# Global Atmosphere Watch Data Acquisition and Quality Assurance System

# (GAW-DAQAS)

## User Requirements Document

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# Deliverables Summary Sheet

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# Executive Summary

*The User Requirements Document describes the functional and non functional requirements on the Data Acquisition and Quality Assurance System (DAQAS) to be developed in the frame of the German contribution to the Global Atmosphere Watch (GAW) programme. GAW-DAQAS shall be installed at the GAW global station operated by the Umweltbundesamt (Federal Environmental Agency) located in the Bavarian Alps at 2650 m above sea level just below Mount Zugspitze, Germany's highest mountain.*

*GAW-DAQAS shall provide a tool for automated acquisition, processing and quality assurance of atmospheric trace gas data, calibration cycle control and report generation. It shall thus contribute to the successful operation of the German GAW global station.*

*In its first development phase, three gas analysers manufactured by Thermo Environmental Instruments Inc. measuring $O_3$, NO, $NO_2$, $NO_X$ and CO shall be controlled by GAW-DAQAS. The CRANOX system of instruments manufactured by ECO Physics AG measuring NO, $NO_2$, $NO_X$, $NO_Y$ and $O_3$ using different measurement principles shall be integrated in a second phase. More instruments may be integrated at a later stage of the project if resources allow to do so.*

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# Preface

The first version of this document has been derived from the information obtained during the kick-off meeting of the project "*Global Atmosphere Watch – Data Acquisition and Quality Assurance System*" (GAW-DAQAS) held 20.-22. November 2002 in the premises of the German *Umweltbundesamt* (Federal Environmental Agency) at *Schneefernerhaus* situated 300 m below Mount Zugspitze (2964 m above sea level).

It was agreed at the GAW-DAQAS kick-off meeting to realise first a prototype system into which a subset of the full intended functionality shall be integrated. This prototype has been installed at *Schneefernerhaus* in the last week of February 2003. The prototype allowed for operational acquisition of data from two TEI instruments measuring $O_3$, NO, $NO_2$, $NO_X$.

Based on the experience gained from operating the prototype, and driven by the necessity of integrating further instruments and more advanced data processing tools, this document is constantly revised. In its actual state, it reflects the requirements on GAW-DAQAS known as of August 2003.

# 1 Introduction

## *1.1 Purpose*

The present User Requirements Document (URD) describes the requirements on the software system GAW-DAQAS (*Global Atmosphere Watch – Data Acquisition and Quality Assurance System)*. GAW-DAQAS shall:

1.) allow automated acquisition and pre-processing of raw data from various trace gas analysers,

2.) trigger and control calibration cycles for each considered analyser,

3.) provide the means for interactive quality control of the raw data and subsequent generation of advanced data products by applying statistical methods,

4.) protect against accidental or malicious loss of raw data and data products.

This URD covers the first stage of the system development process during which three different trace gas analysers shall be integrated into the software system.

The intended readership comprises project management and technical staff on the customer's side as well as project management and software developers on the contractor's side.

This document is a living document and shall be revised whenever additional user requirements are to be integrated or obsolete user requirements are to be removed.

## 1.2 Definitions, acronyms and abbreviations

**Table 1: List of used acronyms and abbreviations**

| Acronym | Explication |
|---|---|
| ASL | Above sea level |
| DAQAS | Data Acquisition and Quality Assurance System |
| DWD | Deutscher Wetterdienst (German Weather Service) |
| ECD | Electron Capture Detector |
| ESA | European Space Agency |
| EUR | End user requirements |
| FID | Flame Ionisation Detector |
| FZK | Forschungszentrum Karlsruhe (Research Centre Karlsruhe) |
| GAW | Global Atmosphere Watch |
| GUI | Graphical user interface |
| IFU | Institut für Atmosphärische Umweltforschung (Institute of Atmospheric Research) as part of the FZK |
| SFH | Schneefernerhaus |
| TEI | Thermo Environmental Instruments Inc. |
| UBA | Umweltbundesamt (German Federal Environmental Agency) |
| UN | United Nations |
| URD | User requirements document |
| VOC | Volatile organic carbon |
| WMO | World Meteorological Organisation (part of the UN) |

**Table 2: Definition of concepts**

| Concept | Explication |
|---|---|
| BTL0 | Bottled zero air, bottled inert air from external provider |
| Level-0 data | Raw data as delivered from an instrument |
| Level-1 data | Flagged and post-calibrated raw data |
| Level-2 data | Quality assured data products obtained through advanced |

| | |
|---|---|
| | statistical methods and direct user interaction |
| SMP0 | Sample zero air, sample air where one or more gases have been catalytically removed. |
| STA0 | Station zero air, trace gas free air |

## 1.3 References

*BSSC(96)2*. Guide to applying the ESA software engineering standards to small software projects, BSSC(96)2, Issue 1, May 1996.

*CRANOX*. Bedienungshandbuch CLD 770 AL ppt, 141p., ECO Physics AG, Dürnten (Switzerland), February 1993.

*ESA PSS-05-0*. ESA Software Engineering Standards, ESA PSS-05-0, Issue 2, February 1991.

*ESA PSS-05-02*. Guide to the user requirements definition phase, ESA PSS-05-05, Issue 1, Revision 1, March 1995.

*ENVIR 100*. Series 100 multigas calibrator. Operating and service manual. Edition 1/90, revision 3, Environics Inc., Tolland (CT), last addendum from March 1998.

*ENVIR 300*. Series 300 computerised ozone analyser. Operating and service manual. Edition 1o/90, revision 6, Environics Inc., Tolland (CT), last addendum from August 1992.

*GAW-URL-01*. GAW home page: http://www.wmo.ch/web/arep/gaw/.

*GAW-URL-02.* Home page of GAW global station Zugspitze / Hohenpeißenberg: http://gawdataeval.tripod.com/

*GAW-80*: Report on the WMO meeting of experts on the quality assurance plan for the GAW, Germisch-Partenkirchen, Germany, 26-30 March 1992 (TD No. 513).

*GAW-86*. Global Atmosphere Watch Guide, 48p., Geneva, AREP/ENV, 1993.

*GAW-89*. Quatrième Conférence Internationale $CO_2$ - Fourth International Conference [on] $CO_2$, 241 p., Carqueiranne, France, 13-17 September 1993.

*GAW-113*. Strategic Plan of the Global Atmosphere Watch (GAW), 83 p., Geneva, AREP/ENV, 1997.

*GAW-114*. Report of the fifth WMO meeting of experts on the Quality Assurance / Science Activity Centres (QA / SACs) of the Global Atmosphere Watch (GAW) jointly held with the second meeting of the coordinating committees of IGAC-GLONET and IGAC-ACE, 99 p., Garmisch-Partenkirchen, Germany, 15-19 July 1996.

*GAW-123*. Report of WMO Meeting of Experts on GAW Regional Network in RA VI, 30 p., Budapest, Hungary, 5-9 May 1997.

*TEI-42C*. Model 42C, trace level chemiluminescence NO-$NO_2$-$NO_X$ analyser, instruction manual, P/N 9993, Thermo Environmental Instruments Inc., Franklin (MA), December 1996.

*TEI-48C*. Model 48C, trace level gas filter correlation CO analyser, instruction manual, P/N 14023, Thermo Environmental Instruments Inc., Franklin (MA), August 2000.

*TEI-49C*. Model 49C, UV photometric $O_3$ analyser, instruction manual, P/N 9999, Thermo Environmental Instruments Inc., Franklin (MA), November 1998.

*TEI-49C-OZO*. Model 49C, Primary standard UV photometric $O_3$ calibrator, instruction manual, P/N 9994, Thermo Environmental Instruments Inc., Franklin (MA), November 1995.

## 1.4 Overview

This URD describes the scientific background of the project GAW-DAQAS and there from draws the requirements on the software system to be developed. Its structure follows the ESA software engineering standards [*ESA PSS-05-0*], in particular the guide to the user requirements definition phase [*ESA PSS-05-02*].

According to the definition given in [*BSSC(96)2*], the project GAW-DAQAS can be considered as small software project (less than 2 person years of working effort). Therefore, the guidelines given in [*BSSC(96)2*] for documenting small software projects have been applied.

This URD is organised as follows: In section 2, the project is described in a general way: project background, capabilities the system shall meet, constraints the system shall respect, characteristics of its users and environment into which the system shall operate. Specific requirements are described in more detail in section 3.

# 2 General description

## 2.1 Project background

In the frame of the GAW programme initiated by WMO (World Meteorological Organisation), the atmospheric background concentrations of various trace gases shall be monitored continuously through a global network of measurement stations. These measurements shall allow early detection of changes of the chemical composition and physical status of the atmosphere in relation to global climatic change. The concentration levels to be measured may be extremely low. It is therefore of utmost importance to assure both quality of raw data acquisition and data evaluation procedures to obtain global comparability of background measurements of the considered trace gases.

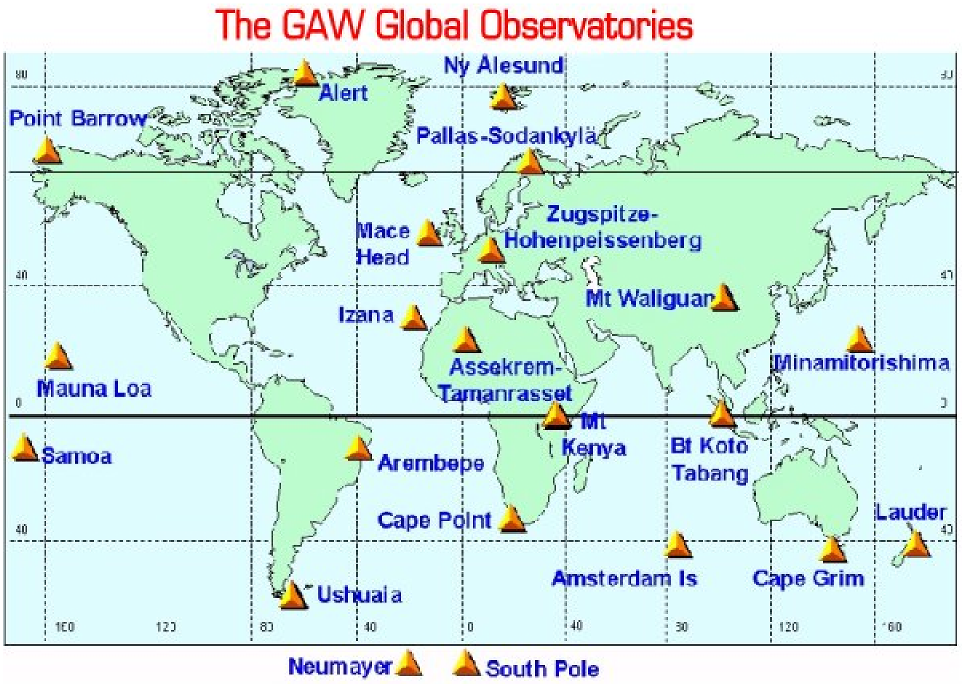


**Figure 1: Geographical distribution of the 22 GAW global observatories.**

The GAW programme has started in 1989. Meanwhile, its measurement network comprises 22 global stations (Figure 1) and about 280 regional stations. The only global GAW station in

Central Europe is located in the Bavarian Alps at 2670 m above sea level (ASL), just below Mount Zugspitze (2963 m ASL), Germany's highest mountain. It is jointly operated by the German *Umweltbundesamt* (UBA, Federal Environmental Agency) and *Deutscher Wetterdienst* (DWD, German Weather Service) at Hohenpeißenberg. Due to its geographical location, the station is situated above the atmospheric boundary layer for more than 60% of year, mainly in autumn and winter. The station is thus suited to monitor the chemical and physical conditions in the uninfluenced lower troposphere which is pre-requisite to detect climatic change. The GAW global station Zugspitze / Hohenpeißenberg provides the GAW contribution for Central Europe. The neighbouring GAW global stations are located on the Irish West Coast (Mace Head) and in Northern Finland (Sodankylä) at distances of 1600 km to the North-West and 2500 km to the North-East, respectively. The neighbouring station to the South is located in Tamanrasset (Algeria) at a distance of 2800 km, and to the East on Mount Waliguan in China.

The most important parameters to be measured in the frame of GAW are the concentrations of various atmospheric trace gases. The instruments available for this purpose at the GAW global station Zugspitze / Hohenpeißenberg are listed in Table 3. More information on GAW can be obtained from the corresponding documents listed in the reference section 1.3 and the official GAW homepage [*GAW-URL-01*]. A dedicated website has been established in order to describe the specific activities at the GAW global station Zugspitze / Hohenpeißenberg [*GAW-URL-02*].

**Table 3: Trace gases measured at the GAW global station Zugspitze / Hohenpeißenberg, Germany.**

| Instrument | Measurement principle | Trace gas |
|---|---|---|
| TEI42C | chemiluminescence | NO, $NO_2$, $NO_x$ |
| TEI48C / TEI48S | photometric | CO |
| TEI49C | photometric | $O_3$ |
| CRANOX | Chemiluminescence in combination with photolytic or catalytic conversion for nitric oxides, photometric for ozone | NO, $NO_2$, $NO_x$, $NO_y$, $O_3$ |
| LEVIN-GC | Gas chromatograph, FID, ECD | $CO_2$, $CH_4$, $SF_6$, $N_2O$ |

| | | |
|---|---|---|
| VOC-GC | Gas chromatograph, FID | VOC, $C_2$-$C_5$ |
| GC-MS | Gas chromatograph, subsequently mass spectrometer | VOC, >= $C_5$ |

## 2.2 General capabilities

The software product to be developed shall be named GAW-DAQAS (Global Atmosphere Watch – Data Acquisition and Quality-Assurance System). During the first development phase of GAW-DAQAS, covered by the present URD, three instruments and their corresponding calibration devices shall be integrated: TEI42C (NO, $NO_2$, $NO_X$), TEI48C (CO) and TEI49C ($O_3$), see Table 3 above. In the second development phase, the CRANOX instruments system ($O_3$, NO, $NO_2$, $NO_X$, $NO_Y$) shall be integrated as well.

The finalised software product GAW-DAQAS shall support the technical staff of the GAW global station Zugspitze / Hohenpeißenberg by providing the following functionalities:

1.) automated acquisition and archiving data of instrumental raw data, including data integrity checks, flagging of possibly erroneous values and alarm triggering,

2.) tools to explore and visualise data to allow the technical staff at SFH to assess the actual gas concentrations as well as the state of all connected instruments at a glance, including an alarming system which informs about values outside pre-defined tolerance ranges,

3.) continuously updated meta data base into which technical staff shall report actions or occurrences which might have an impact on data quality ("*Stationsbuch*" or log book),

4.) interface to the existing independent software tool "*ISAVE*", developed by the Dresden-located *Quodata GmbH*, which is used for interactive quality control and the generation of quality-assured 30-min average values,

5.) automated back-up system in order to minimise data loss due to technical problems or accidental or malicious misuse.

The different components of GAW-DAQAS and their inter dependencies are shown in Figure 2 below.

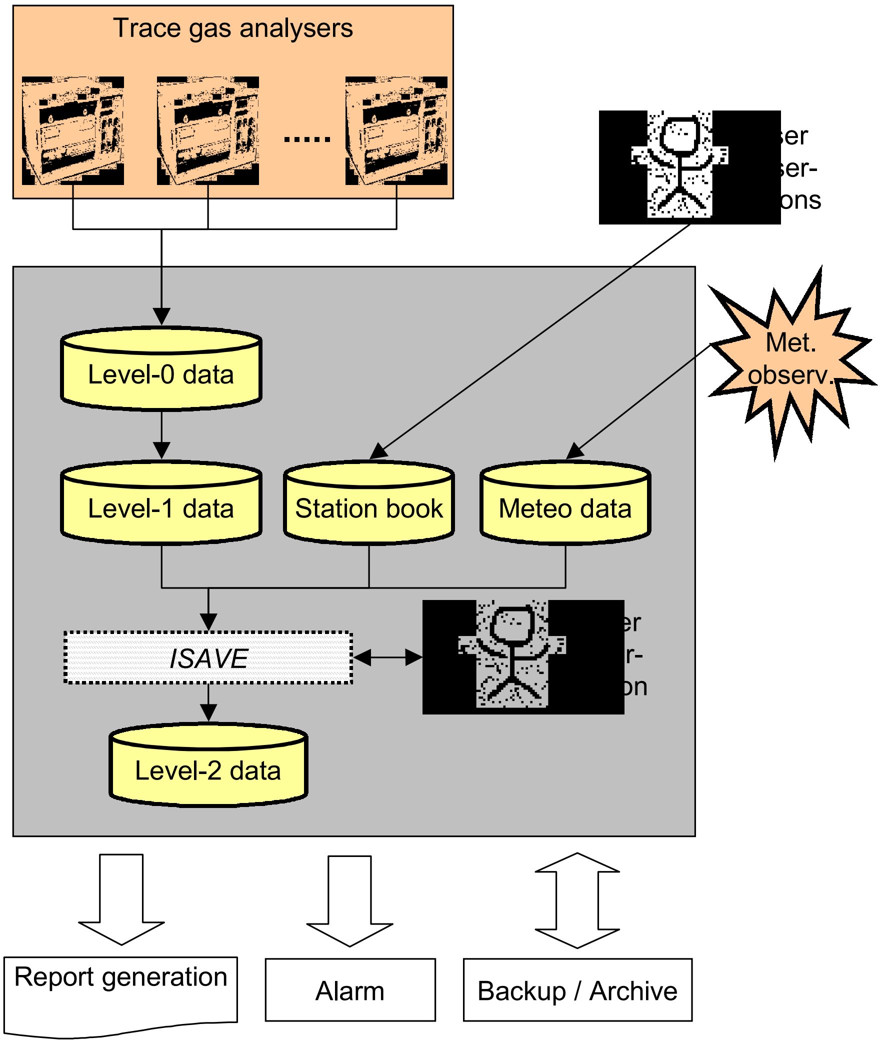


**Figure 2: Interdependencies of the different components of GAW-DAQAS.**

## *2.3 General constraints*

A number of general constraints shall be respected by GAW-DAQAS:

1.) In the frame of the GAW programme, an 80% criterion of data completeness shall be met (GAW report *GAW-80* available as paper copy from LR). This means that data shall be available for at least 80% of a calendar year. To be able to calculate seasonal averages, continuous data loss shall not happen for periods longer than ten days. Missing values should be arbitrarily distributed in time.

2.) The parts of GAW-DAQAS to be used for raw data acquisition and instrument control shall be developed such that that the technical staff of the GAW global station Zugspitze / Hohenpeißenberg is able to integrate new instruments or data evaluation algorithms without the need of assistance from the developers of GAW-DAQAS.

3.) GAW-DAQAS shall be realised for a Windows NT/2000/XP environment on hardware which already exists.

4.) The interactive data processing shall be performed by the existing software package "*ISAVE*". The reason for this is that *ISAVE* has been specifically produced for this purpose and needs just to be adjusted with respect to the interfaces to the raw data and data product databases.

5.) Documentation of the GAW-DAQAS system shall be written in English. The reason for this is that the software product to be developed, as well as the reasons for decisions taken and strategies adopted will be of practical interest to the operating organisations other GAW stations. This all the more, as the GAW programme itself does not provide practical support for data acquisition and quality control.

## *2.4 User characteristics*

The software GAW-DAQAS will primarily be used by the scientific and technical staff of the GAW station Zugspitze / Hohenpeißenberg. Primary users of GAW-DAQAS will thus typically have a university degree in natural sciences or a degree in engineering from a polytechnic university. They will thus mostly dispose of a certain knowledge in scientific or technical programming. However, users of GAW-DAQAS will typically NOT have a university degree in computer science.

The software GAW-DAQAS will be run continuously to acquire raw data. The raw data gathered by GAW-DAQAS will interactively be processed typically about once a week (more frequently, if necessary) in order to produce the data products and reports required for the GAW project.

## 2.5 Operational environment

At the end of the first development phase, three trace gas analysing units shall be controlled by GAW-DAQAS. Each unit consists of two different subunits, the trace gas analyser itself and the corresponding calibration unit providing test gases of precisely known mixing ratios. The following trace gas analysers shall be integrated: TEI42C (NO, $NO_2$, $NO_X$), TEI48S (CO) and TEI49C ($O_3$). At the end of the second development phase, the CRANOX instruments system ($O_3$, NO, $NO_2$, $NO_X$, $NO_Y$) of ECO Physics AG shall be integrated into GAW-DAQAS as well. Details on these instruments are found in Table 4.

**Table 4: Trace gas analysers and complementary instruments to be integrated into the GAW-DAQAS prototype.**

| Instrument | Manufacturer | Serial Number | Interfaces | Remarks |
|---|---|---|---|---|
| TEI42C analyser | Thermo Environmental Instruments | 42CTL-57756-314 | 2 x RS232<br>1 x parallel<br>16 x analogue | |
| TEI48S analyser | Thermo Environmental Instruments | C 048S 52027-290 | 6 x analogue (2 out + 4 control ??) | Only analogue output |
| TEI48C analyser | Thermo Environmental Instruments | 48CTL-68927-362 | 2 x RS232<br>1 x parallel<br>16 x analogue | Does not belong to UBA |
| TEI49C analyser | Thermo Environmental Instruments | 49C-65220-347 | 2 x RS232<br>1 x parallel<br>16 x analogue | |
| MicroCal 5000 | MCZ Umweltanalytik | 97-01-007 | 1 x RS232<br>1 x parallel<br>2 x BNC<br>1 x Data logger | |
| TEI49C calibrator | Thermo Environmental Instruments | 49CPS-58686-319 | 2 x RS232<br>1 x parallel<br>16 x analogue | |
| CRANOX NOy instrument system | ECO Physics AG | 300699 | 4 x RS232<br>2x3+1 analogue | Integration into GAW-DAQAS using analogue outputs |

The way how the different instruments shall be integrated into GAW-DAQAS are sketched in Figure 3 to Figure 6 . Depending on the instrument, different strategies for providing the analysers with calibration gases are appropriate. For the TEI42C (NO, $NO_2$, $NO_X$), the calibration strategy is as follows: standard gas of precisely known concentration is further diluted with inert air in order to provide the low gas concentrations required for the calibration. Alternatively, the TEI42C may be connected to the calibration gas stream provided by the CRANOX system. A decision on the best method for automated calibration of the TEI42C still has to be taken by the UBA staff. In the present state, valves are switched manually by UBA technical staff in order to redirect the calibration gas to the analyser. The calibration procedure for the TEI42C is repeated about once a week.

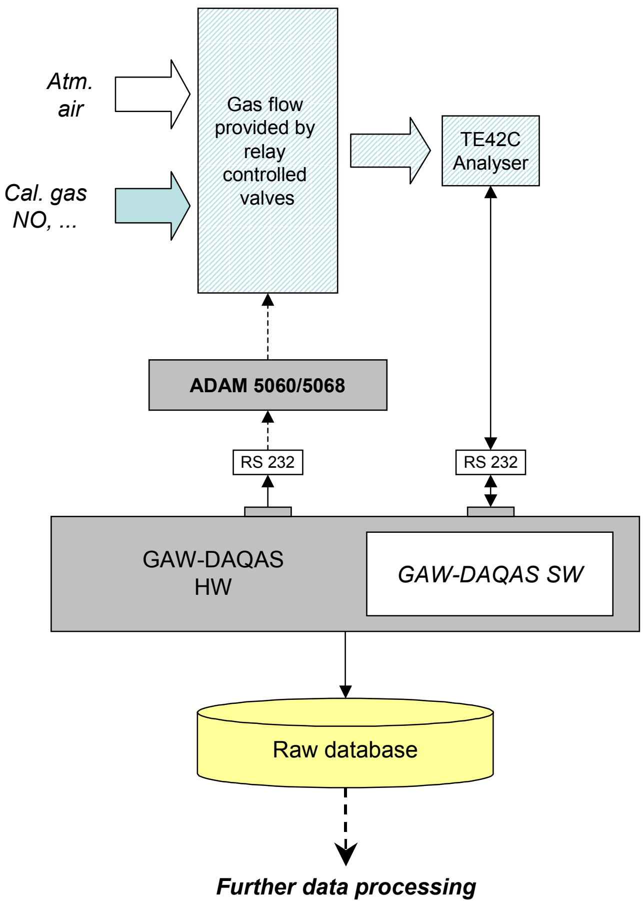


**Figure 3: Integration of the TEI 42C analyser into GAW-DAQAS.**

The TEI48S (CO) requires a different calibration strategy due to its rapidly shifting baseline. A system of valves already has been put into service allowing CPU-controlled switching between calibration gas and atmospheric air every 15 minutes. Besides, calibration cycles using three different CO concentrations are regularly executed.

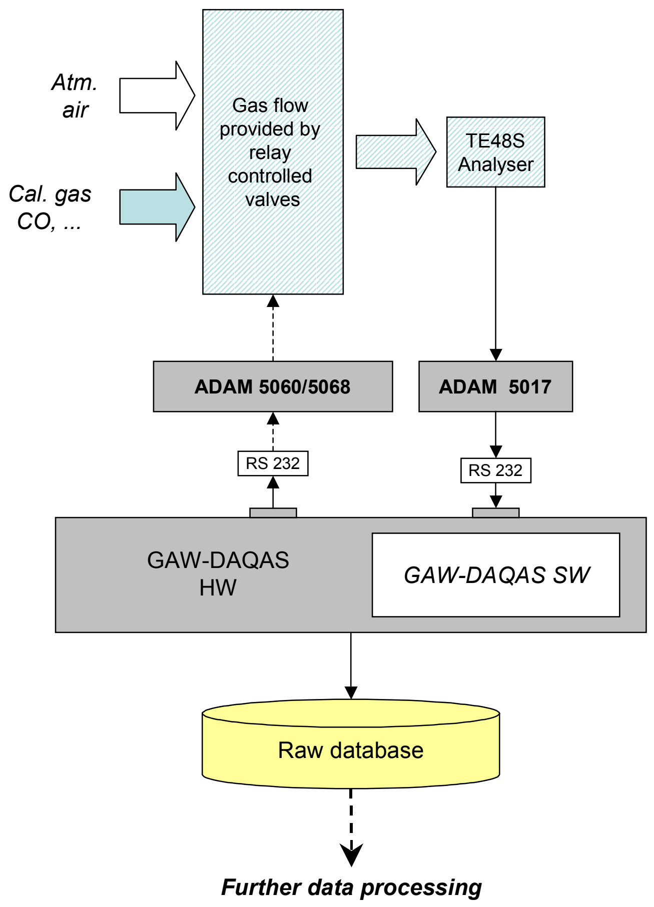


**Figure 4: Integration of the TEI 48S analyser into GAW-DAQAS.**

The TEI49C (O3) disposes of a standard calibration unit from the same manufacturer (TEI49C calibrator) which produces calibration gases of known ozone concentration between 50 and 10.000 µg $m^{-3}$. In the actual state of the system, tubes are switched manually by the technical staff in order to redirect the calibration gas to h e O3 analyser. Different calibration cycles are regularly executed which are repeated at shorter (2-point calibration) or longer (5-point calibration) time intervals.

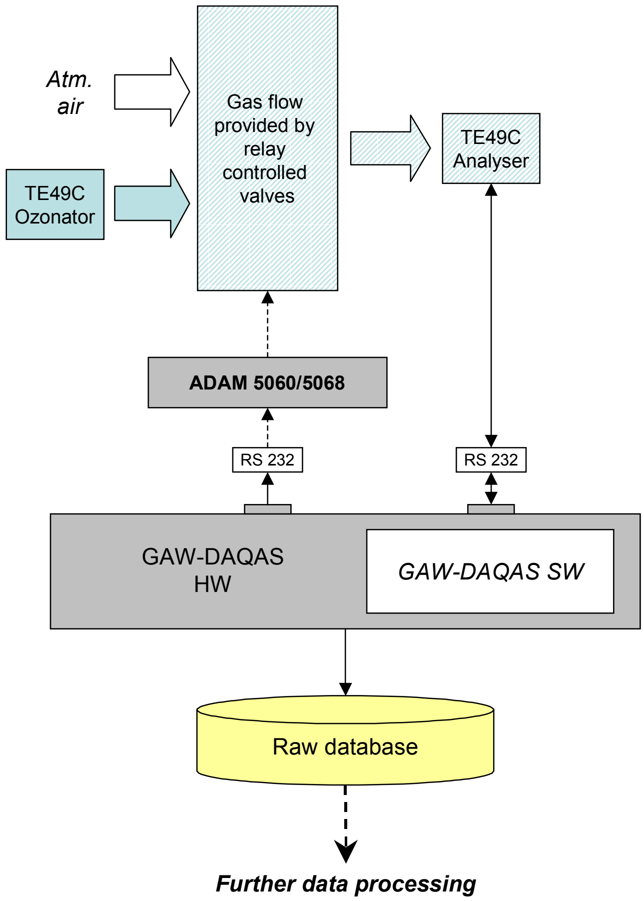


**Figure 5: Integration of TEI 49C into GAW-DAQAS.**

All three TEI trace gas analysers as well as the corresponding calibration units shall be controlled by the software product GAW-DAQAS. GAW-DAQAS shall run on a single PC to which all instruments shall be connected. The CRANOX disposes of internal calibration units which may, at a later stage, also be controlled by GAW-DAQAS. However, while building up experience regarding the operational use of the CRANOX, only the analogue outputs shall be acquired by GAW-DAQAS.

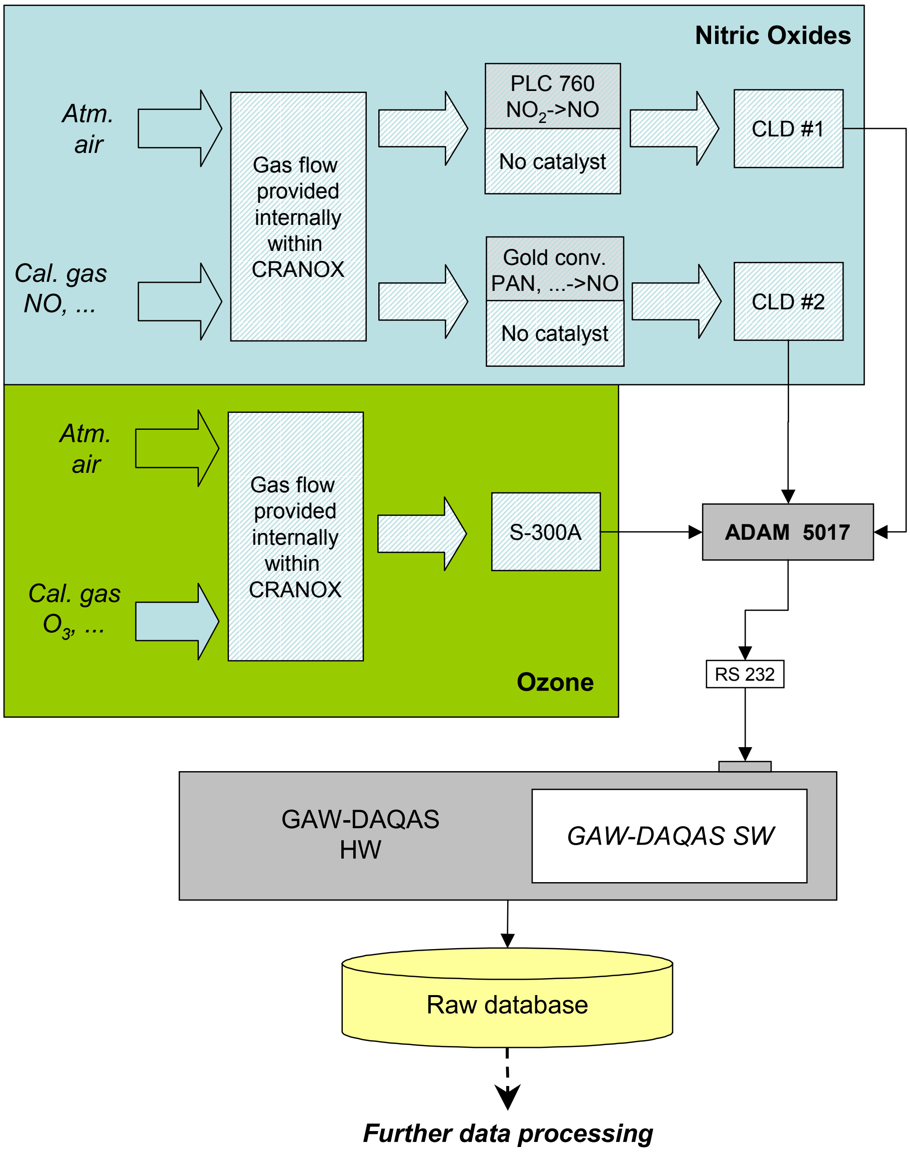


**Figure 6: Integration of the CRANOX instrument system into GAW-DAQAS.**

# 3 Specific requirements

The following subsections describe in detail the specific requirements on GAW-DAQAS. Here, it is distinguished between "*Capability Requirements*" describing the functional requirements to be met and "*Constraint Requirements*" imposed by the technical and organisational environment into which GAW-DAQAS shall operate. Each requirement is given a descriptive title and a unique 14-character identifier. Additionally, its source (responsible person) is specified, a priority between 1 and 3 is attributed and a description in plain English is provided. Only priority 1 requirements shall be realised for the GAW-DAQAS prototype.

## 3.1 Overview

GAW-DAQAS is a complex system which shall integrate a multitude of different data processing tasks which reflect the different requirements on the system. The different data to be processed, their interdependencies as well as the tool used for data processing are depicted in Figure 7. In GAW-DAQAS, we distinguish between three levels of data processing:

1.) Level-0 data: These are unprocessed raw data as received from the instrument.

2.) Level-1 data: These are data products which are obtained through automated processing. In the frame of GAW-DAQAS, Level-1 data consist of post calibrated and flagged concentration values averaged over one minute as well as flagged instrumental parameters obtained at a rate of one per minute. Flags are raised if values are outside pre-defined tolerance ranges.

3.) Level-2 data: These are data products obtained from Level-1 data through direct user interaction. They consist of quality assured 30-min averages for later delivery to the WMO or other organisations.

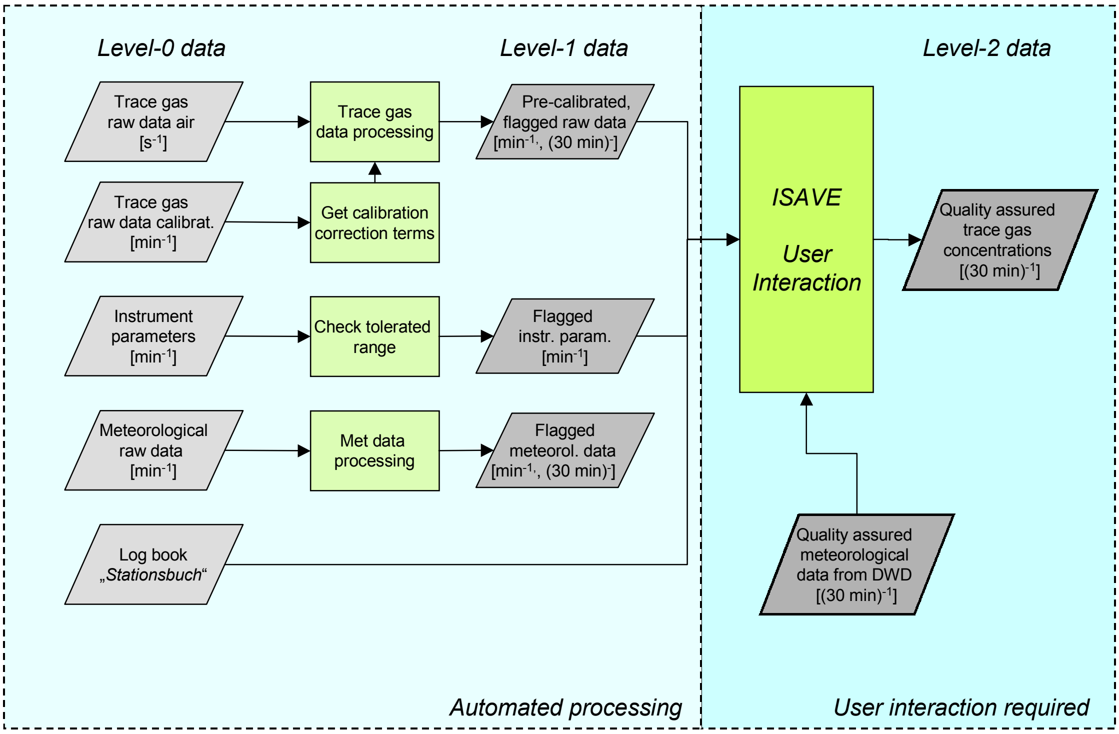


**Figure 7: Processing from Level-0 data to Level-2 data products.**

## *3.2 Capability requirements*

### 3.2.1 Data acquisition CRANOX

*Identifier: REQ-ACQ-CRANOX*

*Source: LR*

*Priority : 2*

*Description:*

Obtain data from the CRANOX instruments system ($O_3$, NO, $NO_2$, $NO_X$, $NO_Y$) and make it available for further processing. Until sufficient knowledge is available to implement automated external control of the CRANOX instrument through the RS-232 interface, data shall be retrieved via the analogue outputs.

The CRANOX system of instruments consists of several sub units: two identical analysers (CLD 770 AL ppt, referred to as CLD #1 and CLD #2), a phytolytic converter (PLC 760) and a gold converter (no acronym) manufactured by ECO Physics AG as well as an ozone calibrator (S-100) and an ozone analyser (S-300A) of Environics Inc (see Table 5).

**Table 5: Sub units of the CRANOX system of instruments.**

| Instrument | Manufacturer | Serial Number | Interfaces | Remarks |
|---|---|---|---|---|
| CLD 770 AL ppt | ECO Physics AG | 77319 | 1 x RS232<br>3 x analogue | Referred to as CLD #1 |
| CLD 770 AL ppt | ECO Physics AG | 77320 | 1 x RS232<br>3 x analogue | Referred to as CLD #2 |
| PLC 760 | ECO Physics AG | 76219 | Internal connection to CLD #1 | |
| Gold converter | ECO Physics AG | ./. | Internal connection to CLD #2 | |
| S-300A | Environics Inc. | 2488 | 1 x RS232<br>2 x analogue | Ozone analyser |
| S-100 | Environics Inc. | 2488 | 1 x RS232 | Ozone calibrator |

The CLD analysers measure the light emitted as chemiluminescence when NO reacts with $O_3$ to $NO_2$ and $O_2$. One of the analysers (CLD #1) is connected to the the photolytic converter PLC 760, which converts very selectively $NO_2$ to NO. Depending on the gas flow (through or bypassing PLC 760), CLD #1 thus measures NO or $NO_X$. The other analyser (CLD #2) is connected to a gold converter, which converts all $NO_Y$ substances (e.g. $HNO_3$, $NH_3$, PAN, etc.) to NO. Depending on the gas flow (through or bypassing the gold converter), CLD #2 thus measures NO or $NO_Y$.

In addition to the instruments required for the measurement of nitric oxides, the CRANOX system also disposes of an ozone analyser and ozone calibrator. Ozone is thus determined twice in parallel (CRANOX and TEI 49C) which allows an efficient identification of measurement errors.

As for the TEI instruments, data shall be retrieved every 10 seconds for the parameters NO, $NO_2$, $NO_X$, $NO_Y$, and $O_3$ (see Table 8), although the sampling rate of the instruments is actually lower.

Detailed information on the CLD instruments and the photolytic converter can be found in [*CRANOX*]. The Environics Inc. ozone analyser and calibrator are described in [*ENVIR 100*, *ENVIR 300*].

**Table 6: Parameters to be acquired from the CRANOX instruments system**

| Parameter | Unit | Acquisition Frequency | Accepted range | Remarks |
|---|---|---|---|---|
| NO | ppb | $0.1\ s^{-1}$ | [0.0, 50.0] | |
| $NO_X$ | ppb | $0.1\ s^{-1}$ | [0.0, 50.0] | |
| $NO_Y$ | ppb | $0.1\ s^{-1}$ | [0.0, 50.0] | |
| $O_3$ | ppm | $0.1\ s^{-1}$ | [50.0, 250.0] | |

### 3.2.2 Acquisition of meteorological raw data

*Identifier: REQ-ACQ-METRAW*

*Source: LR*

*Priority : 3*

*Description*:

Two sources of meteorological data are to be used within GAW-DAQAS:

1.) Data obtained locally at *Schneefernerhaus* by DWD. These data are to be imported in near-real-time into the Level-1 database at a rate of 1 per minute and will provide qualitative information on meteorological parameters required for immediate interpretation of trace gas measurements.

2.) Data processed by DWD. These data consist of quality–assured 30-min average values and shall be used within the interactive *ISAVE* visualisation and analysis tool.

**Table 7: Meteorological parameters to be acquired from DWD**

| Parameter | Unit | Acquisition Frequency | Accepted range | Remarks |
|---|---|---|---|---|
| Wind speed horizontal | $m\ s^{-1}$ | $1\ Min^{-1}$ | [0, 50] | |
| Wind speed vertical | $m\ s^{-1}$ | $1\ Min^{-1}$ | [0, 10] | |
| Wind direction | deg | $1\ Min^{-1}$ | [0, 360] | |
| Air temp. | °C | $1\ Min^{-1}$ | [-50, 50] | |
| Air pressure | hPa | $1\ Min^{-1}$ | TBC | TBC |
| Rel. humidity | TBC | $1\ Min^{-1}$ | [0, 100%] | TBC |
| Global irradiation | $W\ m^{-2}$ | $1\ Min^{-1}$ | [0, 2000] | TBC |
| Horizontal visibility | km | $1\ Min^{-1}$ | [0, 300] | TBC |

### 3.2.3 Data acquisition TEI42C analyser

*Identifier: REQ-ACQ-TEI42C*

*Source: LR*

*Priority : 1*

*Description:*

Obtain data from the TEI42C analyser (NO, $NO_2$, $NO_X$) and make it available for further processing. The data shall be retrieved via the RS-232 serial interface of the TEI42C instrument. Data shall be retrieved every 10 seconds for the parameters NO, $NO_2$, $NO_X$ . Additionally, a number of instrumental parameters shall be retrieved at a rate of one per minute (see Table 8).

Detailed information on the TEI42C analyser can be found in [*TEI-42C*].

**Table 8: Parameters to be acquired from the TEI42C analyser**

| Parameter | Unit | Acquisition Frequency | Accepted range | Remarks |
|---|---|---|---|---|
| NO | ppb | 0.1 $s^{-1}$ | [0.0, 200.0] | |
| $NO_2$ | ppb | 0.1 $s^{-1}$ | [0.0, 200.0] | $NO_2 = NO_x - NO$ |
| $NO_x$ | ppb | 0.1 $s^{-1}$ | [0.0, 200.0] | |
| BKG NO | ppb | 1 $Min^{-1}$ | [-1.0, 1.0] | Background NO |
| BKG NOX | ppb | 1 $Min^{-1}$ | [-1.0, 1.0] | Background $NO_x$ |
| NO COEF | 1 | 1 $Min^{-1}$ | [0.9, 1.1] | Coeff. NO |
| NO2 COEF | 1 | 1 $Min^{-1}$ | [0.9, 1.1] | Coeff. $NO_2$ |
| NOX COEF | 1 | 1 $Min^{-1}$ | [0.9, 1.1] | Coeff. $NO_x$ |
| INTERNAL TEMP | °C | 1 $Min^{-1}$ | [20.0, 40.0] | Instrument temp. |
| REACT TEMP | °C | 1 $Min^{-1}$ | [47.0, 51.0] | Reaction chamber temp. |
| CONV TEMP | °C | 1 $Min^{-1}$ | [350.0, 500.0] | $NO_2$ converter temp. |
| PRES | mm Hg | 1 $Min^{-1}$ | [200.0, 300.0] | Pressare react. chamber |

| | | | |
|---|---|---|---|
| SAMPLE FLOW | l $min^{-1}$ | 1 $Min^{-1}$ | [0.60, 1.20] |
| OZONATOR FLOW | l $min^{-1}$ | 1 $Min^{-1}$ | [0.035, 0.150] |
| PMT VOLTAGE | V | 1 $Min^{-1}$ | [-830, -870] |
| PMT TEMP | °C | 1 $Min^{-1}$ | [-20.0, -1.0] |

### 3.2.4 Data acquisition TEI48S (TEI48C) analyser

*Identifier: REQ-ACQ-TEI48S*

*Source: LR*

*Priority : 1*

*Description:*

Obtain data from the TEI48S (and TEI48C) analysers (CO) and make it available for further processing.

The TEI48S is older than the TEI48C and does not dispose of an RS-232 interface. Instead, it is controlled through six analogue input/output ports. Therefore, an interface is required which converts the controlling commands sent to and the data received from the TEI48S. This interface shall be provided by an RS-485 based data acquisition and control system (ADAM 5000 series by Advantech Co., Ltd., further on referred to as ADAM) and an additional RS-232 to RS-485 converter (see Figure 3).

The TEI48C is a newer instrument which may directly be controlled through the RS-232 serial interface. However, the TEI48C does not belong to UBA and may eventually be given back to its owner in near future.

Both instruments shall be integrated into GAW-DAQAS. Data shall be retrieved at a rate of one measurement per second for the parameter CO. Additionally, a number of instrumental parameters shall be retrieved at a rate of one per minute (see Table 9).

The TEI48C/TEI48S instruments show a significant drift of the baseline. A specific cyclic operation mode is therefore required: after 15 minutes of regular air sampling, the air shall be redirected over a catalyst to remove all CO providing a baseline measurement for another 15 minutes. A full sampling cycle therefore takes 30 min.

Detailed information on the TEI48C analyser can be found in [*TEI-48C*].

**Table 9: Parameters to be acquired from the TEI48S / TEI48C analyser**

| Parameter | Unit | Acquisition Frequency | Accepted range | Remarks |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| CO | ppm | 1 $s^{-1}$ | [0, 10000] | |
| BKG | ppm | 1 $Min^{-1}$ | [-1.0, 1.0] | CO background |
| CO COEF | Ppm | 1 $Min^{-1}$ | [0.9, 1.1] | CO coefficient |
| INTERNAL TEMP | °C | 1 $Min^{-1}$ | [20.0, 40.0] | Instrument temp. |
| CHAMBER TEMP | °C | 1 $Min^{-1}$ | [40.0, 48.0] | React. Chamber temp. |
| PRES | mm Hg | 1 $Min^{-1}$ | [450.0, 600.0] | Press. React. Ch. |
| FLOW | l $min^{-1}$ | 1 $Min^{-1}$ | [0.50, 1.00] | Sample flow |
| BIAS VOLTAGE | V | 1 $Min^{-1}$ | [-120, -100] | IR bias supply voltage |
| AGC INT | Hz | 1 $Min^{-1}$ | [160000, 220000] | Intensity ref. chan. AGC circ. |

### 3.2.5 Data acquisition TEI49C analyser

*Identifier: REQ-ACQ-TEI49C*

*Source: LR*

*Priority : 1*

*Description:*

Obtain data from the TEI49C analyser ($O_3$) and make it available for further processing. The data shall be retrieved via the RS-232 serial interface of the TEI49C instrument. Data shall be retrieved at a rate of one measurement per second for the parameter $O_3$. Additionally, a number of instrumental parameters shall be retrieved at a rate of one per minute (see Table 10).

Detailed information on the TEI49C analyser can be found in [*TEI-49C*], on the TEI49C calibrator in [*TEI-49C-OZO*].

**Table 10: Parameters to be acquired from the TEI49C analyser**

| Parameter | Unit | Acquisition Frequency | Accepted range | Remarks |
|---|---|---|---|---|
| $O_3$ | ppm | 0.1 $s^{-1}$ | [50.0, 250.0] | |
| $O_3$ BKG | ppm | 1 $Min^{-1}$ | [-1.0, 1.0] | Ozone background |
| $O_3$ COEF | 1 | 1 $Min^{-1}$ | [0.9, 1.1] | Ozone coefficient |
| BENCH TEMP | °C | 1 $Min^{-1}$ | [20.0, 40.0] | |
| LAMP TEMP | °C | 1 $Min^{-1}$ | [50.0, 60.0] | Bench lamp temp. |
| LAMP SETTING | % | 1 $Min^{-1}$ | [50, 100] | |
| PRES | mm Hg | 1 $Min^{-1}$ | [450.0, 600.0] | React. ch. Press. |
| FLOW A | l $min^{-1}$ | $Min^{-1}$ | [0.4, 0.8] | Sample flow cell A |
| FLOW B | l $min^{-1}$ | $Min^{-1}$ | [0.4, 0.8] | Sample flow cell B |
| CELL A INT | Hz | $Min^{-1}$ | [55000, 150000] | |
| CELL B INT | Hz | $Min^{-1}$ | [55000, 150000] | |

### 3.2.6 Manual calibration control

*Identifier: REQ-CAL-MANCTL*

*Source: LR*

*Priority : 2*

*Description:*

Provide a user interface for manually controlling the calibration process for the trace gas analysers. Manual control shall allow:

1.) to run a non-standard calibration cycle to allow execution of specific non-standard calibration strategies,

2.) to start one of the pre-defined calibration cycles at any specific time.

The manual calibration control shall also provide a graphical interface for controlling each individual valve of the gas flow for any instrument integrated into GAW-DAQAS.

The user interface for manual calibration control shall guide the technical staff through the different steps of the calibration cycle and shall create the database entries required for subsequent automated data processing of the manually obtained calibration data.

### 3.2.7 Calibration cycle of TEI42C

*Identifier: REQ-CAL-TEI42C*

*Source: LR*

*Priority : 1*

*Description:*

Provide gas flow of known NO, $NO_2$, $NO_X$ concentration for the calibration of the TEI42C analyser. There are two possible approaches to TEI42C calibration:

1.) The calibration gases may be provided by diluting gases of known concentrations using the MicroCal 5000 mass flow controller. The gas flow shall be controlled by sequentially switching valves through the ADAM process control system. Report each processing step, adding a time stamp required for later analysis.

2.) The calibration gases may be redirected from the CRANOX instruments system towards the TEI42C.

***A SOLUTION HAS STILL TO BE DEFINED BY UBA***

### 3.2.8 Calibration cycle of TEI48S (TEI48C)

*Identifier: REQ-CAL-TEI48S*

*Source: LR*

*Priority: 1*

*Description:*

Provide gas flow of known CO concentration for the calibration of the TEI48S (TEI48C) analyser. One calibration cycle is to be realised:

- a daily calibration (3-point method).

During the daily calibration cycle, gases of three different CO concentrations are to be offered to the CO analyser:

1.) the so-called "*test gas*" contains CO higher than the ambient CO concentration levels (typically between 150 and 500 ppb).

2.) The so-called "*target gas*" contains CO concentrations comparable to the ambient CO concentration levels (typically between 50 and 150 ppb).

3.) Besides, air free of CO is to be provided as well.

Each day, the actual execution of the daily calibration cycle is to be shifted in time in order to avoid systematic data loss for a specific time of the day. The sequence of the daily CO calibration cycle is depicted in Figure 8.

The calibration gas is provided by bottled gases of known concentration. The actual concentration values vary between the bottles and must be stored in the database for later analysis. Additionally, CO-free air is provided from three different sources: it is either produced in-house (*station zero air*, STA0), directly generated by catalytically removing the CO from the sample air (*sample zero air*, SMP0), or as well taken from a bottle (BTL0). The gas flow shall be controlled by sequentially switching valves through the ADAM process control system. Report each processing step, adding a time stamp required for later analysis.

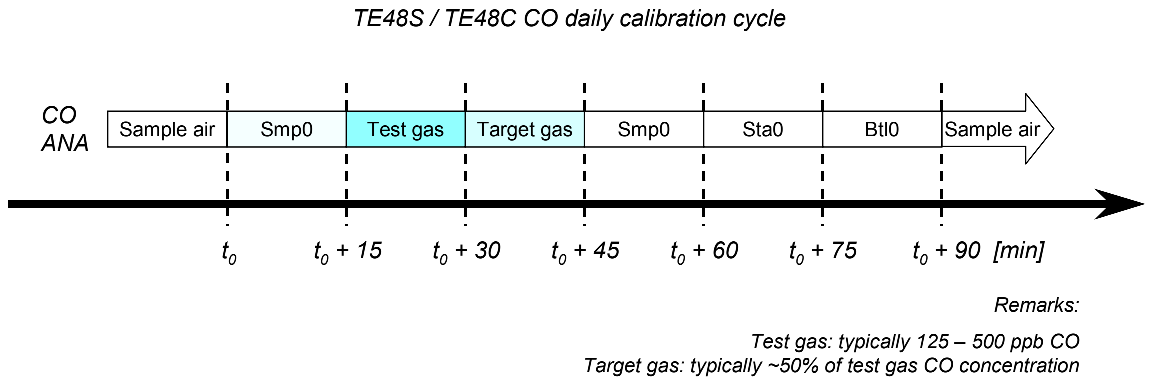


**Figure 8: 3-point calibration cycle for the CO analysers (TEI48S / TEI48C).**

### 3.2.9 Calibration cycle of TEI49C

*Identifier: REQ-CAL-TEI49C*

*Source: LR*

*Priority : 1*

*Description:*

Provide gas flow of known $O_3$ concentration for the calibration of the TEI49C analyser. Two different calibration cycles are to be realised:

1.) A daily calibration (2-point method).

2.) A monthly calibration (5-point method)

During the daily calibration cycle, test gases of two different ozone concentrations are to be offered to the ozone analyser: 0 and 75 ppb. Each day, the actual execution of the daily calibration cycle is to be shifted in time in order to avoid systematic data loss for a specific time of the day. The sequence of the daily calibration cycle is depicted in Figure 9.

During the monthly calibration cycle, test gases of five different ozone concentrations are offered to the ozone analyser: 0, 25, 50, 75 and 150 ppb. The monthly calibration cycle shall be executed each first working day of a month. The sequence of the monthly calibration cycle is depicted in Figure 9.

The calibration gas of the required $O_3$ concentration is produced *in situ* using the TEI49C calibrator. The ozone-free calibration gas is provided by two different means: the so-called “*station zero air*” (STA0) is produced at SFH while the “*sample zero air*” (SMP0) is generated “on-line” by catalytically removing the ozone from the sample air. The main difference between the two types of ozone-free test gases is that the sample zero air is comparable to the sample air in terms of temperature, composition (except ozone concentration), *etc*.

The $O_3$ calibrator is controlled by sending commands over the RS-232 interface. The gas flow shall be controlled by sequentially switching valves through the ADAM process control system. Each processing step is to be reported for later analysis.

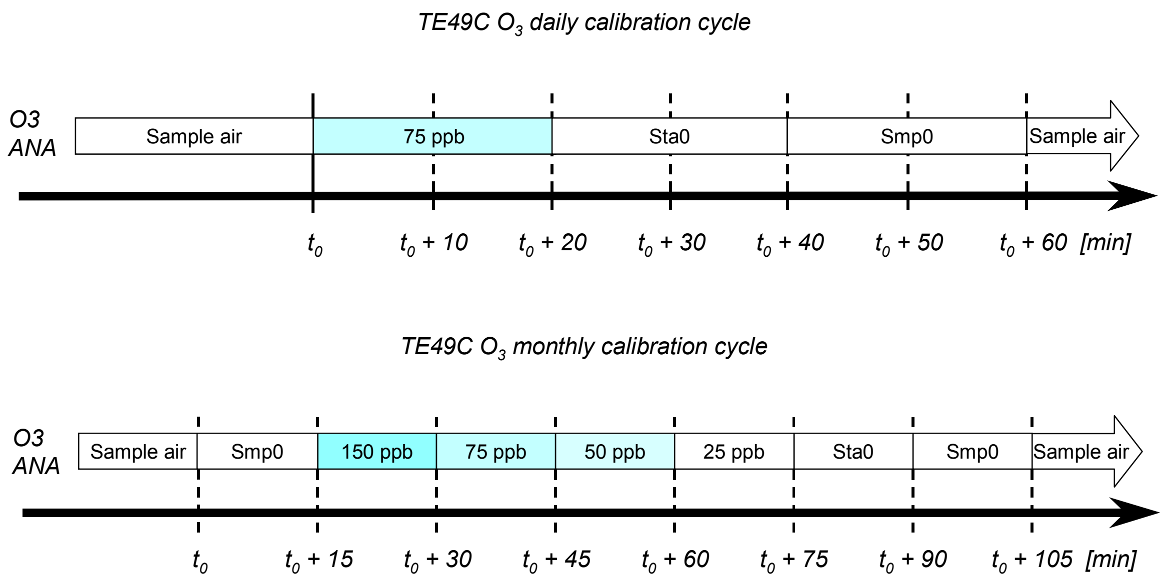


**Figure 9: Daily (2-point, upper panel) and monthly (5-point, lower panel) calibration cycles for the ozone analyser (TEI49C).**

### 3.2.10 Backup and recovery system

*Identifier: REQ-DBS-BACKUP*

*Source: LR*

*Priority : 1*

*Description:*

The back-up and recovery subsystem (referred to as GAW back-up) shall prevent from data losses due to external factors, GAW-DAQAS system failure or accidental misuse. GAW back-up secures two main data types: the source code and configuration information required to operate the GAW-DAQAS system and the data obtained from the operational data acquisition.

The following requirements shall be met by the back-up strategy:

1.) Consider those external factors potentially leading to data loss considered as being of high priority,

2.) Consider the constraints imposed by hardware or network access limitations

3.) Enable rebuilding of the GAW-DAQAS database and system in less than one working day.

### 3.2.11 Level-0 data dump

*Identifier: REQ-DBS-L0DUMP*

*Source: LR*

*Priority: 1*

*Description:*

Dump the raw data stream to and from all instruments without any modification to a file to allow for error analysis and raw data reprocessing in case of necessity.

### 3.2.12 Level-1 products database

*Identifier: REQ-DBS-L1DBSE*

*Source: LR*

*Priority: 1*

*Description:*

Store all data required for further Level-2 data product generation into a database system (raw database). The data to be stored comprise:

1.) One minute trace gas concentration averages with assigned flags,

2.) Instrumental parameters acquired at a rate of one per minute with assigned flags,

3.) 30-min average values of trace gas concentrations and instrumental parameters with assigned flags,

4.) Calibration cycle parameters.

The format of the stored data shall be such as to avoid loss of significant digits. The raw database shall allow to store one full year of data for up to ten instruments. However, later inclusion of further instruments shall not be restricted by the chosen database system. After quality assured data of one year have been delivered to WMO, the corresponding raw data shall be exported from the database into an archive in order to avoid excessive size of the raw database.

### 3.2.13 Level-2 products database

*Identifier: REQ-DBS-L2DBSE*

*Source: LR*

*Priority: 2*

*Description:*

Provide the structures in the database required for storage of Level-2 data products. In the frame of GAW-DAQAS, Level-2 data products consist of 30-min quality-assured average values produced interactively through using the external data visualisation and manipulation tool *ISAVE*. These values shall be used for later delivery to the WMO. The adaptation of the existing version of ISAVE to the new database structure shall be done by the developer of *ISAVE* (Quodata GmbH, Dresden)

### 3.2.14 Meteorological database for quality-assured data

*Identifier: REQ-DBS-METQUA*

*Source: LR*

*Priority: 3*

*Description:*

Provide the structures in the database required for storage of quality-assured 30-min averages of meteorological parameters provided by DWD. These data are to be imported into the *ISAVE* tool for the generation of quality-assured trace gas time series for subsequent delivery to WMO.

### 3.2.15 Station book

*Identifier: REQ-DBS-STBOOK*

*Source: LR*

*Priority : 2*

*Description:*

The station book is a tool to allow users of GAW-DAQAS to log any activity or occurrence that might influence the operation of the GAW station. This information shall be used for general documentation purposes and later interactive data processing. The activity and occurrence logs shall be stored in the GAW-DAQAS database to allow queries relating occurrences directly to measured parameters. Provide specific entry masks and data views to facilitate the GAW staff the management of the station book. There shall be no limitation in entry length for comments. In its first version, contents, entry masks and data views of the station logbook shall closely follow the existing ACCESS implementation. If required, the data model shall be optimised. Additionally, information on the exact concentrations of the bottled test gases used for the calibration shall be included.

### 3.2.16 Calibration coefficient correction

*Identifier: REQ-PRC-CALCOC*

*Source: LR*

*Priority : 2*

*Description:*

Provide actual correction terms for the instrument calibration coefficients. The trace gas analysers are regularly calibrated, typically once per year, typically in external labs such as the *Fraunhofer-Institut*. The instrumental calibration coefficients may change significantly between two subsequent calibrations. In order to provide actual trace gas concentrations with best accuracy, it is necessary to apply correction terms which reflect the actual state on an instrument. Different intermediate calibration cycles are therefore applied for each instrument (see sections 3.2.7, 3.2.8, 3.2.9). These intermediate calibration cycles shall be automatically processed immediately after a calibration cycle has been finished. The aim is to provide linear correction terms relating pre-corrected and corrected target parameters.

In order to assess if an intermediate calibration has been successful, the measured concentrations shall be compared with the corresponding target concentrations. Only if the differences between measured and target concentrations are within pre-defined confidence levels, correction terms shall be calculated and applied to the actual data. If this is not the case, the latest valid correction terms shall be applied. In any case, the latest intermediate calibration shall be visualised on request. All derived correction terms shall be stored to allow further analysis of the instrument stability.

**Table 11: Tolerated deviations between measured and target concentration for the different intermediate instrumental calibrations.**

| Instrument | Calibration for | Tolerated deviation zero gas | Tolerated deviation target conc. (TC) |
|---|---|---|---|
| TE 42C | NO | ±x1 ppb | ±\|x1 + y1% TC\| ppb |
| TE 48S | CO | ±x2 ppm | ±\|x2 + y2% TC\| ppb |
| TE 48C | CO | ±x3 ppm | ±\|x3 + y3% TC\| ppb |

| | | | |
|---|---|---|---|
| TE 49C | O3 | ±x4 ppb | ±\|x4 + y4% TC\| ppb |

### 3.2.17 Flag generation

*Identifier: REQ-PRC-FLGGEN*

*Source: LR*

*Priority : 2*

*Description:*

Assign flags to Level-1 and Level-2 data products to inform GAW staff about data quality. Flag generation for subsequent storage into the database is limited to data quality related to data availability. The reason for this limitation is that flags based on predefined tolerance ranges require reprocessing of the whole database in case a tolerance range is changed. The flags shall be stored together with the corresponding values. The flags listet in xxx shall be assigned.

**Table 12: Flags to be used within GAW-DAQAS.**

| Flag | Value | Description |
|---|---|---|
| SUSPICIOUS | 0 | A value could be calculated but should be handled with care (e.g. few valid values in time interval) |
| VALID | 1 | No apparent problems encountered |
| NO DATA | 4 | No values available (e.g. no data from instrument, not enough data for statistical calculations) |
| NO DATA VALUE | -999 | Value assigned to parameter in case "NO DATA" flag is raised |

### 3.2.18 ISAVE integration

*Identifier: REQ-PRC-ISVINT*

*Source: LR*

*Priority : 2*

*Description:*

Implement interfaces for import of data from the raw database into the data visualisation and manipulation tool *ISAVE* as well as for export from *ISAVE* into the Level-2 database. A pre-requisite for starting this activity is the finalisation of the raw data acquisition up to Level-1 data product generation.

### 3.2.19 Level-1 product generation

*Identifier: REQ-PRC-LEVEL1*

*Source: LR*

*Priority: 1*

*Description:*

The latest valid correction terms shall be applied to the instrumental raw data to provide actual trace gas concentrations with the best possible accuracy. 1- minute averages shall be calculated and stored from the trace gas concentrations. Statistical methods shall be applied to minimise the effects of outliers on the results as follows:

1.) The median shall be used to calculate the average for all trace gas concentration measurements.

2.) If three or more valid values per minute interval are considered as “VALID”, the median is calculated and the “VALID” flag is raised for the 1-minute average.

3.) If less than three values per minute interval are considered as valid, the median is calculated as arithmetic mean (two values) or is set equal to the one and only valid value. In this case, the “SUSPICIOUS” flag is raised for the minute average.

4.) If no valid value is available for the one minute interval, the “NODATA” value is assigned and the “TIME OUT” flag is raised for the minute average.

30-minutes averages shall be derived for all measured trace gas concentrations from the 1-minute averages as follows:

5.) The median, arithmetic mean and standard deviation shall be used to characterise the 30-minutes averages.

6.) If 20 or more 1-minute averages are considered as “VALID” within a 30-minutes interval (“2/3 criterium”), median, arithmetic mean and standard deviation are calculated and the “VALID” flag is raised for the 30-minutes averages.

7.) If between 10 and 19 1-minute averages are considered as “VALID” within a 30-minutes interval, median, arithmetic mean and standard deviation are calculated and the “SUSPICIOUS” flag is raised for the 30-minutes averages.

8.) If less than 10 1-minute averages are considered as “VALID” within a 30-minutes interval, the “NODATA” value is assigned to median, arithmetic mean and standard deviation and the “TIME OUT” flag is raised for the 30-minutes averages.

The 30-minutes averages are not quality-assured and shall only be used for internal purposes of the UBA GAW global station at SFH.

The raw data used to derive Level-1 data shall not be stored in the GAW-DAQAS database. However, raw data are available from the raw data stream written directly on a storage medium (see section 3.2.11)

### 3.2.20 Level-2 product generation

*Identifier: REQ-PRC-LEVEL2*

*Source: LR*

*Priority: 2*

*Description:*

Generate Level-2 data products from Level-1 data products. Level-2 data products consist of 30-min average values. The first value of a day is given at 00:30 MEZ (MEZ = UTC+1) and represents all values obtained between 00:00 and 00:30 MEZ. The last value of a day is given at 24:00 MEZ and represents all values obtained between 23:30 and 24:00 MEZ.

Level-2 data products are derived using the external *ISAVE* software produced by Quodata GmbH, Dresden.

#### 3.2.21 Report generation

*Identifier: REQ-REP-LEVEL2*

*Source: LR*

*Priority: 2*

*Description:*

Generation of reports, including data delivery, from the Level-2 data product database for different purposes:

1.) Internal UBA reports

2.) Data delivery to DWD

3.) Data delivery to WMO

The different reports require customer-specific contents and formats (“Langen” data format for delivery to WMO, DWD data format for delivery to the German Weather Service, further data formats to account for specific UBA requirements.

A tool to generate these reports has already been developed by LR under MS Visual Basic, further on referred to as LR_REPGEN. GAW-DAQAS shall provide a tool to export of data from the DAW-DAQAS database for direct input to LR_REPGEN. To do so, the exported data shall comprise 30-min averages for a period of time interactively specified by the user. The exported data must follow a specific column-based file structure in the EXCEL *.csv (ASCII) file format, that is columns are separated by a semicolon. The first line is a header line identifying the data in the respective columns. The actual data follows in lines 2, …, N. LR_REPGEN identifies the columns by their position, the pre-defined suite of columns must therefore strictly be followed

**Table 13: Identifiers and Units of export data format for LR_REPGEN.**

| Column No. | Identifier | Unit |
|---|---|---|
| 1 | JUL_KAL | None |
| 2 | JJMMTT | None |
| 3 | DAY OF MONTH | None |
| 4 | MEZ (HHMM) | None |

| | | |
|---|---|---|
| 5 | CO2 | ppmV |
| 6 | CH4 | ppbV |
| 7 | O3 | ppbV |
| 8 | CO | ppbV |
| 9 | NO | ppbV |
| 10 | NOx | ppbV |
| 11 | N_RADIOAK | bq/m^3 |
| 12 | BE7 | bq/m^3 |
| 13 | L_DRUCK | hPa |
| 14 | GLB_STR | W/m^2 |
| 15 | DIF_STR | W/m^2 |
| 16 | TEMP | °C |
| 17 | TAUP | °C |
| 18 | REL_FEU | % |
| 19 | NOy | ppbV |
| 20 | DIR_STR | W/m^2 |
| 21 | S_DAUER | h |
| 22 | SICHTW | km |
| 23 | N2O | ppbV |
| 24 | SF6 | ppbV |

Missing values shall be filled by the value –999. Additional columns may be added if required. The values shall be given out in decimal format as accurately as required. Formatting shall be such as to allow comfortable viewing of the exported data in an editor.

### 3.2.22 System surveillance

*Identifier: REQ-REP-SYSSRV*

*Source: LR*

*Priority: 2*

*Description:*

Generate status reports on the actual state of GAW-DAQAS itself and the various connected trace gas analysers. The reports shall cover a one week period from Monday morning 00:00 to Sunday evening 23:59. They shall be delivered as formatted ASCII file.

The following analysis shall be performed for GAW-DAQAS:

1.) Availability of GAW-DAQAS in per cent

The following analysis shall be performed for each trace gas analyser:

2.) Overall availability of the instrument in per cent

3.) List of unavailability periods (beginning, end and duration)

4.) List of time periods when instrumental parameters were outside tolerance intervals (beginning, end and duration)

5.) List of time periods when derived trace gas concentrations were outside tolerance intervals (beginning, end and duration)

6.) List of actual calibration coefficients used during the reporting interval (instrument calibration coefficients and actual correction terms)

### 3.2.23 Level-1 data product visualization

*Identifier: REQ-VIS-LEVEL1*

*Source: LR*

*Priority : 1*

*Description:*

A Graphical User Interface (GUI) shall be provided to allow the technical staff at SFH

1. to be always informed about the actual concentration levels of the atmospheric trace gases,
2. to be alarmed in case trace gas concentrations or instrumental parameters are outside pre-defined tolerance ranges,
3. to visually inspect time series of trace gas concentrations or instrumental parameters stored in the raw data base,
4. to visually inspect the latest intermediate calibration for each trace gas.

Ad 1.): trace gas concentrations of all instruments connected to GAW-DAQAS shall be presented in the form of a table. If an instrument does not directly provide concentration units, its raw values shall also be displayed.

Ad 2.) In case a trace gas concentration or an instrumental parameter is outside its tolerance range (see Table 8, Table 9, Table 10), a pop-up window shall appear on the screen providing detailed information on the suspicious value. Eventually, an acoustic alarm may also be triggered.

Ad 3.) Time series covering the actual day and the full previous day shall be provided for both trace gases and instrumental parameters. Additionally, historical data from the database shall be accessed and visualised through the data visualisation window.

Ad 4.) The latest intermediate calibration for each trace gas shall be graphically represented as follows:

- Measurement of the trace gas concentration as time series
- Horizontal lines indicating the corresponding target concentrations

## *3.3 Constraint requirements*

### 3.3.1 GAW-DAQAS hardware

*Identifier: URD-CON-HDWARE*

*Source: LR*

*Priority : 1*

*Description:*

GAW-DAQAS shall operate on hardware which has been specifically acquired for this purpose and which has been used operationally for data acquisition at SFH since 2001. The hardware consists of one PC (Pentium II) equipped with two 8 GB SCSI hard disk drives operating under RAID level 1. Several ADAM I/O modules are available for relay control and acquisition of analogue signals. The operating system originally installed is MS Windows NT 3.5. It may be changed to MS Windows 2000/XP in case of necessity. The GAW-DAQAS hardware shall allow simultaneous connexion of at least 10 RS232 interfaces. The GAW-DAQAS hardware shall be connected to the UBA intranet.

A portable computer of similar specifications is available in order to replace the main PC in case of failure. The portable computer shall be equipped such as to replace the main GAW-DAQAS hardware system within two hours. This requires parallel installation of both hard- and software on the portable computer.

### 3.3.2 English documentation

*Identifier: URD-CON-ENGLSH*

*Source: LR*

*Priority : 1*

*Description:*

All technical documentation shall be written in English. This will allow to present the analysis of the identified requirements on GAW-DAQAS, as well as the strategies chosen to fulfil these requirements, to the operating institutions of GAW regional or global stations worldwide. It will also facilitate to generate information for the planned GAW-DAQAS website.

### 3.3.3 Maintainability

*Identifier: URD-CON-MNTNBT*

*Source: LR*

*Priority : 1*

*Description:*

GAW-DAQAS shall be operated independently by GAW staff after its final installation and subsequent training. In this respect, operating GAW-DAQAS means:

1.) Shutting down and restarting each component of GAW-DAQAS: scheduler, database, back-up process,

2.) Modifying existing calibration cycles,

3.) Filling gaps in the database using the direct log of the raw data stream.

Integration of UBA staff during the development phase of GAW-DAQAS shall enable continuous competence building at UBA.

To ensure maintainability, an architectural design is required which provides clear and well documented interfaces.