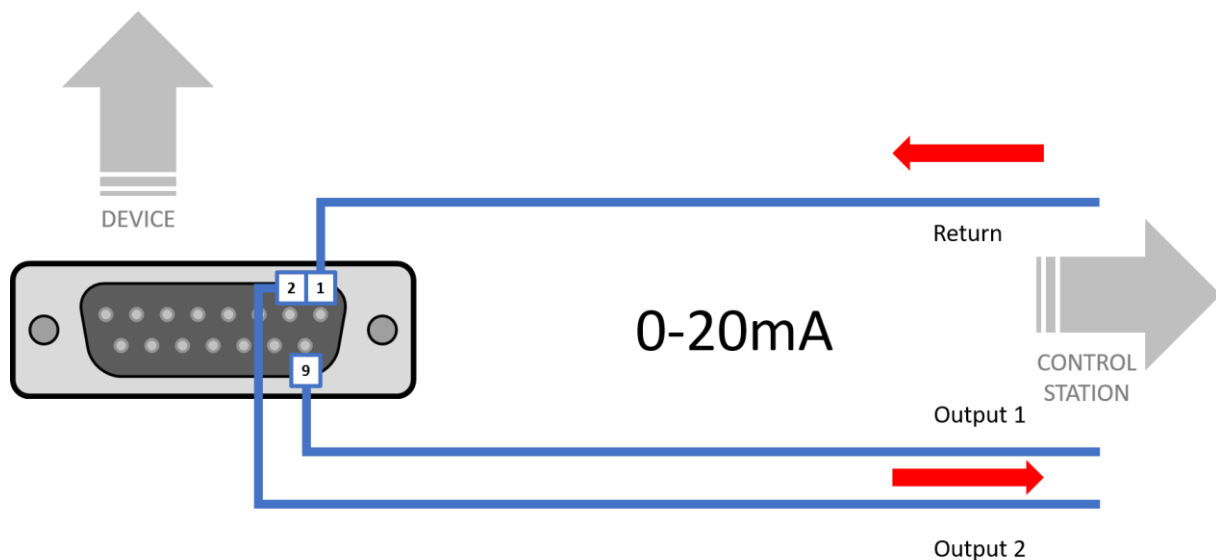
Outside this sub-interval a mA-error value and a mA-idle value can be defined.

The error value is set when a measurement has failed to produce a valid concentration.

The idle value is set when no valid concentration is available yet or when the interval mode is not active.

9.13.2 Electrical Interface

The current loop must be connected to the **Signal Converter – I/O Ports** socket at the rear of the housing according to the following diagram:



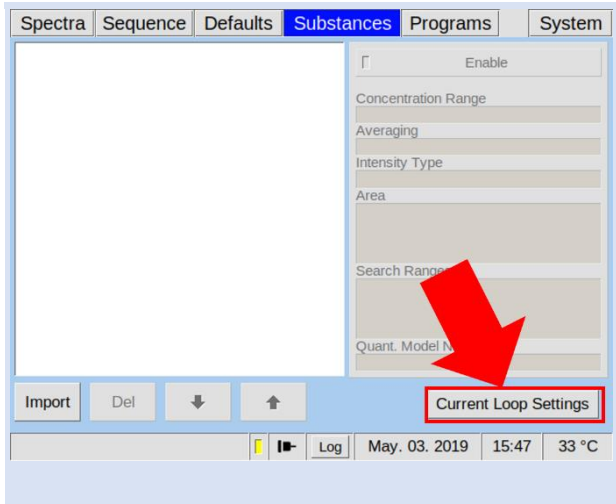
9.13.3 Configuring the Current Loop



INFORMATION!

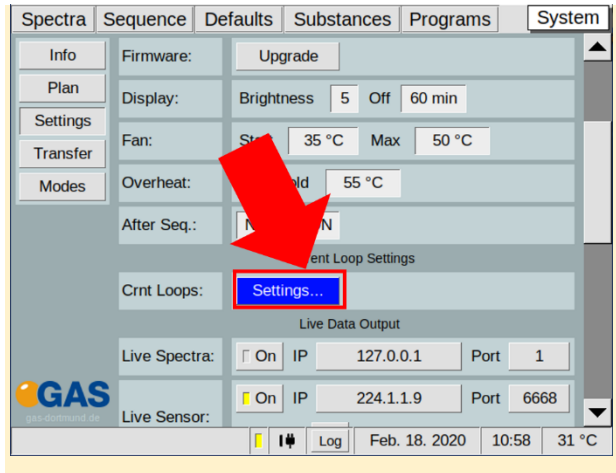
For concentration value output through the 0-20mA current loop the socket **Signal Converter – I/O Ports** at the rear of the housing must be connected to an appropriate cable to a display unit.

1a



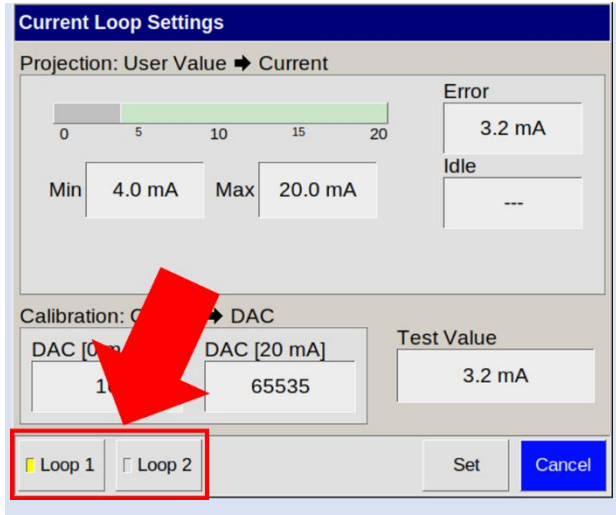
Open dialog:
Substances > **Current Loop Settings**.

1b
 Option



Optional open dialog:
System > **Settings** > **Settings**.

2



Select **Loop 1** or **Loop 2**.
Loop1: Output of the first substance result.
Loop2: Output of the second substance result.



INFORMATION!
 Only two substance results can be transferred. These must be at the first and second position in the substance list.

3

Current Loop Settings

Projection: User Value → Current

0 5 10 15 20

Min 4.0 mA Max 20.0 mA

Error 3.2 mA

Idle ---

Calibration: Current → DAC

DAC [0 mA] DAC [20 mA] Test Value

16 65535 3.2 mA

Loop 1 Loop 2 Set Cancel

In **Projection: User Value**

-> **Current** set **Min** and **Max** value of the concentration range to the range 0 mA – 20 mA.

4

Current Loop Settings

Projection: User Value → Current

0 5 10 15 20

Min 4.0 mA Max 20.0

Error 3.2 mA

Idle ---

Calibration: Current → DAC

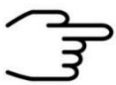
DAC [0 mA] DAC [20 mA] Test Value

16 65535 3.2 mA

Loop 1 Loop 2 Set Cancel

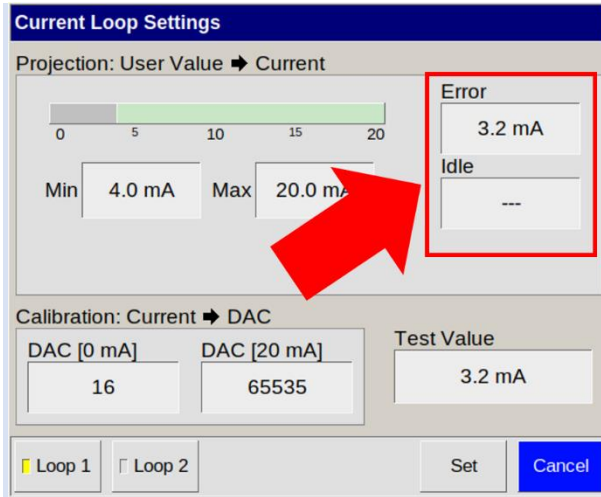
In **Calibration: Current ->**

DAC set **DAC [0 mA]** and **DAC [20 mA]** calibrate to 0-20 mA by observing the outputted mA value on the external display unit. The values on the picture are examples. The values for DAC [0 mA] and DAC [20 mA] are preset by G.A.S. but **must be adapted by the user.**

**INFORMATION!**

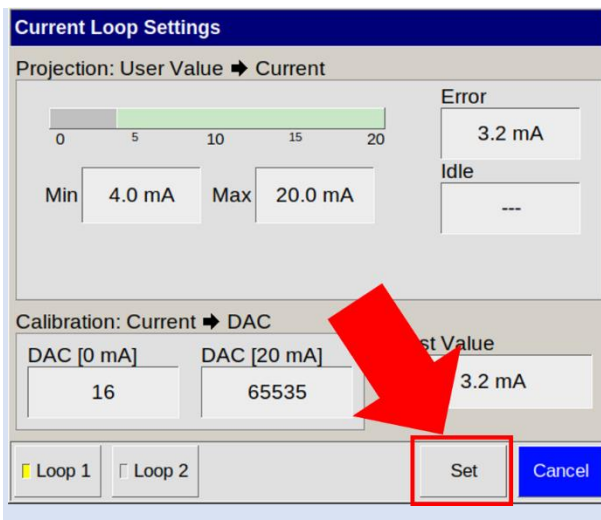
The values for DAC [0 mA] and DAC [20 mA] are preset. The correct values for DAC [0 mA] and DAC [20 mA] must be adapted by the user.

5



When desired set mA values for error and idle state with **Projection User Value -> Current Error** and **Idle**.

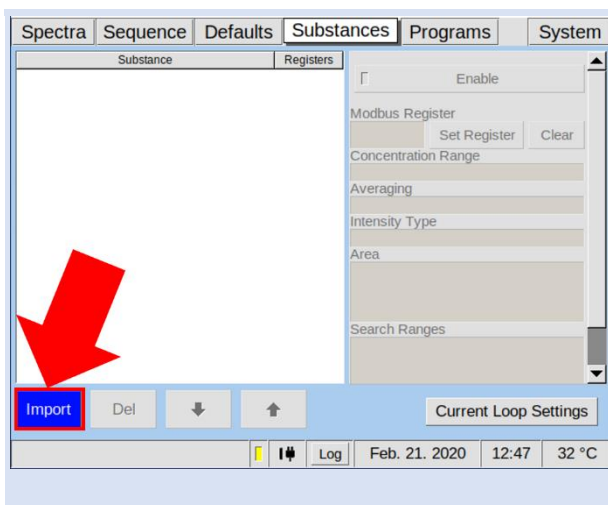
6



Close the dialog with **Set**.

9.14 Workflow: Modbus TCP Setup

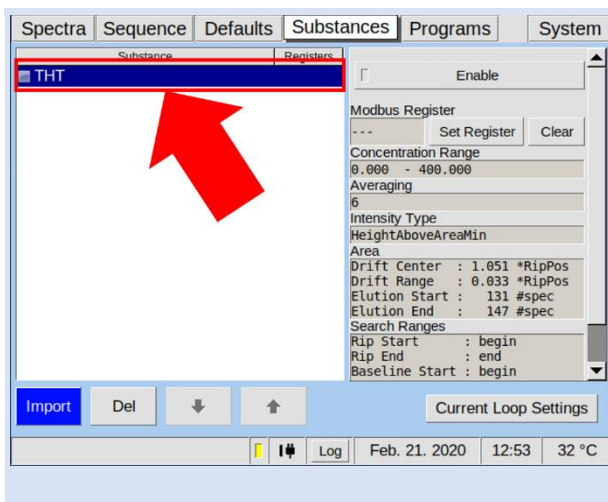
1



Open dialog:

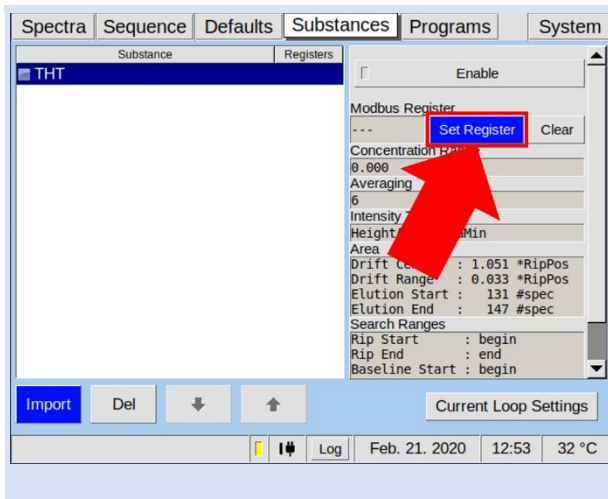
Substances > **Import** to import a substance file list named **calibration.gsd**

2



Select a Substance to setup the Modbus TCP register.

3



Select **Set register** to open the **Setup Dialog**.

4

Enter First Register (Total size will be 6)

Min: 7
Max: 120

7 8 9
4 5 6
1 2 3
0

Clear
←

OK Cancel

In **Setup Dialog** enter the Register Values.

5

Spectra Sequence Defaults Substances Programs System

Substance	Registers
<input checked="" type="checkbox"/> THT	7-12

Enable

Modbus Register
7 - 12 Set Register Clear

Concentration Range
0.000
Average
6
Inter
HeightAl
Area
Drift Cent : 1.051 *RipPos
Drift Range : 0.033 *RipPos
Elution Start : 131 #spec
Elution End : 147 #spec
Search Ranges
Rip Start : begin
Rip End : end
Baseline Start : begin

Import Del ↓ ↑ Current Loop Settings

Log Feb. 21. 2020 13:06 31 °C

In **Substances Window** the entered **Register range** is displayed.

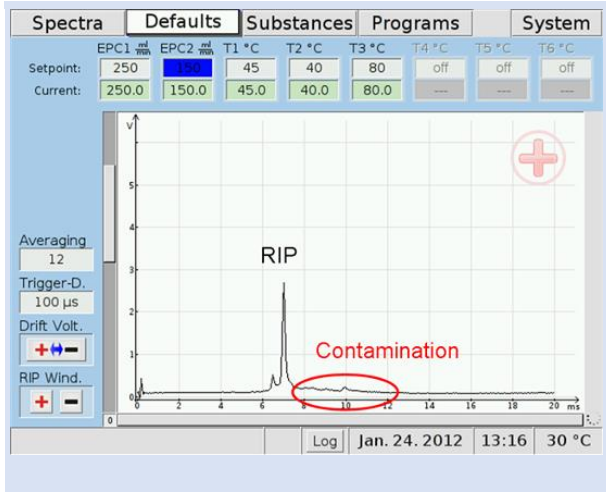
9.15 Workflow: Start Cleaning mode



INFORMATION!

In case of contamination it is helpful to activate the cleaning mode to clean the system.

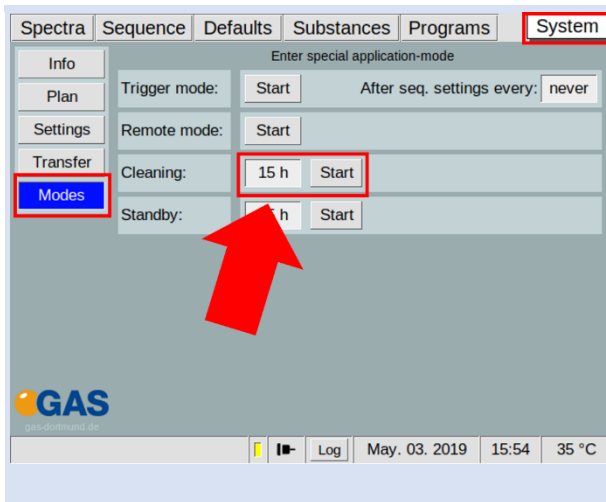
1



In case of contamination it is helpful to activate the cleaning mode to clean the system.

The frequency of cleaning interval is depending on the character and quantity of the samples.

2

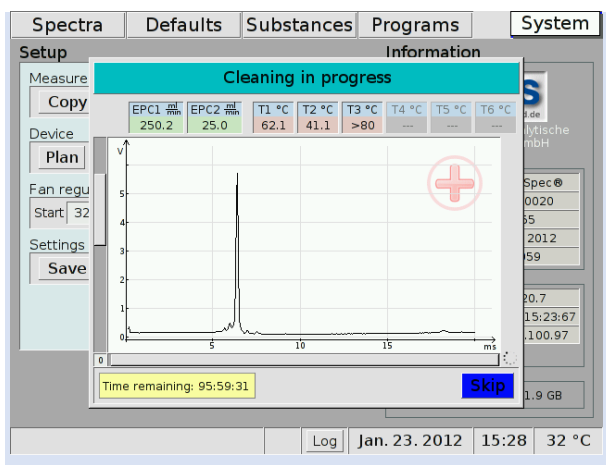


Select **System** > **Modes** > **Cleaning [x h]** and set the cleaning duration time.

Select **Start** to start the cleaning process.

All temperatures are set up to their maxima.

3



During the cleaning process a Cleaning window appears. During this process no other activities can be executed. This process can be skipped at any time.

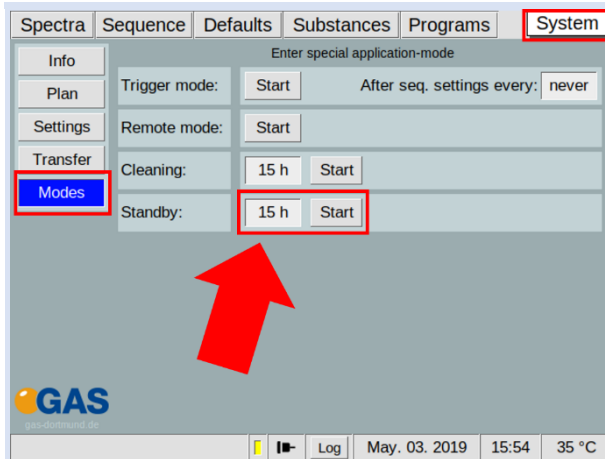
9.16 Workflow: Start Standby mode



INFORMATION!

It is recommended not to switch off the device during measurement breaks. Using the Standby mode ensures the cleanness of the system and a quick readiness to measure.

1

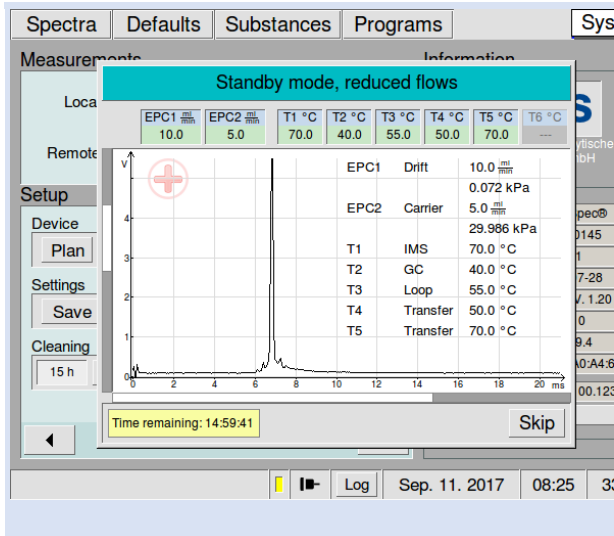


Select **System** > **Modes** > **Standby [x h]** and set the standby duration time.

Select **Start** to start the Standby process.

Driftgas (EPC1) is set to **10 ml/min** and Carriergas (EPC2) is set to **5 ml/min**.

2



During the standby process a Standby Window appears.

During this process no other activities can be executed.

This process can be skipped at any time.

9.17 Workflow: Remove the Housing Cover



DANGER!

Before all work on the device switch off the device and pull out the power plug!

1



Switch off the device and pull out the power plug.

2a



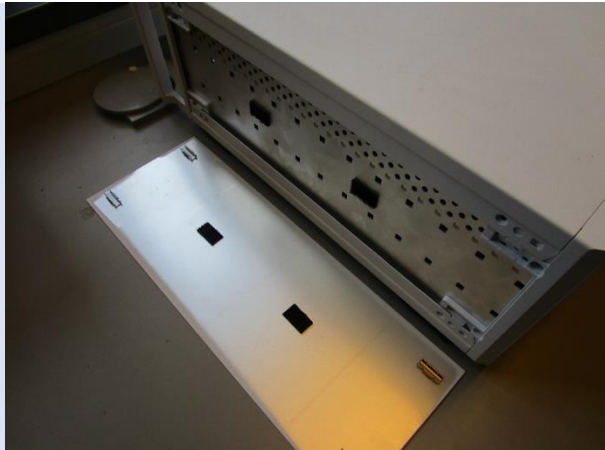
Open the side-covers of the case carefully using a screwdriver.

2b



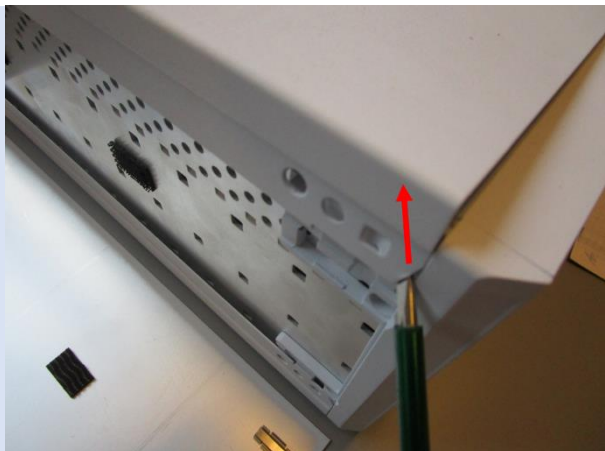
Remove the side-covers of the case carefully

2c



Removed side-cover.

3a



Open the top-cover of the case carefully using a screwdriver.

3b



Remove the top-cover of the case carefully

4



Device without top cover.

9.18 Workflow: Change Capillary Column



DANGER!

Before all work on the device switch off the device and pull out the power plug!

1



Necessary tools:

1. Small slotted screw driver
2. T10 Torx screwdriver
3. 8mm wrench
4. 1/16 " Swagelok screw connections
5. Teflon Ferrule with hole (depending on the column dimensions)
6. Column cutter
7. Capillary column

2



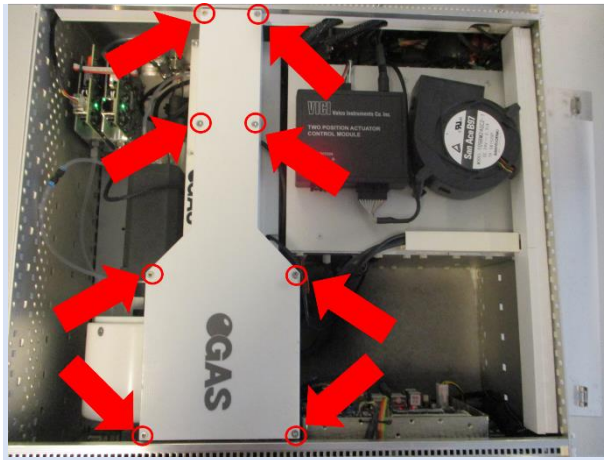
Switch off the device and pull out the power plug.

3



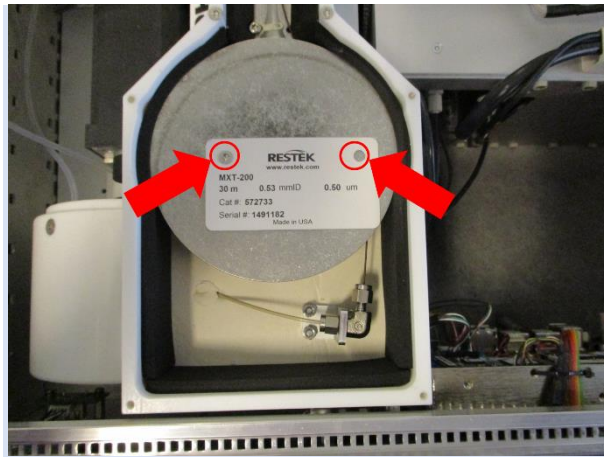
Remove the top cover.
For detailed information see [Workflow: Remove Housing Cover](#)

4



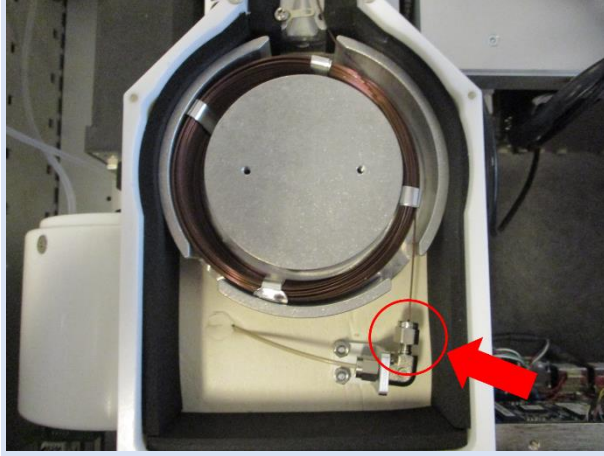
Release all screw of the oven-cover and remove it.

5



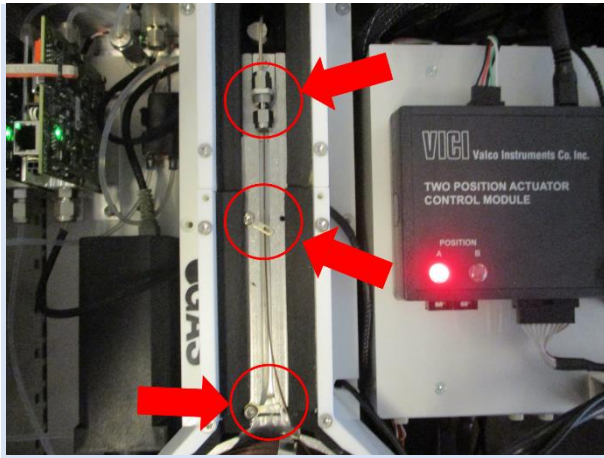
Release all screw of the inner oven-cover and remove it.

6



Open the capillary-column-connectors using a 8 mm open-end-wrench.

7

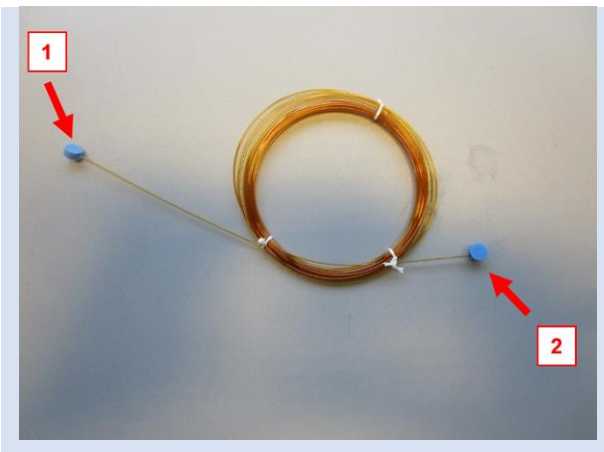


Open the capillary-column-connectors using a 8 mm open-end-wrench.

Also open the transfer line securing holder.

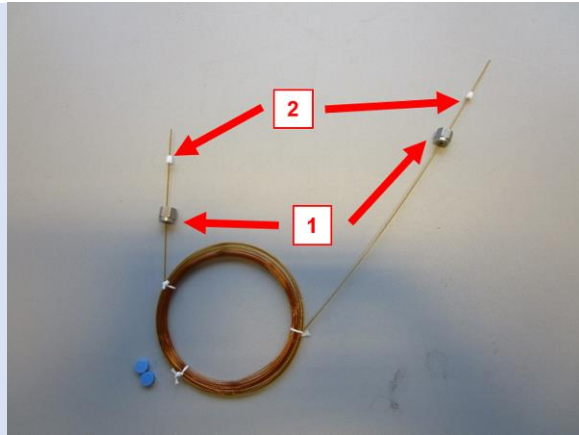
Remove the capillary column.

8



Remove the blind bolts (1) + (2) of the capillary column

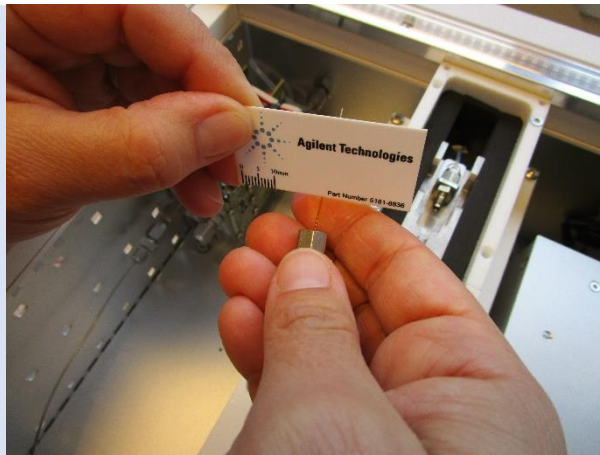
9



Insert the 1/16" screw connectors and the Teflon-ferrules with hole.

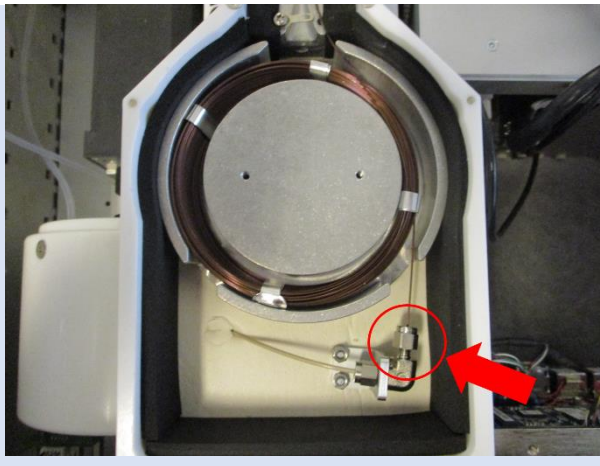
Ensure that the distance between ferrule and column end is about 5 mm.

10



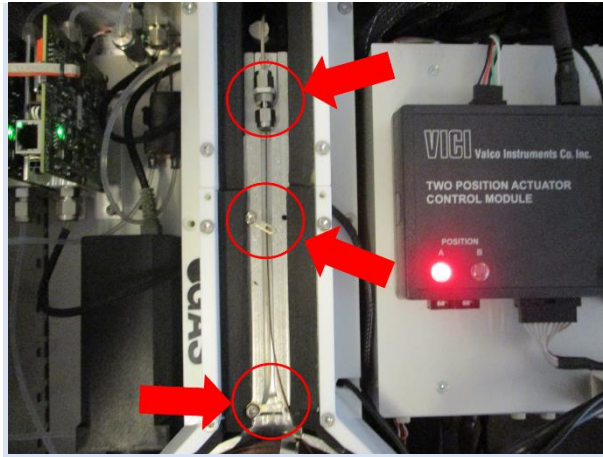
Put the new capillary column into the oven. If necessary cut the ends of the column.

11



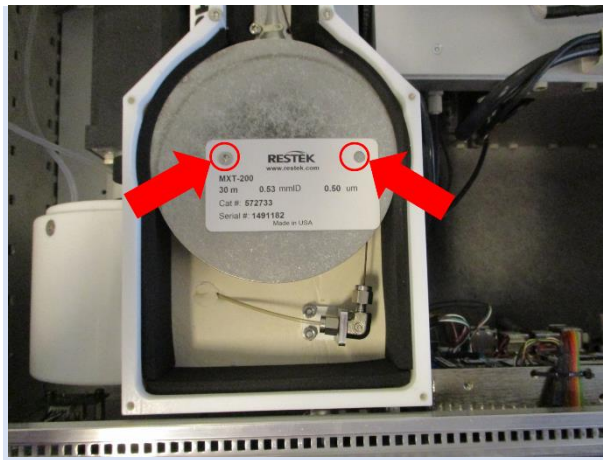
Connect the capillary-column-connector using two 8 mm open-end-wrench.

12



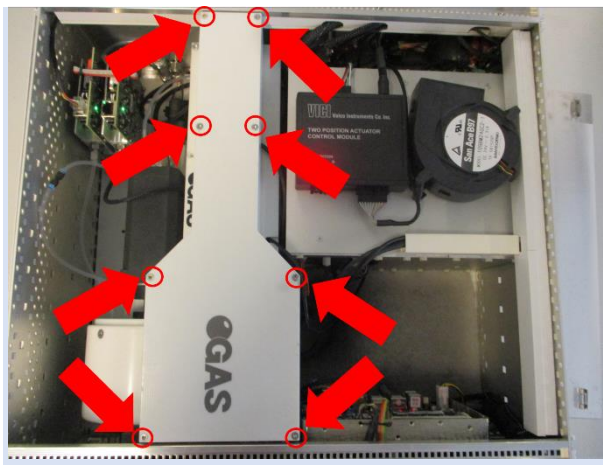
Connect the capillary-column-connector using two 8 mm open-end-wrench. Also close the transfer-line securing holder.

13



Mount the screws of the inner oven cover. Make sure that the column labeling is screwed on.

14



Mount the screw of the oven cover.
Attach the top cover, the bottom cover and the side cover.
Install all connections and switch on the device.

9.19 Workflow: Change sample pump unit



INFORMATION!
Only authorized, trained and technically instructed people are allowed to do these work steps.



DANGER!
Before all work on the device **switch off the device** and **pull out the power plug!**

1



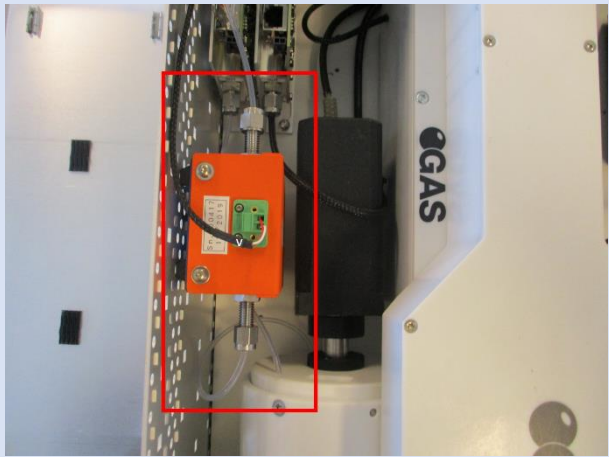
Switch off the device and pull out the power plug.

2



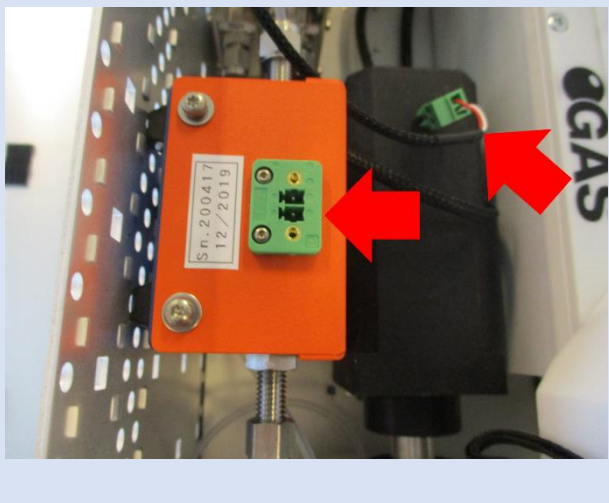
Remove the top cover.
For detailed information see **Workflow: Remove Housing Cover**

3



Top view of installed sample pump unit.

4



Remove the plug.

5



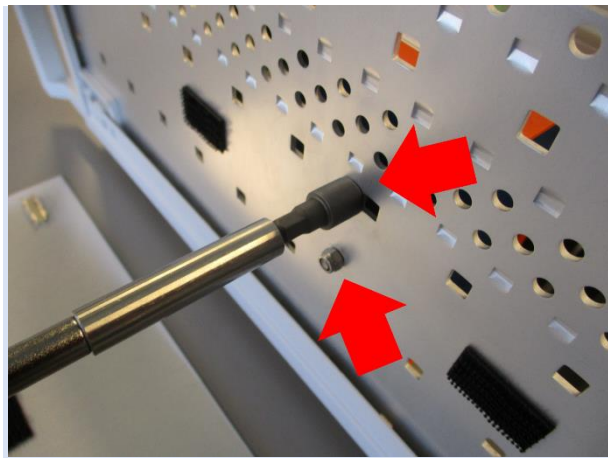
Loosen front connector.

6



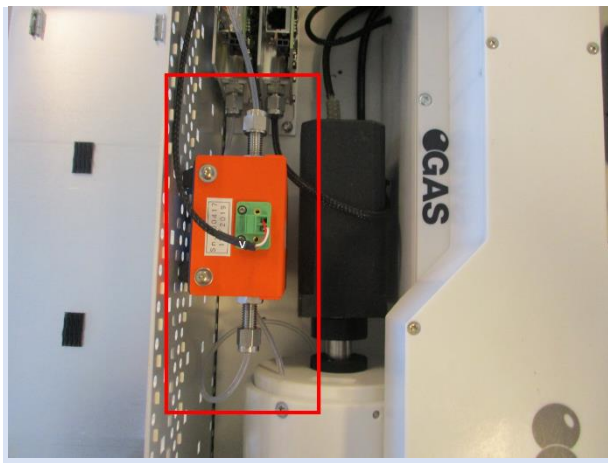
Loosen rear connector.

7



Loosen the fixing screws and remove the sample pump unit.

8



Insert a new sample pump unit and mount it in reverse order.

9.20 Workflow: Change high voltage circuit board



INFORMATION!

Only authorized, trained and technically instructed people are allowed to do these work steps.



DANGER!

Before all work on the device **switch off the device** and **pull out the power plug!**

1



Switch off the device and pull out the power plug.

2



Loosen three Screws at the front of the device.

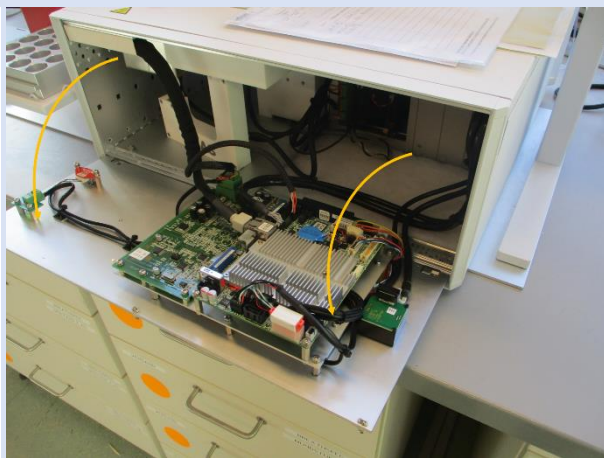
3



Remove the top cover.

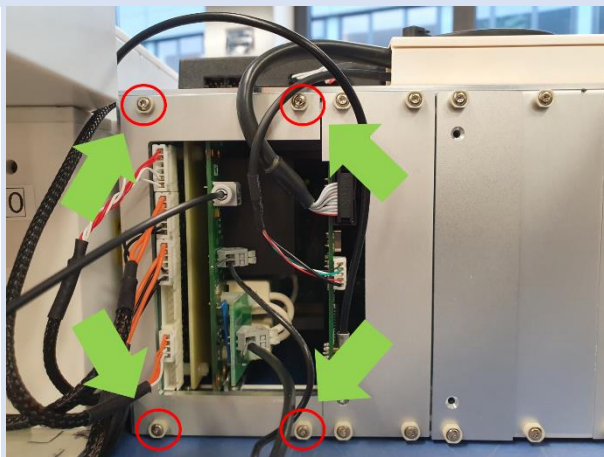
For detailed information see [Workflow: Remove Housing Cover](#)

4



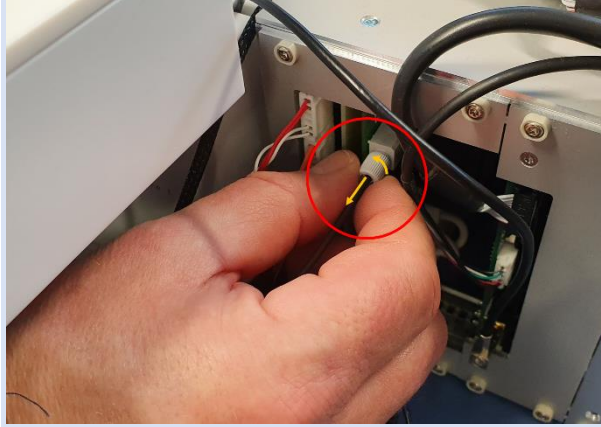
Open the front panel.

5



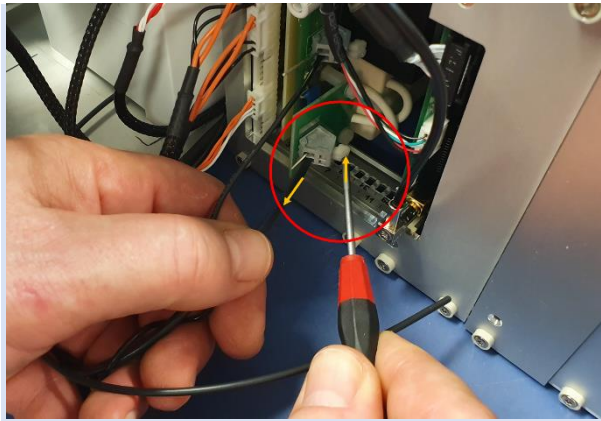
Loosen four screws with T8 screwdriver and remove the coverplate.

6



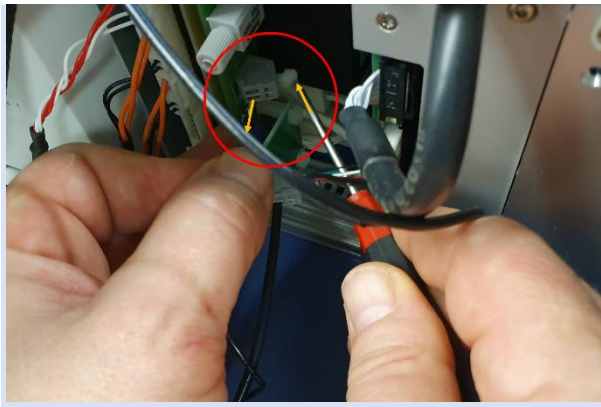
Loosen the nut from transmitter and pull out fibre-optical-cable.

7



Push the button and pull out high voltage wire

8



Push the button and pull out ground wire

9



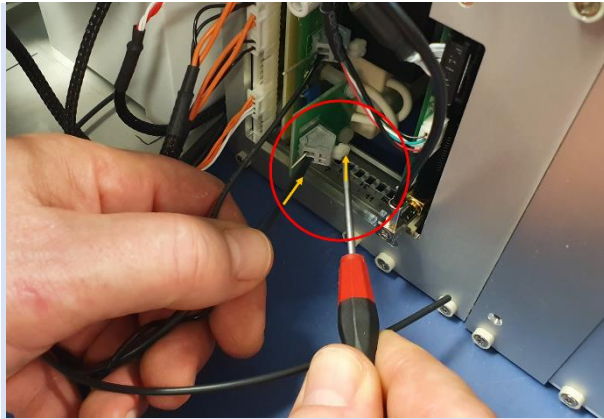
Pull the circuit board out of the casing profile

10



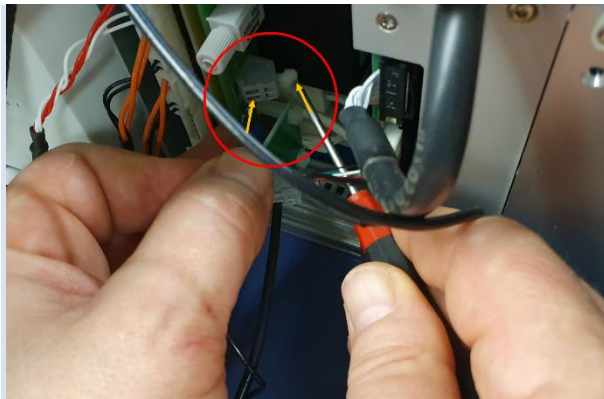
Insert the new circuit board

11



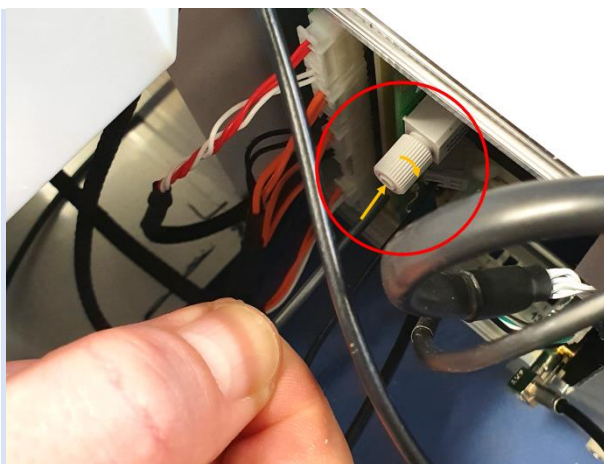
Push the button and reinsert the ground wire

12



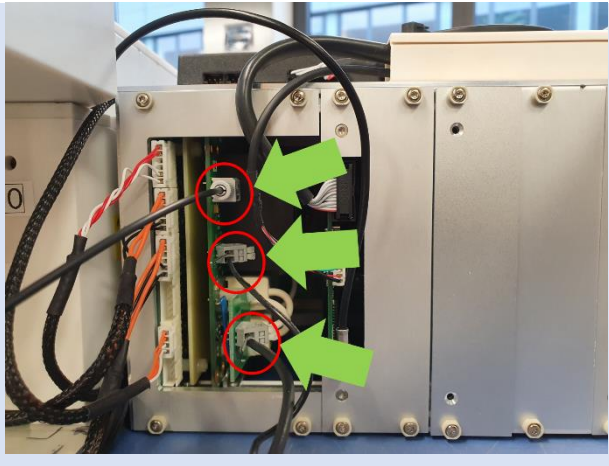
Push the button and reinsert the high voltage wire

13



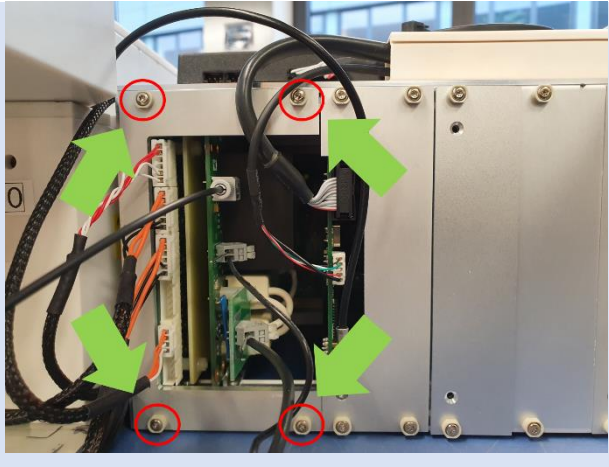
Reinsert the optical fiber cable and tighten the screw connection.

14



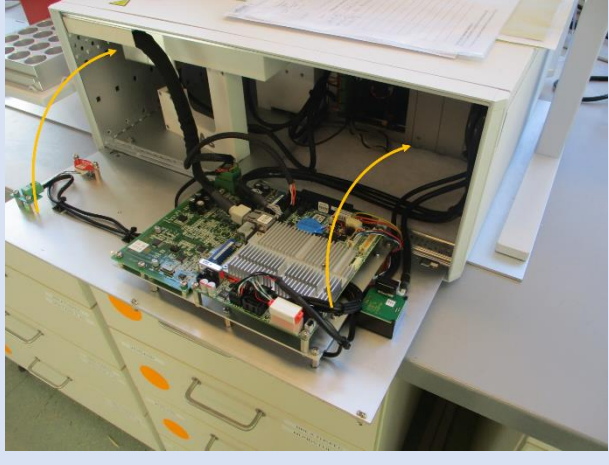
View of the three connected wires.

15



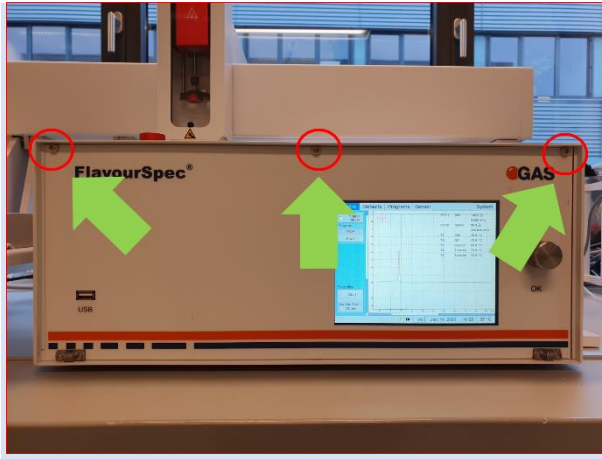
Replace the cover plate and tighten the four screws.

16



Close the front plate and attach the top cover.

17



Tighten the three screws of the frontplate.

9.21 Workflow: Reinitialize the 6-Port-Valve



INFORMATION!

Only authorized, trained, and technically instructed people are allowed to do these work steps.

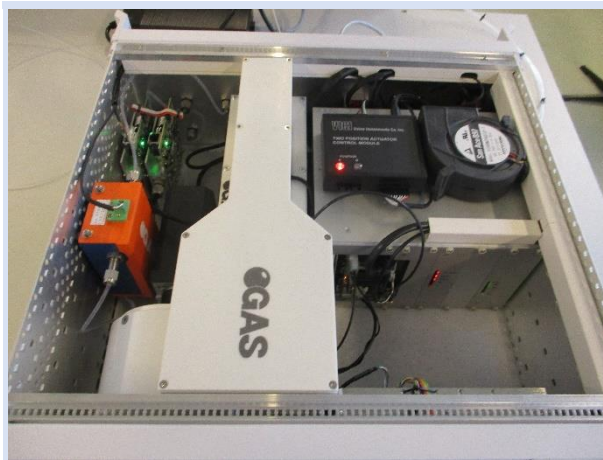


DANGER!

The device must be operated in the open state.

Be very careful!

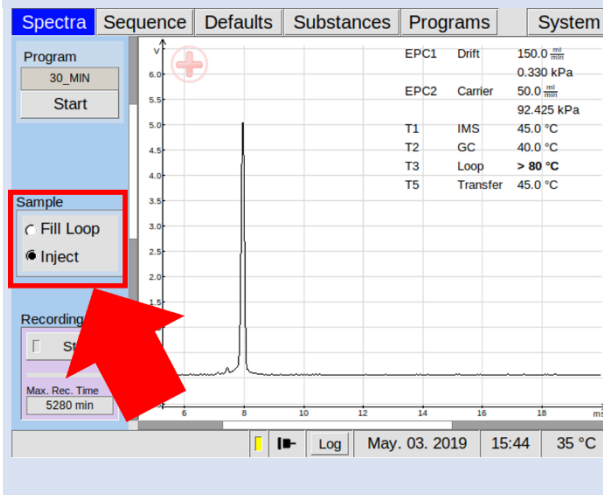
1



Remove the top cover.

For detailed information see [Workflow: Remove Housing Cover](#)

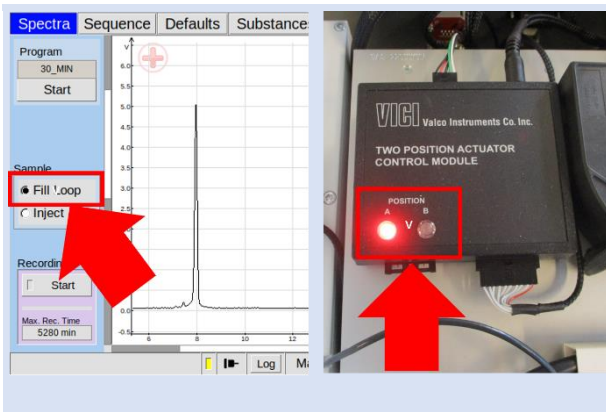
2a



Select **Spectra** > **Sample**.

Switch valve **several times** between position **Fill Loop** and **Inject**.

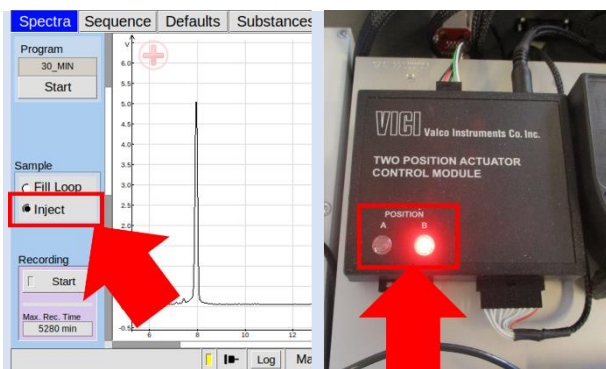
2b



Valve position Fill Loop:

Controller **LED in POS-A**

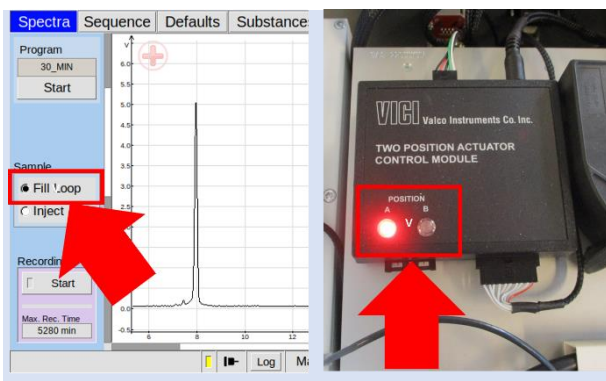
2c



Valve position Fill Loop:

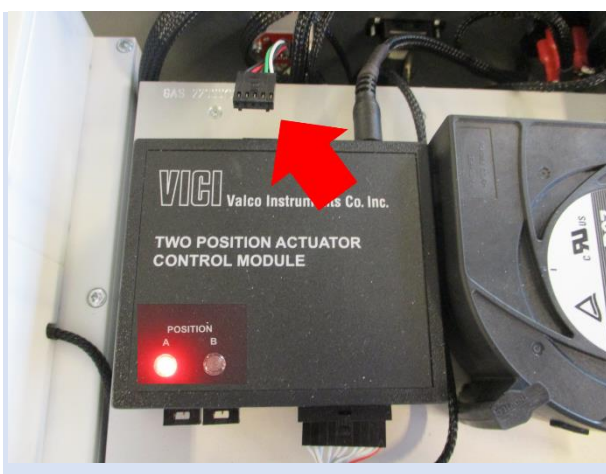
Controller **LED in POS-B**

3a



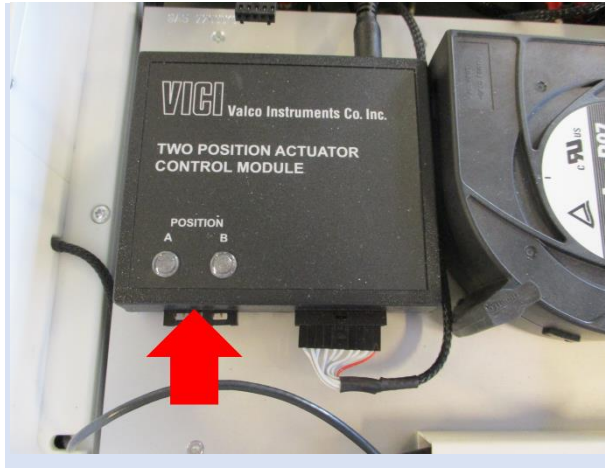
Switch Valve to position
Fill Loop

3b



Disconnect the **five-pin
plug** of the valve
controller.

4



Switch the valve as long as both controller LEDs are off.

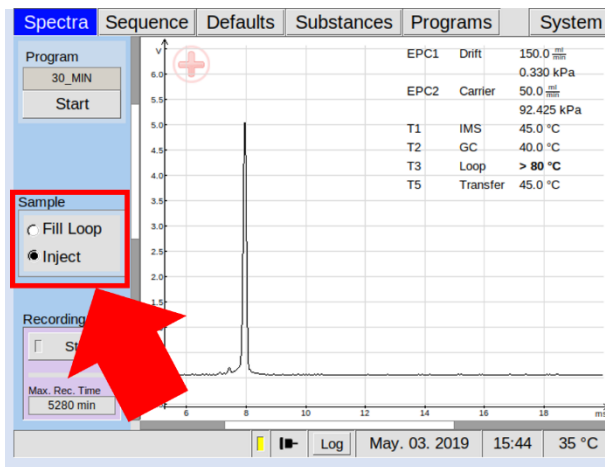
The valve is now in **initialization mode**.

5



Replug the **five-pin connector** of the valve controller.

6



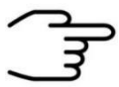
Switch valve about **eight times** between position **Fill Loop** and **Inject**.

The switching noise is extended.

8



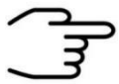
The controller finds a position again and the **switching noise is normal** again.



INFORMATION!

If the valve cannot find a position or the switching noise does not return to normal, repeat the procedure.

9.22 Workflow: Change filter set CGFU



INFORMATION!

It is recommended change the filter set of the Circular gas flow unit periodically. The recommended maintenance interval is every **6 month**.



DANGER!

Before all work on the device switch off the device and pull out the power plug!

1



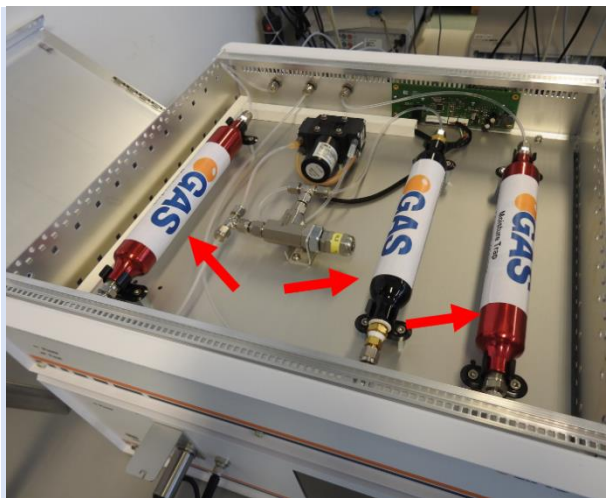
Switch off the device and pull out the power plug.

2



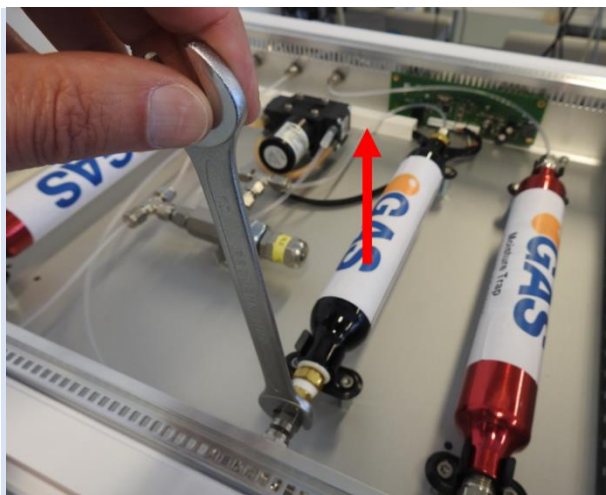
Remove the side-covers of the CGFU-case carefully with a small screwdriver and remove the cover.

3



The two molecular sieve cartridges (Red) and the activated carbon cartridge (Black) must be replaced periodically **every 6 month**.

4



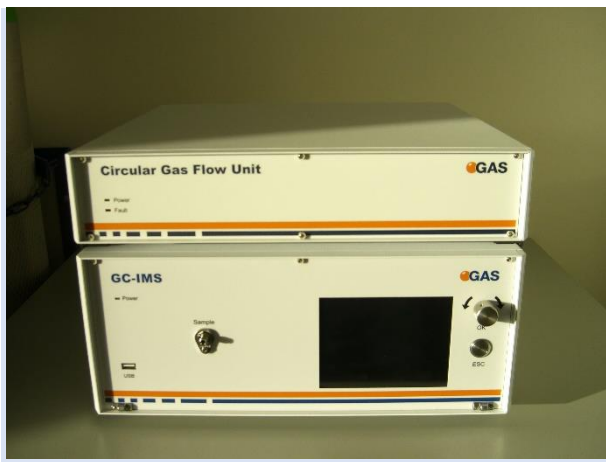
Loosen the connectors with a spanner and remove the cartridges in upwards direction.

5



Insert a new cartridge into their clips and tighten the connector screws.

6



Attach the top cover.
Connect the power plug
and switch on the device.

9.23 Workflow Firmware Upgrade

The firmware of G.A.S. IMS devices can be upgraded by the user with an upgrade file – named update.gas - provided by G.A.S.

This file has to be put on an empty USB storage device (e.g. 'USB stick' / 'USB thumb drive') formatted as a FAT32 file system.



INFORMATION!

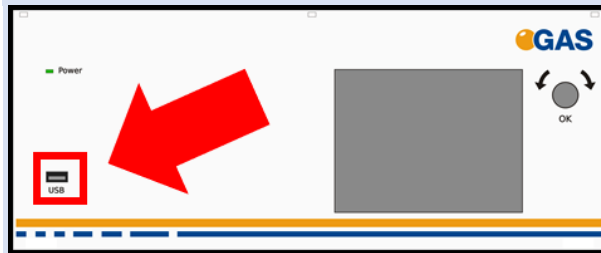
The USB storage device must be formatted to FAT32. Consult your system administrator on formatting USB devices.



INFORMATION!

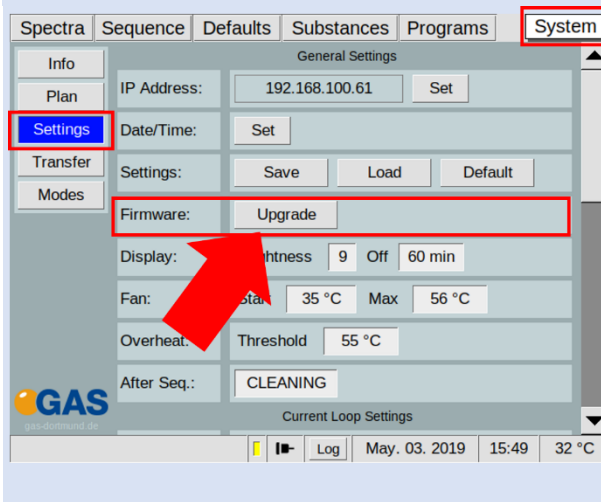
Do not turn off the device during the upgrade process!

1



Connect the **USB device** (**FAT32-formatted**) with the upgrade file – named **update.gas** - provided by G.A.S. to the **USB socket** at the front side of the housing.

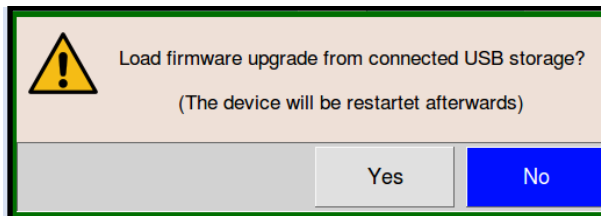
2



Open page:
System > **Settings**.

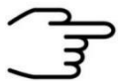
Press:
Firmware > **Upgrade**.

3



A confirmation dialog opens.

Press **Yes** to start the process.



INFORMATION!

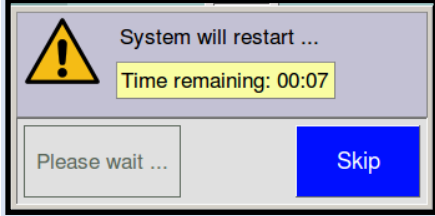
Do not turn off the device during the upgrade process!
Do not remove the USB device!

The upgrade process will take one minute or more depending on the tasks that are performed during the process.

4

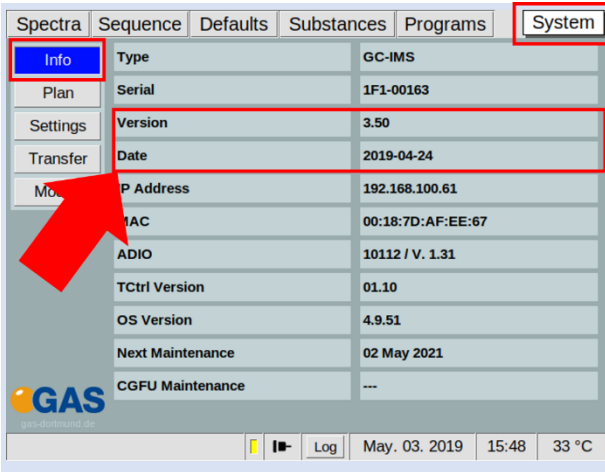


Wait until the process is completed and a system restart dialog opens.

5  Wait for the device to restart or press **Skip** to restart the device immediately.

6  **Now:** Remove the connected USB device from the **USB** socket at the front side of the housing.

7  Wait until the device has started and the user interface is visible on the screen.

8  Open page: **System** > **Info**.
Verify that the new firmware version has been installed.



The device firmware has been upgraded.

9.24 Workflow: Creating diagnostic information for support



INFORMATION!
The following steps are necessary to compile the required diagnostic information. Please stick on consecution as listed below.

1



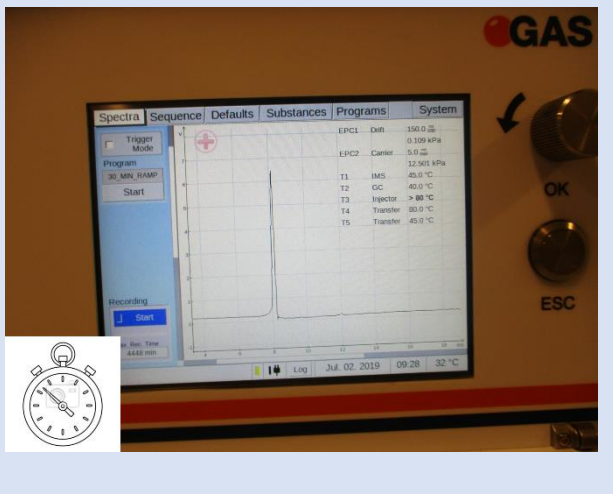
Take a picture of the instrument label on the rear side.

2



Switch on the device. Power LED front and switch (rear) have to be illuminated.

3



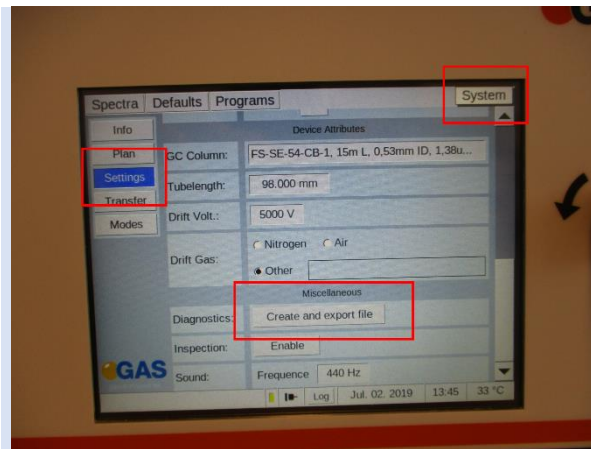
Inform how long it takes to boot up and to display of GUI in seconds. In case of error take a photo of the display.

4



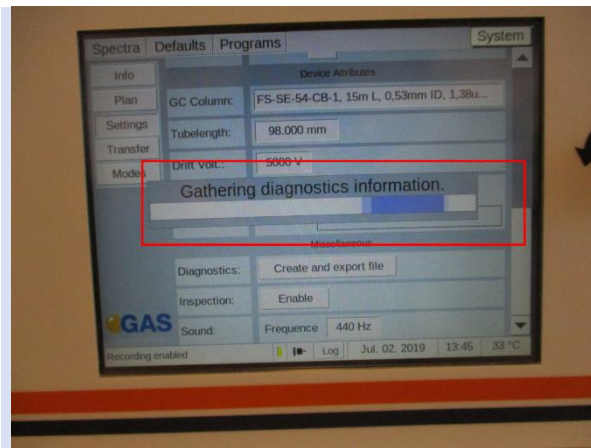
Insert a **FAT32 formatted USB-stick** into the **USB slot** at the front of the device.

5



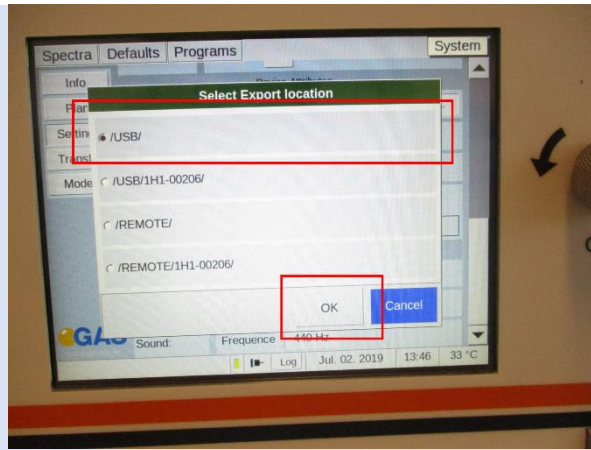
In **System Window** > **Transfer** select Settings and start the diagnostic file compilation by selecting the **Create and Import file Button**.

6



The diagnostic file is created.

7



Select Export Location
/USB/ and press **OK**.

8

Name
Diag_1H1-00203_190702_144931.gas

Send the **diagnostic file**
and the **photos** taken by
user by data transfer to
support@gas-dortmund.de

9.25 Workflow: Packing for return transport



INFORMATION!

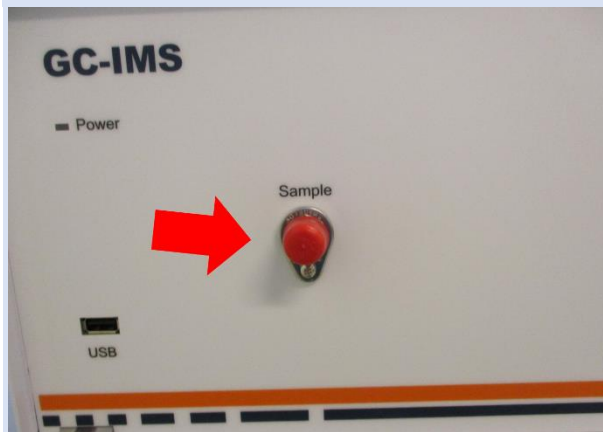
It is recommended to **use the original transport box** for a safe return transport.



INFORMATION!

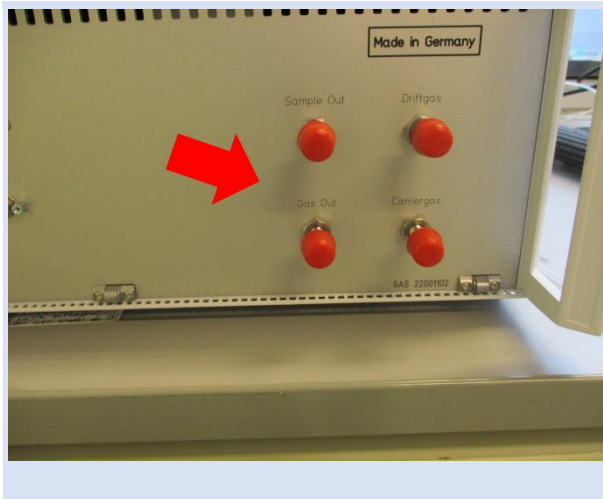
It is recommended to **to send the transport box on palett** for a safe return transport.

1



Close all gas connections with the red caps on the front side of the device.

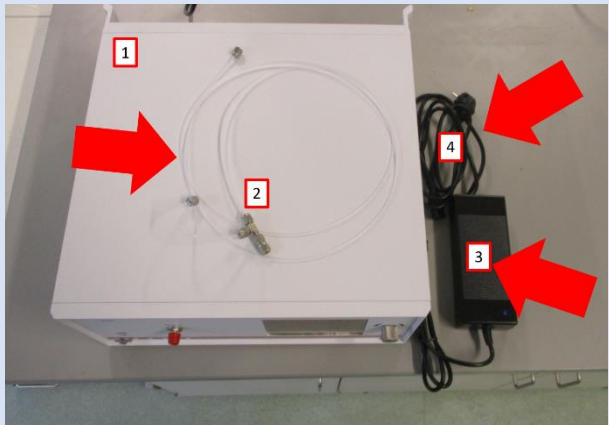
2



Close all gas connections with the red caps on the rear side of the device.

BreathSpec® – User Manual

3



Minimum scope of delivery for the return transport: Device 1, Hoses 2, power supply 3 and plug 4

4



It is recommended to return the system in the original box and on palett. Further accessories can be supplied optionally.

9.26 Workflow: Manual modification of the sample description attribute.

The attribute sample description can be changed manually in the measurement file. For this purpose a text editor is required, e.g. the free editor **Notepad++** [<https://notepad-plus-plus.org/>].



INFORMATION!

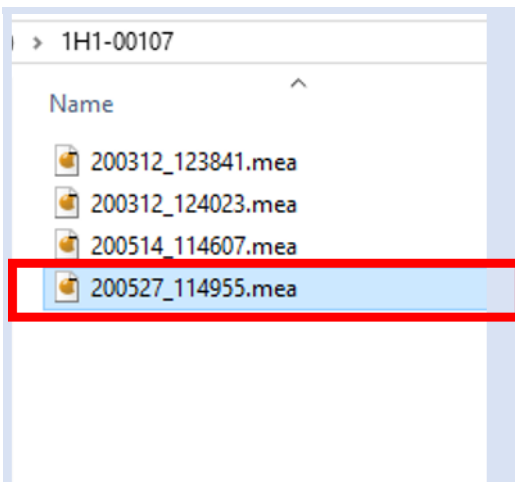
Only authorized, trained and technically instructed people are allowed to do these work steps. Please contact us in any case before you start working.

Only use the recommended text editor notepad++ [<https://notepad-plus-plus.org/>].

Wrong input can corrupt the measurement file.

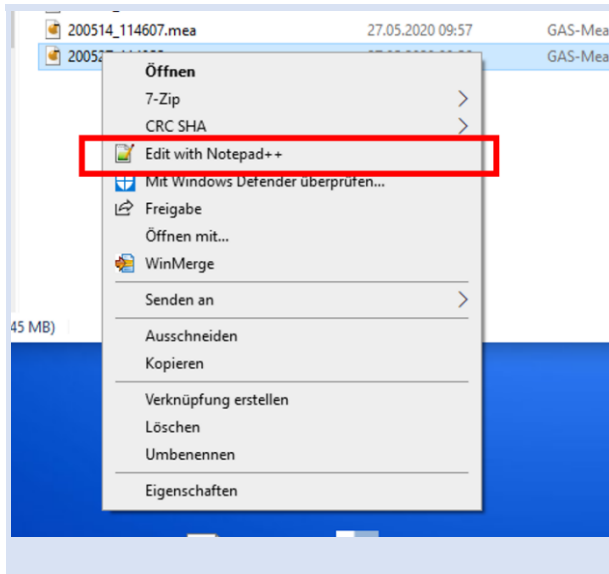
Only work with a copy of the measurement file.

1



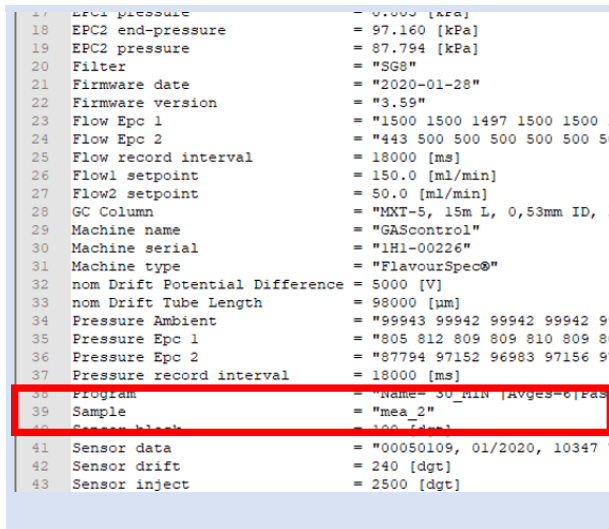
In windows explorer **select a copy** of the measurement file.

2



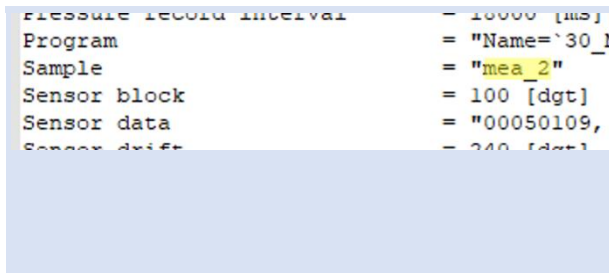
With **right click** on measurement file select **Edit with Notepad++**.

3



In the opened measurement file find the attribute **Sample**.

4



Change sample description **(Entry between the quotation marks)**. **Save the measurement file.**

10 Appendix

10.1 Technical data: BreathSpec®

Dimensions	<ul style="list-style-type: none"> • Housing: 19"-compatible • Height: 184.5 mm • Width: 449 mm • Depth 435 mm • Weight: ca. 15 kg
Operational conditions	<ul style="list-style-type: none"> • Temperature range: +5 °C ... +40°C • Humidity: 0-90 % RH, non-condensating
Electrical Connectors	<ul style="list-style-type: none"> • 2 x RS232 DE9 plug • 1 x I/O DA15 socket • 1 x Ethernet RJ45 IEEE 802.3 100BASE-T • 1 x USB 2.0 Host (USB A Connector) • 1 x XLR 3-pole male, for power supply
Power Supply	<ul style="list-style-type: none"> • Input line voltage: Grounded AC, 85 to 264V • Input line frequency: 47-63 Hz • Input current: < 2.8 A • Output voltage: 24 VDC • Output current: 9.2 A internal • Power consumption: < 221 Watt
Cooling	<ul style="list-style-type: none"> • Axial ventilator, temperature-controlled, max. 5.5 m³/h
Gas connectors	<ul style="list-style-type: none"> • 3 mm stainless steel Swagelok-connector.
Internal hoses	<ul style="list-style-type: none"> • PFA
IMS-parameters	<ul style="list-style-type: none"> • Drifttube length: 53 mm • Electrical field strength: 500 V/cm • Resolution: ~ 45 • Operating temperature: 35–80°C
Ionisation source	<ul style="list-style-type: none"> • Radioactive - Tritium H³ (β⁻ Radiation)

Data acquisition	<ul style="list-style-type: none">• Sample-Rate: 150 kHz• Resolution: 14 bits• Trigger-duration: 100 µs• Trigger-repetition rate: 30 ms• Transimpedance: 3 V/nA typ.
Drift voltage	<ul style="list-style-type: none">• 2,7 kV Positive/negative Driftvoltage switchable
Sampling system	<ul style="list-style-type: none">• 6-port-valve• Sample loop: 1 mL (other volumes available on request)• Operation temperature: 35 – 80 °C (default 45 °C)• Temperature display accuracy: ± 1°C• Temperature control accuracy: ± 0,1 K
Data storage	<ul style="list-style-type: none">• Internal storage volume• Data transfer via LAN-connection via SMB, SFTP or TFTP (G.A.S. variant of TFTP)
Operation	<ul style="list-style-type: none">• 6.4" TFT Touchscreen• Pushable rotary knob
Standard Gaschromatic Capillary Column (Other Column types only on request)	<ul style="list-style-type: none">• Standard Stationary Phase:<ul style="list-style-type: none">• (Polyethethylene glycol)• Capillary column<ul style="list-style-type: none">• Identification: MXT-WAX• Film thickness: 0,5 µm• Column length: 30 m• ID: 0.53 mm• OD: 0.68 mm
Column oven	<ul style="list-style-type: none">• Operation temperature: 35 – 80 °C• Temperature-display accuracy: ± 1°C• Temperature-control accuracy: ± 0.1 °C
Flow Control EPC1 Driftgas	<ul style="list-style-type: none">• Type: Differential pressure control• Input Pressure: 3.0 bar (300 kPa) – 6.0 bar (600 kPa)

	<ul style="list-style-type: none">• Output Pressure Stability: 0.01%• Output Pressure Linearity: 0.05%• Operation flow rates: 0 – 500 mL/min
Flowcontrol EPC2 Carriergas	<ul style="list-style-type: none">• Type: Differential pressure control• Input Pressure: 3.0 bar (300 kPa) – 6.0 bar (600 kPa)• Output Pressure Stability: 0.01%• Output Pressure Linearity: 0.05%• Operation flow rates: 0 – 150 mL/min (depending on the GC-Column dimensions)
Consumables	<ul style="list-style-type: none">• Gas nitrogen 5.0 quality or Synthetic air 5.0 quality
Cleaning mode	<ul style="list-style-type: none">• IMS, column and sampling system are heated up to > 80°C (~ 100 °C).

10.2 Technical data: I/O Interface

Device Connector Specification		
Analog output	Output type Non-loaded voltage Maximum output signal Maximum output load (burden resistance) Accuracy Linearity error Temperature coefficient Output Ripple (RMS)	Isolated active current output 0-22 mA < 20 V < 25 mA 500 Ohm better than 0.5 % < 10 µA (guaranteed monotonic) < 1µA/K (t.b.d. < 10 µA)
Digital input	Input type Off-state voltage On-state voltage Input current	Isolated opto-coupler input < 1 V 5 .. 30 V < 20 mA depending on input voltage
Digital output	Output type Maximum open circuit voltage Maximum on-state saturation voltage Maximum on-state current	Isolated passive transistor output 30 V 2 V 20 mA
Relais output	Contact material Rated current Switching power Max. Switching voltage Min. Recommended contact load	AgPd alloy 0.1 A 12 VA, 3 W 24V DC, 120V AC 1 mA at 1 V DC
Isolation	Isolation type ¹ Surge voltage category Pollution degree Rated insulation voltage <hr/> ¹ All in-/outputs are isolated from instrument	basic insulation according to EN 61010 II 2 100 V DC or 100 Vrms AC

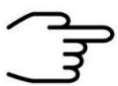
Device Connector Pinout

Connector type	D-Sub DA-15 female	
Analog output	Return ² Internal shunt Current output <hr/> ² PIN 1 is common return for both analog outputs and for digital transistor output	Pin 1 Pin 2 Pin 9
Digital input	Negative Positive	Pin 4 Pin 5
Digital output	Negative ³ Positive	Pin 1 Pin 6
Relais output	Common NC NO	Pin 11 Pin 3 Pin 13



INFORMATION!

- Relais is energized if no fault was detected.
- Relais will de-energized not later than 40 seconds after MCU failure
- Availability of I/O is device dependent.
- Do not connect any other pins.



INFORMATION!

- If an external trigger is inserted into the run of a triggered running measurement is applied, it is completely ignored. A MessageBox with Time(s) of occurrence is displayed and must be confirmed.

BreathSpec® – User Manual

- None Error output via current loop or digital output. Only via Modbus, a bit is set for "external error" (error codes) at current measurement.
- On the BreathSpec the current measurement remains unaffected by this.

10.3 Ionisation Source Specification



INFORMATION!

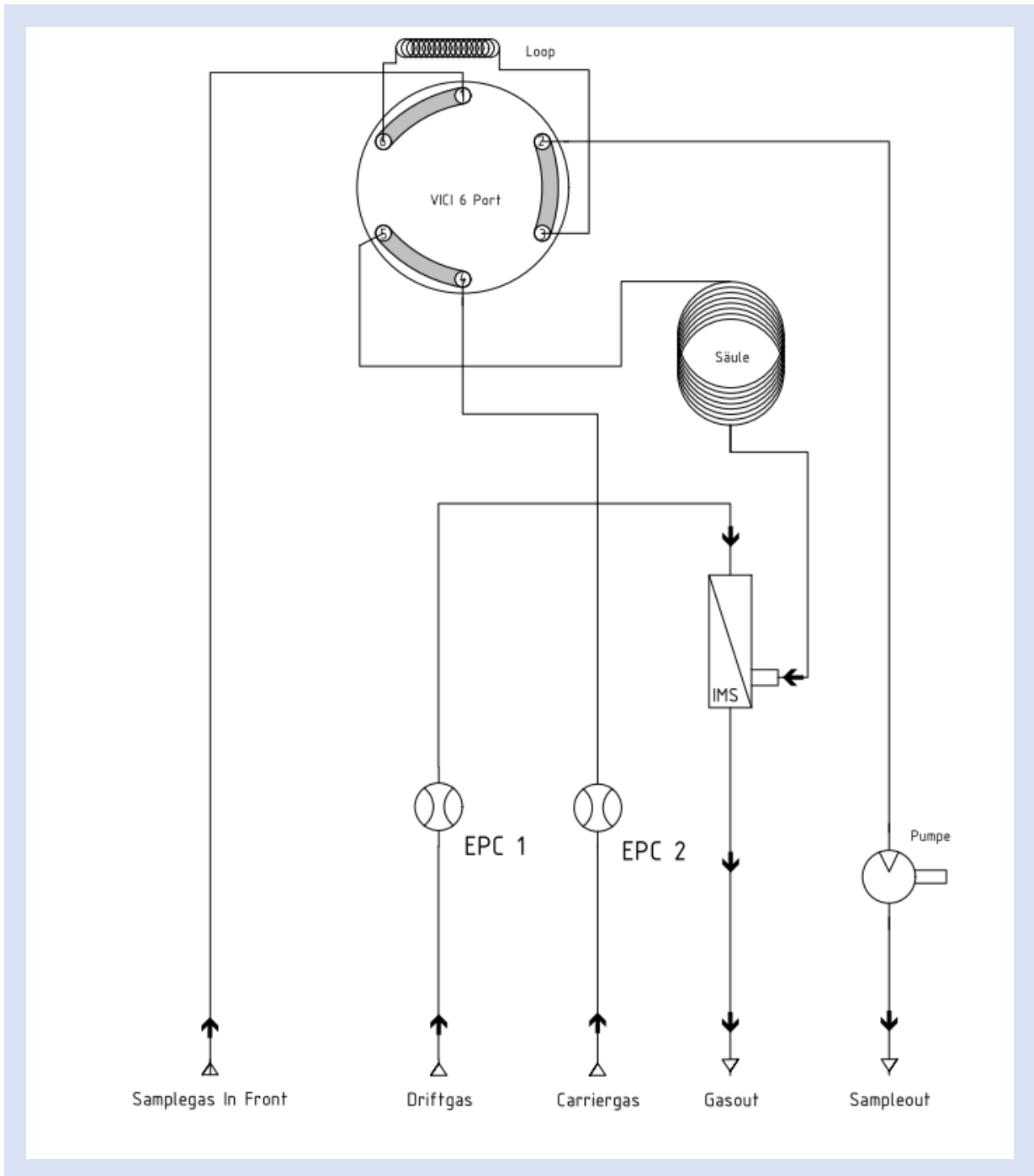
The permission and exemption limits are regulated by the Radiation Protection Ordinance and the European Union Council Directive 96/26/EURATOM in accordance with the regulations of the International Atomic Energy Authority (IAEA).

Source Type	Tritium H³, Solid-state bonded
Activity	Below the exemption limit of 1 GBq for tritium acc. to Table B (column 2) of Article 26, of the Directive 2013/59 EURATOM of December 5 th , 2013
Radiation Type	β⁻-Radiation
Radiation Energy	Average energy: 5.68 keV Maximum energy: 18.7 keV
Full Duration Half Maximum (FDHM)	12.3 years
Bracking radiation	2×10^{-7} (mSv / h x GBq) $H_{\text{Brake}} = A \times h_{\text{Br}} \times (1\text{m} / r)^2$ $h_{\text{Br}} = 0.257 \times 10^{-4} \times (E_{\beta\text{max}} / \text{MeV}) \times 2$
Attenuation of Radiation	Air: 4 mm Water: < 100 μm Tissue: < 100 μm

BreathSpec® – User Manual

	Below the exemption limit of a dose rate of 1 $\mu\text{Sv/h}$ at a distance of 0.1 m from any accessible surface of the apparatus acc. to Article 26, of the Directive 2013/59 EURATOM of December 5 th , 2013
Mounting Location and Type	Fixed inside the device and not accessible from the outside. The source cannot be touched directly.

10.4 Technical drawing: Internal Gasflow



10.5 Current Loop Interface (optional)

Output Type	Isolated active current output 0-20 mA
Non-loaded Voltage	< 20 V
Maximum Output Signal	< 22 mA
Maximum Output Load (burden resistance):	500 Ohm
Accuracy	Better than 1 %
Connector Type	D-Sub DA-15 female
Used Pins	Current output 1: Pin 9 Current output 2: Pin 2 Return: Pin 1



INFORMATION!

- Do not connect any other pins.

Current Loop Settings Values (Min, Max, Default and Example Values)

Result Value-Range	Min 0mA, Max 20 mA (Default: 4,0 mA – 20 mA)
DAC-Range	Depending on Current Loop generation
Error Value	Min 0 mA – Max 1024 mA (Example: 22 mA – 981 mA)
Idle Value	Min 0 mA – Max 65535 mA (Example: 20 mA – 54559 mA)

10.6 Modbus TCP Specification

Register Layout

Offset	Register	Content
1-6	40001-40006	<u>Header Information</u> for the <u>latest results</u> .
7-125	40007-40125	The <u>latest results</u> are mapped to these registers.
126-132	40126-40132	<u>Header information</u> for the <u>previous results</u>
133-250	40133-40250	The <u>previous results</u> are mapped these registers.

Registers in Header

Register	Datatype	Information
1	16bit unsigned Integer	The amount of results that are available.
2	16bit unsigned Integer	A 16bit encoded error code . For the possible errors see Error Codes page 216 . In case of multiple errors, the error codes are added together.
3	32bit unsigned Integer	Time in seconds since 01.01.1970 00:00 encoded into a 32bit Integer split up into this and the following register. Contains the two least significant bits.
4		Second part of the encoded time from register 3. Contains the two most significant bits.
5	Unused	

6	Unused	
---	--------	--

Substance at Register *n*

Register	Datatype	Information
n	32bit unsigned Integer	The concentration (multiplied by 1000 for a possible three decimal point precision) encoded into a 32bit Integer split up into this and the following register. The unit for this concentration is specified in the corresponding calibration and can be seen in Substance window of your device. The precision of this calculated value can be looked up in the corresponding calibration protocol for this substance. Contains the two least significant bits.
n+1		Second part of the encoded concentration (multiplied by 1000 for a possible three decimal point precision) from register n. Contains the two most significant bits.
n+2	16bit unsigned Integer	Shows you whether the substance has been enabled (=1) or disabled (=2) for evaluation.
n+3	16bit unsigned integer	A 16bit encoded status of the substance result. See Status codes pages 216 for further information.
n+4	-	Unused
n+5	-	Unused

Error codes

Bit	Value	Information
	0	No Error
0	1	Unknown Error. Source of Error unknown.
1	2	Error concerning current . Only used in special applications.
2	4	The temperature of a component has not reached the designated value
3	8	The flow of one or more pressure controllers has not reached the designated value
4	16	Storage problems. E.g. cannot write to the device
15	32768	Multiple Trigger

Status codes

Bit	Value	Information
0	1	Concentration within range
1	2	Concentration is below the calibrated range
2	4	Concentration is above the calibrated range
3	8	Invalid
3-15	16-32768	Unused

10.7 Troubleshooting

10.7.1 Error message list

Error message	Drift voltage supply.
<i>Description</i>	<i>Drift voltage error</i>
Action	Fatal Error! Contact the G.A.S. service hotline.
Error message	Can't save measurement.
<i>Description</i>	<i>The measurement file could not be saved to the internal memory.</i>
Action	Export and save all Measurement of the internal storage and clear the storage. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	smb connection failed:
<i>Description</i>	<i>Samba (Service Message Block SMB) connection failed.</i>
Action	Check network cable, network shares and IP-address. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	sftp connection failed:
<i>Description</i>	<i>Secure File Transfer Protocol (SFTP) connection failed.</i>
Action	Check network cable, network shares and IP-address. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	No USB-Storage found.
<i>Description</i>	<i>Mounting of the USB-Stick failed.</i>
Action	Ensure that a USB-Stick is insert. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. If that still does not help contact the G.A.S. service hotline.

Error message	Unable to unmount USB-Storage.
<i>Description</i>	<i>Unmounting of the USB-Stick failed.</i>
Action	Remove the USB-Stick and restart the device. Check the USB-Stick, optionally reformat it. Insert the USB-Stick and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	No program selected.
<i>Description</i>	<i>At program start no program was detected</i>
Action	Create and select a program. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Drift gas flow too low. Aborting...
<i>Description</i>	<i>At program start the drift gas flow is too low. Programstart will be refused.</i>
Action	Increase the back pressure. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Stop recording first.
<i>Description</i>	<i>If recording is activ a programstart is refused.</i>
Action	Deactivate recording and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Can't initialize drift supply. Program can not be started.
<i>Description</i>	<i>Drift voltage error</i>
Action	Fatal Error! Contact the G.A.S. service hotline.
Error message	Invalid program.
<i>Description</i>	<i>The selected program has no instructions.</i>
Action	Complete the program and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Not enough storage space left. Please delete or copy measurement or choose a shorter program.

BreathSpec® – User Manual

<i>Description</i>	<i>The internal storage has not enough storage space left.</i>
Action	Export and save all Measurement of the internal storage and clear the storage. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Hardware access failure
<i>Description</i>	<i>Error when switching the drift voltage polarity.</i>
Action	Fatal Error! Contact the G.A.S. service hotline.
Error message	Valve set to Inject. Loop not filled! Proceed? OK or Chancel
<i>Description</i>	<i>Valve start position is set to Inject instead of Fill loop.</i>
Action	Set valve start position manually to Fill loop. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Can't import calibration.gsd
<i>Description</i>	<i>The file „calibration.gsd“ was not found.</i>
Action	Create the file „calibration.gsd“ and import it with an USB-Stick. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	No measurements stored.
<i>Description</i>	<i>No measurements stored on the internal storage.</i>
Action	Do a measurement. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Folder cannot be created :
<i>Description</i>	<i>When exporting the device subfolder could not be created.</i>
Action	Check the external storage. Check network cable, network shares and IP-address. Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new

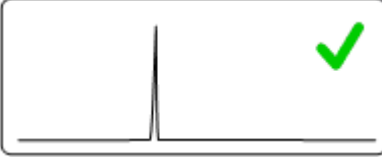
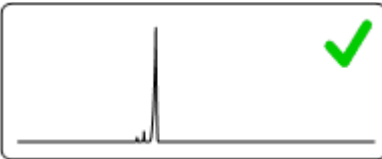

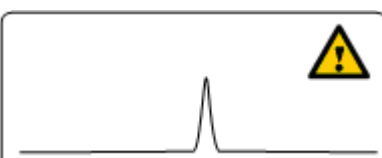



	one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	No measurement files transferred
<i>Description</i>	<i>No measurement are transferred to an external storage.</i>
Action	Check the external storage. Check network cable, network shares and IP-address. Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	No measurements stored.
<i>Description</i>	<i>No measurements were deleted, because no measurements are available.</i>
Action	Do a measurement. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	RTC read error.
<i>Description</i>	<i>Date and time setting failed.</i>
Action	Restart the system and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Save settings failed.
<i>Description</i>	<i>Setting data could not be save on a USB-stick.</i>
Action	Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Load settings failed.
<i>Description</i>	<i>Setting data could not be load from a USB-stick</i>

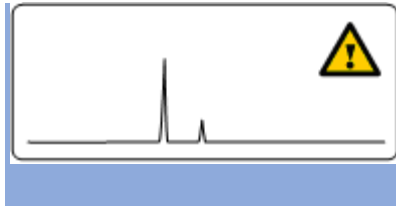
BreathSpec® – User Manual

Action	Repeat the procedure. Restart the system and repeat the procedure. Check write protection of the USB-Stick. Ensure that the USB-Stick is FAT32 formatted. Reformat the USB-Stick. Replace the USB-Stick with a new one. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Do you really want to relabel loop volume? It will be stored in all following measurements.
<i>Description</i>	<i>Sample loop setting is change manually.</i>
Action	Confirm or abort the dialog.
Error message	Can't set static ip!
<i>Description</i>	<i>Setup of the static IP-address failed.</i>
Action	Check the network settings. Contact your administrator. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Can't request DHCP:
<i>Description</i>	<i>Setup of the dynmaic IP-address failed.</i>
Action	Check the network settings. Check DHCP-server. Contact your administrator. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Valve set to Inject. Loop not filled
<i>Description</i>	<i>Valve setting is set to position "Inject" and not to "Fill loop". Sample loop could not be filled.</i>
Action	Abort program and set valve to position „Fill loop“ manually.
Error message	Trigger recieved while running program.
<i>Description</i>	<i>During the program run a new trigger signal will be received. The program run is aborted.</i>

Action	The device get a wrong trigger signal. Check the external trigger programming. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Stop recording first.
<i>Description</i>	<i>When starting the trigger mode recording is activated.</i>
Action	Deactivate recording and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Select program first.
<i>Description</i>	<i>When starting the trigger mode no program is activated.</i>
Action	Select a program and repeat the procedure. If that still does not help contact the G.A.S. service hotline.
Error message	Can't read calibration.gsd
<i>Description</i>	<i>The import of the calibration.gsd. file failed. The file was not found.</i>
Action	Ensure that the file calibration.gsd exist and is placed in the measurement subfolder of the device. Check network cable, network shares and IP-address. Repeat the procedure. If that still does not help contact the G.A.S. service hotline.

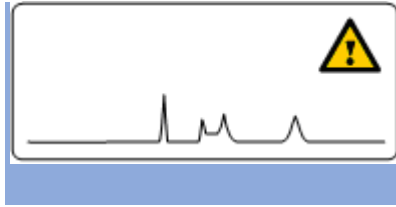
10.7.2 IMS-Spectrum Examples

Schematic of IMS spectrum	Spectrum description	reasons / suggestions
	Clean spectrum	Perfect
	Clean spectrum, up to two extra signals left hand side of the RIP	Perfect
	RIP shifted to lower drift times	<ul style="list-style-type: none"> - elevated temperature - reduced pressure
	RIP shifted to higher drift times	<ul style="list-style-type: none"> - low temperatures - elevated pressure
	RIP deformed	<ul style="list-style-type: none"> - gas quality out of specifications - device needs to be flushed for some time - flows not in range
	RIP base deformed yet visible	<ul style="list-style-type: none"> - gas quality out of specifications - device needs to be flushed for some time - flows not in range
	RIP deformed towards tailing	<ul style="list-style-type: none"> - gas quality out of specifications - device needs to be flushed for some time - flows not in range



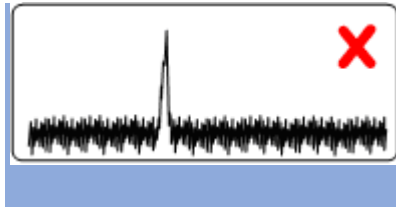
Minor impurities

- gas quality out of specifications
- device is polluted > run system cleaning



Major impurities

- gas quality out of specifications
- device is polluted > run system cleaning



Elevated noise

Contact G.A.S. support



No signal

Contact G.A.S. support

10.7.3 Troubleshooting / How to...



INFORMATION!
 This chapter is a collection of possible practical problems and serves as a guide for making an initial assessment. It makes no claim to completeness.

Symptom	Device does not start
<i>Possible Cause</i>	<i>Problem with the electrical power supply</i>
Action	Check the current power supply and restart the system. If that still does not help contact the G.A.S. service hotline.
Symptom	Device freezes during start procedure.
<i>Possible Cause</i>	<i>Problem with the Firmware</i>
Action	Restart the system. If that still does not help contact the G.A.S. service hotline.
Symptom	Start procedure paused
<i>Possible Cause</i>	<i>Hardwarecheck during the start procedure</i>
Action	Wait up to 5 min. Normally the start procedure continues. Restart the system. If that still does not help contact the G.A.S. service hotline.
Symptom	Temperature and/or gas flow values will not be displayed
<i>Possible Cause</i>	<i>Problem with hardware/firmware communication</i>
Action	Restart the system. If that still does not help contact the G.A.S. service hotline.
Symptom	Screen is black while device is on.
<i>Possible Cause</i>	<i>Screensaver is active</i>
Action	Using the pushable rotary knob to activate the screen. If the screen can't be reactivated then restart the system. If that still does not help contact the G.A.S. service hotline.

Symptom	Gasflow set-values cannot be achieved.
<i>Possible Cause</i>	<i>Backpressure too low</i>
Action	Set up the back pressure at least to 3 bar. If that still does not help contact the G.A.S. service hotline.
<i>Possible Cause</i>	<i>Hardware failure</i>
Action	Contact the G.A.S. service hotline.
Symptom	Temperature set-values cannot be achieved.
<i>Possible Cause</i>	<i>Hardware failure</i>
Action	Contact the G.A.S. service hotline.
Symptom	No display of measurement values during monitoring
<i>Possible Cause</i>	<i>Hardware failure</i>
Action	Contact the G.A.S. service hotline.
Symptom	No Reaction Ion Peak (RIP) will be displayed.
<i>Possible Cause</i>	<i>Device is in negative mode</i>
Action	Switch the drift voltage into positive mode. If that still does not help contact the G.A.S. service hotline.
<i>Possible Cause</i>	<i>Hardware failure</i>
Action	Contact the G.A.S. service hotline.
Symptom	No or small Reaction Ion Peak (RIP) will be displayed.
<i>Possible Cause</i>	<i>Insufficient gas quality</i>
Action	Check quality of operating gas (5.0 or better) and use moisture trap.
Action	When using the CGFU-unit, replace the CGFU-filters.
<i>Possible Cause</i>	<i>System contamination</i>
Action	Start cleaning mode.

Symptom	Find signals from the prior measurement run in the chromatogram
<i>Possible Cause</i>	<i>The measurement runtime is too short.</i>
Action	Increase the measurement run time
Symptom	The actual size of the measurement file is too large
<i>Possible Cause</i>	<i>Average setting too low.</i>
Action	Increase the Average setting or shorten the runtime (recommended averaging: 6).
Symptom	The measurement signals cannot mapped well.
<i>Possible Cause</i>	<i>Average setting is too high.</i>
Action	Decrease the Average setting (recommended averaging: 6).
Symptom	EPC2 Maximum flow of 150 ml/min is not reached.
<i>Possible Cause</i>	<i>The reachable maximum flow depends on the dimensions of the installed column.</i>
Action	Get the specified maximum flow from Analytical approval. If that still does not help contact the G.A.S. service hotline.
<i>Possible Cause</i>	When using a CGFU unit the total flow (EPC1 and EPC2) is limited to 400ml/min.
Action	No Action
Symptom	Six-Port-valve doesn't switch
<i>Possible Cause</i>	<i>Lost connection</i>
Action	Restart the system. If that still does not help contact the G.A.S. service hotline.
Symptom	Six-Port-valve switching noise sounds strange
<i>Possible Cause</i>	<i>Initialization lost</i>
Action	Reintializise the Six-Port-Valve
Symptom	No sample signals are displayed during a measurement.

<i>Possible Cause</i>	<i>Sample-Pump has failed</i>
Action	Set pump capacity to 100%. The pump device must be audible loud. Turn the pumping power back to the working flow. In addition, the flow can be measured using a flowmeter at the sample inlet and outlet. If that still does not help change sample pump.
Symptom	Drift time fluctuates
<i>Possible Cause</i>	<i>System is untight</i>
Action	Check all gas supply connections of operating gas.
Action	Check all gas supply connections of GC-column.
Symptom	Retention time fluctuates
<i>Possible Cause</i>	<i>System is untight</i>
Action	Check all gas supply connections of operating gas.
Action	Check all gas supply connections of GC-column.

10.8 Consumables / Spare Parts



Part number: 4000 1000

Power supply with Power plug



Part number: 9510 0003

Gas tube Kit: (BreathSpec 4G1)

- Driftgas/Carriergas Adapter with 0,15 m PFA-Tubes with 3mm Swagelok Connectors (1piece)
- 0,65m 3mm PFA Tubes with 3 mm Swagelok-Connector (2 Pieces)
- 2 m 3mm PFA Tubes with 3 mm Swagelok-Connector (2 Pieces)



Part number: 9510 0004

Gas tube Kit: (BreathSpec 4G2)

- Driftgas/Carriergas Adapter with 0,15 m PFA-Tubes with 3mm Swagelok Connectors (1piece)
- 0,65m 3mm PFA Tubes with 3 mm Swagelok-Connector (2 Pieces)
- 2 m 3mm PFA Tubes with 3 mm Swagelok-Connector (6 Pieces)



Part number: 8900 1094

Molecular sieve 200 ml with 1/8" connections
(1 piece)

(Labuse)



Part number: 8900 1101

Molecular sieve 120 ml with 1/8" connections
(1 piece)

(Attachable to device)



Part number: 8101 1532

Standard-capillary column MXT-WAX
Lenght 30 m, ID 0,53 mm, Filmthickness 0,5
µm, Winding ID 80 mm
(1 piece)

(Other column types only on request)



Part number: 8103 1001

Teflon Ferrules for capillary column with ID
0,53 mm
Connection 1/16", Hole 0,8mm, T max. =
250°C

Package size: 10 Pieces



Part number: 1303 0036

Connection Kit for capillary column connection 1/16"

Package size: 2 Pieces



Part number: 9510 0000
LAN Cable (1 piece)



Part number: 9510 0002

Blind plug Set (5 pieces)



Part number: 1305 0013

Torx Tool Kit

- Torx Screwdriver 8 mm (1 piece)
- Torx Screwdriver 10 mm (1 piece)



Part number: 1305 0008

Torx Screwdriver 30 mm (1 piece)



Part number: 2603 2100

CGFU Connection cable (1 piece)



Part number: 8001 1707

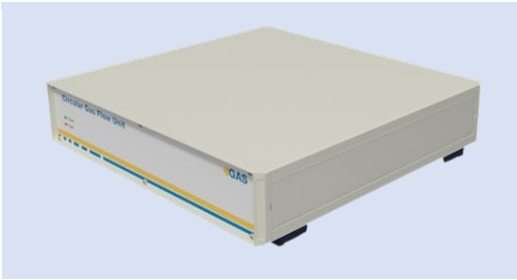
BreathSpec Transport box Length = 75 cm,
Height = 40 cm, Width = 59 cm
(1 piece)



Part number: 8003 0001

GC-IMS Transport palett (60 x 80 cm)

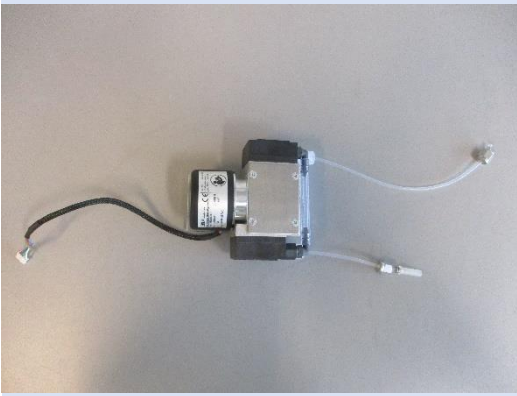
BreathSpec® – User Manual



Part number: 4600 000 000
Circular Gas Flow Unit with accessories



Part number: 8900 1104
Circular Gas Flow Unit exchange filterset.



Part number: 4000 0930
Circular Gas Flow Unit pump.



Part number: 4600 500 000
Nitrogen Generator with accessories
(example picture)



Part number: 8204 1100

μTD with accessories



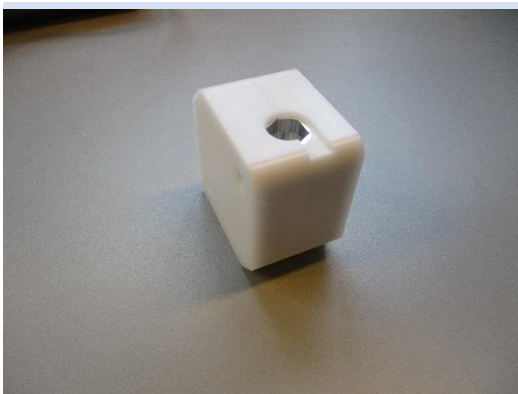
Part number: 8205 0000

Laptop Computer (different design) including software for control and evaluation



Part number: 4000 2130

Luer Adapter (1 piece)



Part number: 4000 2100

Luer Adapter Heater (1 piece)

BreathSpec® – User Manual



Part number: 8900 1058

Sampling Syringe 5ml syringe for Luer Adapter) (100 pieces)



Part number: 8900 1057

- Reservoir tube (100 pieces)



Part number: 8900 1000

- Mouthpieces (100 pieces) different color possible



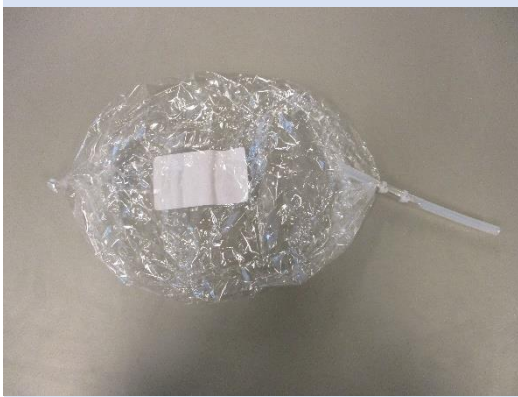
Part number: 8900 1059

Inner Syringe Body (2ml syringe) (50 pieces)



Part number: 4000 0940

Sample pump



Part number:

Sampling Bag (10 pieces)



Part number:

Sampling Bag Adapter (10 pieces)

10.9 Corresponding G.A.S. Documents and Tutorials



INFORMATION!

- BreathSpec Quickstart Manual
- CGFU User Manual (optional)
- Airsense uTD Handbook (optional)
- μ TD GC-IMS Additional Information Quickstart (optional)
- Sequence Designer Manual
- IMS Control TFTP-Server Manual
- Tutorials Sequence Designer
- Tutorials VOCal
- Manuals VOCal

10.10 Table of Figures

Figure 1: Ion Mobility Spectrometer - Basic Relations	29
Figure 2: Ion Mobility Spectrometer -Working Principle	30
Figure 3: IMS Predominant Ionization (positive polarization)	31
Figure 4: Protone Affinities of VOC's	31
Figure 5: GC-IMS measurement 3D	32
Figure 6: BreathSpec® device plan (exemplary)	35
Figure 7: Six-Port Valve - Position Fill Loop and Inject	36
Figure 8: BreathSpec® (Version 4G1) - Housing of device - Front.....	37
Figure 9: BreathSpec® (Version 4G1) - Housing of device - Rear	39
Figure 10: BreathSpec® with Airsence μ TD (Version 4G2) - Housing of device - Top	41
Figure 11: BreathSpec® (Version 4G2) with Airsence μ TD - Housing of device - Front	42
Figure 12: BreathSpec® (Version 4G2) with Airsence μ TD - Housing of device - Rear	44
Figure 13: Device Type / Serial Number Plate.....	46
Figure 14: Operating Interface - Overview.....	47
Figure 15: Operating Interface - Windows Selection Bar	48
Figure 16: Operating Interface - Status Bar	49
Figure 17: Operating Interface – View Control Bar	50
Figure 18: Operating Interface - Low Pressure Alarm Box	51
Figure 19: Operating Interface - High Pressure Alarm Box	52
Figure 20: Operating Interface - Spectra Window.....	53
Figure 21: Start Program	54
Figure 22: Recording Check Box.....	55
Figure 23: Recording Check Box.....	55
Figure 24: Operating Interface - Sequence Window	56
Figure 25: Operating Interface - Sequence Window - Processing	57
Figure 26: Operating Interface - Defaults Window	58
Figure 27: Drift Voltage Windows - positive and negative Mode.....	60
Figure 28: Flow and Temperature Control (Example).....	61
Figure 29: Operating Interface - Substances Window	62
Figure 30: Substance List Control panel.....	63
Figure 31: Substance selection 1	63
Figure 32: Substance selection 2	64
Figure 33: Substance selection 3	64
Figure 34: Substances Window	65
Figure 35: Information about the last Modbus TCP Connection	65
Figure 36: 32 bit split up into 16 bit registers	66
Figure 37: First 25 registers of an example Modbus result.	66
Figure 38: Substance Calibration Information Area	67
Figure 39: Recognized Substances Window	68
Figure 40: Operating Interface - Programs Window	69
Figure 41: Measurement Control Panel	71
Figure 42: Selected Program Window	72
Figure 43: Selected Program Window Control Panel	73
Figure 44: Flow Ramps	74
Figure 45: Operating Interface - System Window	76
Figure 46: Operating Interface - System Info Window	77

BreathSpec® – User Manual

Figure 47: Operating Interface - System Plan Window	78
Figure 48: Operating Interface - System Settings Windows 1	79
Figure 49: Operating Interface - System Settings Window 2	80
Figure 50: Operating Interface - System Settings Windows 3	82
Figure 51: Operating Interface – Snapshot Window	85
Figure 52: Operating Interface – Snapshot Window in detail (example EPC2 pressure)	86
Figure 53: Operating Interface - Simplified View Window.....	88
Figure 54: Operating Interface - System Transfer Window.....	89
Figure 55: Operating Interface - System Modes Window	91
Figure 56: Operating Interface - Trigger Mode Window.....	92
Figure 57: Operating Interface - Remote Mode Window	94
Figure 58: Operating Interface - Cleaning Mode Window	96
Figure 59: Operating Interface - Standby Mode Window	97
Figure 60: Error Information Window	98
Figure 61: Log Messages Dialog Window	99
Figure 62: IP Adress Input Dialog Windows	100
Figure 63: Date and Time Input Dialog Window	101
Figure 64: Text Input Dialog Window.....	102
Figure 65: Number Input Dialog Window (Example).....	103
Figure 66: IP Adress Input Dialog Windows	Fehler! Textmarke nicht definiert.
Figure 67: Date and Time Input Dialog Window ...	Fehler! Textmarke nicht definiert.
Figure 68: Text Input Dialog Window.....	Fehler! Textmarke nicht definiert.
Figure 69: Number Input Dialog Window (Example).....	Fehler! Textmarke nicht definiert.