GRUAN OZONESONDE TECHNICAL DOCUMENT

Version 1.1.0.3

Purpose of this Guide

This Document to GCOS Reference Upper Air Network (GRUAN) ozonesonde operations provides both mandatory operating protocols and non-mandatory recommendations for measurements of vertical ozone profiles using ozonesondes within GRUAN. This Document relies on the standard operating protocols, instrument selection, and uncertainty estimates and calculations from the WMO/GAW Report #201 [Smit et al., 2014], Assessment of Standard Operating Procedures for Ozone Sondes (ASOPOS) panel recommendations, and the large body of peer-reviewed literature on ozonesondes. This Document also builds on the GRUAN Manual and Guide to Operations (herein referred to as GCOS-171). As in the GRUAN Manual and Guide, mandatory operating protocols are distinguished by the words ‘shall’ or ‘must’ while guidelines are distinguished by the words ‘could’ or ‘should’.

The primary goal of GRUAN is to provide vertical profiles of reference measurements suitable for reliably detecting changes in global and regional climate on decadal time scales. GRUAN’s goals have been agreed to by GCOS (Global Climate Observing System) and WMO (World Meteorological Organization). Ozone is classified as a priority 2 essential climate variable (ECV) within GRUAN. GRUAN ozonesonde measurements will provide a calibrated reference standard for global satellite-based measurements of atmospheric ozone. GRUAN ozonesonde measurements will also ensure that potential gaps in satellite measurement programmes do not invalidate the long-term ozone record, and will provide data to fully characterize the properties of the atmospheric column. Because ozone is a key radiatively active gas, vertically resolved measurements of the ozone profile are essential for characterizing radiative transfer through the atmosphere column.

From Section 6.1 of GCOS-171

“GRUAN will not prescribe the use of specific instruments in the network since the emphasis is not on prescribing an instrument, but rather on prescribing the capabilities required of an instrument and allowing individual sites to select an instrument that achieves those capabilities.”

This GRUAN Ozonesonde Technical Document includes frequent references to the requirements described in the GRUAN Guide to Operations (GCOS-171), and provides additional ozonesonde-specific requirements not described in GCOS-171. It defines the requirements on random and systematic uncertainty and long-term stability for the operations of all ozonesonde instruments in use at GRUAN sites. This Document establishes the philosophy under which GRUAN ozonesondes shall operate and inform current and future GRUAN sites of the expected modus operandi for ozonesonde operations at GRUAN sites. The overall framework under which an ozonesonde will operate in GRUAN is hereafter referred to as the ‘GRUAN Ozonesonde Programme’.
The GRUAN community is not the international authority on ozonesonde operations. This Document has been developed in close collaboration with international leaders in the development of ozonesonde standard operating procedures (SOPs). These are the principals in the WMO ozonesonde community (Dr. H. Smit/Research Centre Jülich GmbH, and collaborators who developed ASOPOS), the Network for Detection of Atmospheric Composition Change (NDACC) working group, and the principals in the Southern Hemisphere ADDitional OZonesondes (SHADOZ) network.

Relevant information from this GRUAN Ozonesonde Technical Document is expected to be incorporated into the WMO Manual on the Global Observing System (WMO-No. 544) and the Guide on the Global Observing System (WMO-No. 488). This Guide may be additionally supported by a series of technical documents listed on the GRUAN web site at http://www.gruan.org.
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1 INTRODUCTION

1.1. Ozone heritage

Ozone is a key trace gas in Earth’s atmosphere. In the stratosphere it absorbs incoming solar radiation in the UVC (<280 nm) and UVB (280-320 nm) portions of the spectrum. Because radiation at these wavelengths has sufficiently high energy to be detrimental to biological systems, the stratospheric ozone layer provides an essential screen thus protect life on Earth’s surface. During the latter half of the 20\textsuperscript{th} century the stratospheric ozone layer was depleted, most severely over Antarctica, as a result of anthropogenic emissions of ozone depleting substances. As a result of the successful implementation of the Vienna Convention for the Protection of the Ozone Layer and its Montreal Protocol (including amendments and adjustments to the Protocol), emissions of ozone depleting substances have declined dramatically and the status of the ozone layer is expected to return to a mid-20\textsuperscript{th} century state in the second half of the 21\textsuperscript{st} century.

The effects of ozone are not always positive. Ozone is a key component of photochemical smog and high levels of ozone are associated with poor air quality. The common saying is that ozone is ‘nice from far but far from nice’. Ozone in the troposphere also acts as a strong oxidizer and this removes many compounds, including toxic substances, from the air. Ozone levels therefore play a role in determining the tropospheric lifetimes of many compounds. Ozone is also a greenhouse gas, absorbing outgoing infrared radiation from Earth’s atmosphere. Because of its importance both as an absorber of incoming solar UV radiation, and as an absorber of outgoing infrared radiation, it is essential that changes in ozone concentrations throughout the atmosphere are carefully monitored.

The vertical distribution of ozone in the atmosphere can be monitored using a range of different techniques including satellite-based (solar occultation, limb-sounding, nadir viewing) instruments, balloon-borne \textit{in situ} instruments (ozonesondes, dropsondes), and ground-based remote sensing systems (lidars and microwave radiometers). Ozonesondes fulfil an important role in this suite of techniques by providing very high vertical resolution ozone profiles from the surface to the middle stratosphere with small measurement uncertainties, capable of making measurements during periods of no sunlight, and can be easily deployed from remote locations such as ships or small islands.

A number of quasi-independent ozonesonde measurement programmes have been established globally to monitor changes in the vertical distribution of ozone. The WMO/GAW\textsuperscript{1}, SHADOZ and NDACC communities have established an expert panel, ASOPOS (Assessment of Standard Operating Procedures for Ozonesondes), to develop standard operating procedures for ozonesonde measurement programmes. This Document builds considerably on the large body of material already developed by ASOPOS [Smit et al., 2012].

\textsuperscript{1} A complete list of all acronyms appearing in this Document is provided at the end of the document.
Because long-term satellite-based measurements of ozone in the troposphere and UTLS are not currently available, the ozonesonde record provides the primary source for deriving ozone trends in the troposphere and UTLS, especially in the climate sensitive region around the tropopause. When combined with satellite-based measurements of ozone, they can provide a global, multi-decadal data set extending from the surface to the mesosphere for long-term ozone trend detection (Bodeker et al., 2012).

There are challenges in making ozonesonde measurements such that will meet the needs of GRUAN users (see Section 1.2). While instruments may be well calibrated, because instruments are seldom recovered after flight, each well calibrated instrument is discarded after each profile measurement. Ensuring inter-instrument calibration in an environment where instruments from different manufacturing batches may show systematic biases, presents a challenge.

1.2. The purpose of ozonesondes within GRUAN

As detailed in GCOS-112, GRUAN’s objectives are to:

i) Provide long-term high quality climate records;

ii) Constrain and calibrate data from more spatially-comprehensive global observing systems (including satellites and current radiosonde networks); and

iii) Fully characterize the properties of the atmospheric column.

To achieve these goals with respect to ozone, sites within the network should provide vertical profiles of reference measurements of ozone for reliably detecting changes in global and regional climate, on multi-decadal time scales, for major climatically distinct regions of the globe. Changes in ozone, both in the stratosphere and troposphere are known to drive changes in global and regional climate. Reference within GRUAN means that, at a minimum, the observations are tied to a traceable standard, that the uncertainty on the measurement has been determined, and that the entire measurement procedure and set of processing algorithms are properly documented and accessible (Immler et al., 2010). Within this framework, ozonesonde measurements are classified as ancillary measurements.

Potential uses of such ancillary measurements include:

i) Providing measurements at GRUAN sites that complement the priority 1 measurements of temperature, pressure and water vapour and priority 2 measurements of ozone.

Understanding changes in the vertical distribution of ozone is required to understand changes in the vertical distribution of temperature.

ii) Providing redundant measurements of the ozone profile.

The four key user groups of GRUAN ozonesonde ozone profiles are the same as those identified in the GRUAN Guide to Operations, viz.:

i) The climate detection and attribution community. Understanding changes in the vertical distribution of ozone is essential to understanding changes in the thermal structure of the atmospheric column.
ii) The satellite community. Validating satellite-based measurements of ozone is recognized as an essential requirement of the GRUAN ozonesonde programme.

iii) The atmospheric process studies community. High vertical resolution measurements of the ozone profile, with well resolved measurement uncertainties, provide key data for understanding atmospheric processes. Many aspects of stratospheric dynamics and the dynamics associated with stratosphere-troposphere exchange can be studied using ozone profiles from ozonesondes. Ozonesonde measurements have played a key role in determining ozone loss rates in the Arctic vortex (Rex et al., 1998).

iv) The numerical weather prediction (NWP) community.

1.3. Organization and design of the GRUAN Ozonesonde Programme

GRUAN operates under the joint governance of GCOS and WMO as a WIGOS Implementation Project. A defining attribute of GRUAN is the standardisation and centralization of data processing with the goal of ensuring network-wide homogeneity of the resultant data products.

1.3.1. Terminology

A GRUAN Ozonesonde Programme is an ozonesonde measurement programme implemented at a site and having been assessed and certified as defined in Sections 3.1 and 3.2.

A GRUAN Ozonesonde instrument is one of the instruments employed in a GRUAN ozonesonde programme. These are balloon-borne electrochemical concentration cell (ECC) ozone sensors measure high vertical profiles of ozone, pressure, temperature, and relative humidity. ECC ozone sensors are described in Section 2.1.

A GRUAN Ozonesonde Product is an ozone product resulting from the measurements made within a GRUAN ozonesonde programme. A GRUAN Ozonesonde Product is always produced by the GRUAN Ozonesonde Analysis Software System (GOASS, see Section 3.7) designed to implement the requirements and recommendations defined in this document.

1.3.2. Responsibilities

The GRUAN Task Team on Sondes (TTS), in consultation with the GRUAN Lead Centre and Task Team on Ancillary Measurements, is responsible for integrating best ozonesonde measurement practices into GRUAN operations. These best practices shall be synthesized in the form of requirements and recommendations compiled in this Document and shall be implemented in all certified GRUAN Ozonesonde Programmes.

GRUAN sites hosting a GRUAN Ozonesonde Programme shall use a designated system of methods, techniques and facilities in full compliance with the requirements and recommendations detailed in this document. For any given GRUAN Ozonesonde Programme, this system will not be changed without advanced notice to the TTS and GRUAN Lead Centre.

GRUAN Ozonesonde Programmes incorporate a programme to validate the stability and uncertainty of the measurements, agreed with WG-GRUAN, and managed in detail by the GRUAN TTS and GRUAN Lead Centre. This assurance programme comprises three mandatory components, which are the GRUAN Standard Operating Procedures (SOPs) for all GRUAN ozonesonde instrument calibration (described in Section 3.5), the RSLaunchClient (described in Section 3.6), and the GOASS (described in Section 3.7).
The design of GRUAN Ozonesonde Programmes shall recognise the heterogeneity of the network of sites, many of which will have primary responsibility to networks other than GRUAN. GRUAN Ozonesonde Programmes shall integrate, where possible and when feasible, with other international long-term monitoring programmes.

GRUAN Ozonesonde Programmes shall be responsive to the latest technological and scientific progress in ozonesonde measurement techniques and observational requirements. Non-GRUAN ozonesonde development work can continue at a GRUAN site in collaboration with the TTS until mature and validated, at which point any improvements can be introduced into GRUAN operations with the agreement of the TTS and GRUAN Lean Centre.

WG-GRUAN, the GRUAN Lead Centre and TTS will act as the interfaces between GRUAN and the community of users of GRUAN ozonesonde products.

1.4. Implementation of GRUAN Ozonesonde Programmes

The implementation of the GRUAN Ozonesonde Programmes, as a whole, and specific issues relevant to an individual Ozonesonde Programme shall be guided by the TTS and WG-GRUAN. These two teams will work with other relevant expertise in support of GRUAN and coordinate with the GRUAN Lead Centre.

A GRUAN Analysis Team for Network Design and Operations Research (GATNDOR) shall undertake focused, short-term research to address specific topics identified by the WG-GRUAN. The work will be conducted in coordination with the TTS and with other GCOS programmes when appropriate.

The WG-GRUAN and TTS shall use this report which establishes standard operational procedures (SOPs) and metadata requirements for all GRUAN Ozonesonde Programmes. The TTS shall evaluate the appropriateness of uncertainty estimates, the usefulness of particular measurements and operational procedures, synthesize the available knowledge, and develop recommendations to improve GRUAN measurements and operations. The TTS and WG-GRUAN shall confer regularly to evaluate the current status of GRUAN observations, to identify weaknesses, and to incorporate new scientific understanding into GRUAN. The expertise of these teams shall also be used to support the Lead Centre in guiding individual sites through changes in instrumentation and operating procedures without impacting long-term measurement time series.

The GRUAN Lead Centre shall identify sites where instrument operators need training, re-training, and organise cost-efficient training courses for the network at appropriate locations, as advised by the appropriate TTS, to encourage uniformity of instrument operation between sites. The Lead Centre may liaise with National Metrological Institutes in this regard.

All activities associated with the implementation of GRUAN are the responsibility of the institution/organization hosting the GRUAN site and should, as far as possible, be met through national funding. To best serve the needs of the climate monitoring and research communities, it is essential that GRUAN is cognizant of the evolving science that drives the measurements and accuracy of the GRUAN data. The ozonesonde instrumentation deployed and the observing schedules may differ between sites, as agreed with WG-GRUAN as part of the site assessment.
and certification process, but the methods of observation used with the main observing systems are expected to be uniform between all GRUAN sites.

1.5. Links to partner networks and satellite-based measurement programmes

In the original charter for GRUAN (GCOS-92) it is stated that ‘where feasible, the GRUAN sites should be co-located and consolidated with other climate monitoring instrumentation’. GRUAN Ozonesonde Programmes shall not be run in isolation of existing ozonesonde networks and GRUAN is not intended to replace existing networks. GRUAN Ozonesonde Programmes are likely to operate in the framework of existing networks such as the Network for the Detection of Atmospheric Composition Change (NDACC) and SHADOZ (Southern Hemisphere ADditional OZonesondes), and to leverage off the expertise available in these networks and e.g. through the GAW (Global Atmosphere Watch) scientific advisory group for ozone. As a result, close and regular coordination between the governing bodies of these networks and with the WG-GRUAN and GRUAN TTR+AM is required. This coordination can be achieved by having members of the WG-GRUAN and TTR+AM attend steering group meetings of partner networks and by inviting co-chairs or steering group members from partner networks to attend WG-GRUAN and GRUAN TTR+AM meetings.

Where an existing ozonesonde measurement system meets the operational requirements of GRUAN, the first priority is to encourage that site to join GRUAN. In such cases operational requirements should be optimized to meet the needs of both parties.

1.5.1. NDACC (Network for the Detection of Atmospheric Composition Change)

NDACC comprises more than 70 remote-sensing research sites for observing and understanding the physical and chemical state of the stratosphere and upper troposphere and for assessing the impact of stratospheric changes on the underlying troposphere and on global climate. A number of NDACC sites fly ozonesonde and NDACC has a standing working group on ozonesondes, water vapor sondes, and aerosol sondes.

1.5.2. GAW (Global Atmosphere Watch)

GAW is as a coordinated network of observing stations, associated facilities and related scientific assessment activities, and supplies basic information to be used by policy-makers [Global Atmosphere Watch Guide, GAW Report No.86, 1993]. As a major component of GAW, the global network of ozone sounding stations provides the longest time series of the vertical ozone distribution between surface and 30-35 km altitude [GAWSIS, http://www.empa.ch/gaw/gawsis ].

1.5.3. Atmospheric Radiation Measurement (ARM) Programme

The goal of the U.S. Department of Energy ARM programme is to study changes in climate, land productivity, oceans or other water resources, atmospheric chemistry, and ecological systems that may alter the capacity of the Earth to sustain life. This includes improving the atmospheric

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2 http://www.wmo.ch/web/arep/gaw/gaw_home.html
A dedicated Data Quality (DQ) Office provides ARM with a number of tools to ensure the high quality of the collected data. The potential use of these tools in GRUAN must be explored to ensure network-wide homogeneity of the GRUAN ozonesonde measurements. The ARM DQ Office has developed a suite of sophisticated data quality visualization tools that may be of interest to GRUAN Ozonesonde Programmes.

1.5.4. SHADOZ (Southern Hemisphere Additional Ozonesondes)

SHADOZ (Southern Hemisphere Additional Ozonesonde) is a project to augment and archive ozonesonde data from over a dozen tropical and sub-tropical sites and has become the central repository for vertical profiles of ozone in the tropics/sub-tropics. Prior to the creation of SHADOZ, tropical ozonesonde data were accessible via campaigns or collaborative associations with specific operating site representatives. Started in 1998 by NASA's Goddard Space Flight Center, and other US and international co-investigators, SHADOZ is an important tool for equatorial tropospheric ozone research. The rationale for SHADOZ is to: (1) validate and improve model and remote sensing techniques for estimating tropical ozone, (2) contribute to climatology and trend analyses of tropical ozone and (3) provide research topics to scientists and educate students, especially in participating countries [Thompson et al., 2003a; 2003b, 2004, 2007, 2012]. SHADOZ is envisioned as a data service to the global scientific community by providing a central public archive location via the internet: http://croc.gsfc.nasa.gov/shadoz. SHADOZ data are mirrored at the Aura Validation Data Center (AVDC) and are deposited to WOUDC. While the SHADOZ website maintains a standard data format for the archive, it also informs data users of the differing sites' preparation techniques and data treatment. Data from launches from various SHADOZ supported field campaigns, such as, the Indian Ocean Experiment (INDOEX), Sounding of Ozone and Water in the Equatorial Region (SOWER) and Aerosols99 Atlantic Cruise are also available.

1.5.5. WOUDC (World Ozone Ultraviolet Data Centre)

WOUDC operates under the auspices of the WMO/GAW programme to archive ozone and ultraviolet in-situ instrument data. Data is contributed to WOUDC at no cost and provides an independent storage and backup of instrument data. Like SHADOZ, WOUDC is a web-based, public access archive (www.woudc.org) and provides enhanced user search capabilities and visualizations. The WOUDC gets guidance from the WMO Science Advisory Groups (SAGs) for issues related to both ozone and UV.

1.5.6. Link to satellite-based measurement programmes

Ozonesonde measurements have historically provided a key data set for validating satellite-based measurements of ozone. GRUAN Ozonesonde Programmes, with their well characterized measurement uncertainties and network wide homogeneity are expected to provide a database of vertically resolved ozone that will be essential for validating satellite-based measurements of the vertical distribution of ozone. Because the GRUAN ozonesonde measurements are likely to serve a wide range of end-users within the satellite measurement community, WG-GRUAN and
TTR+AM members shall be assigned to liaise with key clients within the satellite community to ensure that GRUAN ozonesonde data products are tailored, where possible, to best meet the needs of this community. Once GRUAN ozonesonde data sets are available, pilot studies on enhanced combined data sets using these reference measurements e.g. generating site atmospheric state best estimates (SASBEs) for ozone, need to be undertaken. The GRUAN ozonesonde measurements provide an essential database for removing offsets and drifts between separate satellite-based measurement series within the limitations imposed by the uncertainties on the GRUAN ozonesonde measurements.
2 GRUAN OZONESONDE TECHNIQUES AND MEASUREMENT PRINCIPLES

This section provides the GRUAN Ozone sonde Programmes and user community with essential knowledge of the way ozonesondes measure profiles of ozone. For further comprehensive reviews of the ozonesonde measurement technique, the reader should refer to the publications mentioned in this section.

Ozonesondes are small, lightweight balloon-borne instruments that use an electrochemical technique to make in situ measurements of ozone from the surface of the Earth to an altitude determined by balloon burst, typically 30 to 35 km [Smit et al., 2002]. The sonde is interfaced to a standard meteorological radiosonde for transmission of the data to the ground and is usually flown together with the radiosonde as part of the same package. The package is carried aloft by a rubber balloon similar to that used for radiosonde measurements, though in this case a 1000-1200 g balloon is typically used rather than the standard 300 g meteorological balloon. The package ascends through the atmosphere at ~6 m.s\(^{-1}\) and, with a measurement frequency of ~2 seconds, results in a vertical resolution of less than 15 m. Ozonesondes constitute the most important data source with long term-data coverage for the derivation of ozone trends with sufficient vertical resolution, particularly in the important, climate sensitive, altitude region around the tropopause.

As defined in GCOS-171:

“A reference measurement result typically arises from a defined measurement procedure that involves standards traceable to national or international standards as maintained at National Metrological Institutes (NMIs). For GRUAN, a reference measurement is one where the uncertainty of the calibration and the measurement itself is carefully assessed. This includes the requirement that all known biases have been identified and corrected, and, furthermore, that the uncertainty on these bias corrections has also been determined and reported. An additional requirement for a reference measurement is that the measurement method and associated uncertainties should be accepted by the user community as being appropriate for the application.”

To produce GRUAN ozonesonde reference measurements, mandatory and recommended processing procedures have been established such that the ozonesonde data products derived shall be reproducible at any time in the future. Section 2 describes the data processing procedures required for each component of the ozonesonde measurement technique. The GRUAN Ozonesonde Programmes and centralized ozonesonde data processing facility shall apply these procedures to create the standard reference GRUAN ozonesonde data product (see Sections 3.5 - 3.7).

As of the time of the development of this Technical Document, the Electrochemical Concentration Cell (ECC) sonde (Komhyr, 1969) is the only type of ozonesonde being flow and therefore this document focusses solely on SOPs for the ECC sonde type. Two other types of sondes, namely the Brewer-Mast (BM) sonde (Brewer and Milford, 1960) and the Japanese manufactured Carbon Iodide (Cl) sonde (Kobayashi and Toyama, 1966) are no longer being
flown operationally. In the last decade long-term BM sonde sites have changed to ECC sondes.

The homogenization of time series that use BM and ECC sondes at the Uccle, Belgium, site has been undertaken by De Backer [1999] using results from dual BM/ECC sonde launches [De Backer et al., 1998] – see also Section 7.2 on the use of transfer functions for homogenizing time series that include BM and ECC sondes. Dual flight campaigns at the Payerne, Switzerland, site showed no detectable differences between their BM and ECC sondes [Stübi et al., 2008]. Since the late 2000s, Japanese sites have switched from using CI sondes to using ECC sondes. While Nakamura et al. [2008] conducted inter-comparison studies for CI and ECC sondes, transfer functions between the two sensors have not yet been derived.

2.1 The Ozonesonde Measurement

The ECC instrument consists of a non-reactive teflon gas-sampling pump connected to an ECC ozone sensor, and an electronic interface that connects the ozone sensor to a radiosonde for data telemetry (see Figure 1 of Komhyr, 1995). The instrument is encased in a polystyrene weatherproof box during flight. Measurements of ozone partial pressure, the sonde’s pump temperature, motor voltage and current, air temperature, air pressure and humidity are transmitted to a ground receiving station. Winds derived from GPS-enabled measurements became available in the early 2000s.

The ECC sensor measures ozone using iodine/iodide electrode reactions [Vetter, 1967]. Two platinum electrodes are immersed in separate cathode and anode chambers, also called half cells, of differing concentrations of potassium iodide (KI) solution. The anode cell contains a solution saturated with KI. Both cells contain an equal concentration of potassium bromide (KBr) and a phosphate buffer to maintain a neutral pH. An ion bridge connecting the two chambers, allows ions to flow between the two cells but prevents mixing, thereby preserving their respective concentrations.

Ambient air containing ozone ($O_3$) is pumped into the cathode cell and reacts with iodide ($I^-$) to form iodine ($I_2$) based on the aqueous reaction:

$$2KI + O_3 + H_2O \rightarrow I_2 + O_2 + 2KOH \quad \text{Rxn. 1}$$

To maintain electrochemical equilibrium iodine is converted back to iodide on the platinum electrode resulting in the release of two electrons by the following reactions:

In the cathode cell: \[ 3I^- \rightarrow I_3^- + 2e \quad \text{Rxn 2} \]

In the anode cell: \[ I_2 + 2e \rightarrow 2I^- \quad \text{Rxn. 3} \]

The total cell reaction is the redox reaction: \[ 3I^- + I_2 \rightarrow I_3^- + 2I^- \quad \text{Rxn. 4} \]

Rxn 2 and 3 are rate determining reactions and result in the transfer of ion to the electrode surfaces. An equilibrium exists between $I_2$ and $I_3^-$(tri-iodide) when the concentrations of $I^-$ are kept constant.
As a result of the reactions detailed above, each ozone molecule entering the sensor causes two electrons to flow through the ECC’s external circuit, which is measured as a current. The resulting electrical current is linearly proportional to the concentrations of ozone in the sampled air. The electrochemical technique assumes no secondary reactions take place and a 1:1 stoichiometric relationship of the \( \text{I}_2 : \text{O}_3 \) ratio is maintained. The relationship between ozone and the electrical current (measured in \( \mu \text{A} \)) is computed using:

\[
P_{\text{O}_3} = 4.307 \times 10^{-4} (I_M - I_{BG}) T_p \Phi \psi
\]

where

\( P_{\text{O}_3} \) = Ozone partial pressure (mPa)
\( I_M \) = Cell current (\( \mu \text{A} \))
\( I_{BG} \) = Cell background current (\( \mu \text{A} \))
\( T_p \) = Ozonesonde pump temperature (K)
\( \Phi \) = Pump flow rate (s/100cm\(^3\))
\( \psi \) = Pump flow conversion efficiency (1/pump flow correction factor, unitless)

The constant, \( 4.307 \times 10^{-4} \), is the half ratio of the ideal gas constant to Faraday’s constant.

Measurement techniques and uncertainty estimates for each variable in Eqn. 1 are reviewed below. The cell current, \( I_M \), and pump temperature, \( T_p \), are in situ measurements while the cell background current, \( I_{BG} \), and flow rate, \( \Phi \), are measured during pre-flight preparations under ambient laboratory conditions and are assumed to remain constant throughout the flight. While it is preferable that the conversion efficiency, \( \psi \), is determined for each flight, unless automated, this can be very time consuming and as a result \( \psi \) values are usually taken from a table of pump flow measurements made at varying low pressures to account for the decrease in pump efficiency at low temperatures. Uncertainties on \( \psi \) are expected to be smaller if they are determined individually for each flight rather than taken from a table (which needs to also provide the statistical uncertainty on the \( \psi \) values). \( \psi \) values vary with ECC sensor type and are further explained in Section 2.5.

### 2.2 Measuring the background current

The background current (\( I_{BG} \)) is the residual current measured by the sonde when sampling ozone-free air. Conventional processing of the sonde telemetry assumes that the background current remains constant during flight and the same assumption is made when processing ozonesonde data within GRUAN. As seen in Equation 1, the background current is subtracted from the ECC sensor current to infer the ozone partial pressure. In the initial conditioning procedure, both cathode and anode cells are filled with sensing solution and stored for no less than 3 days prior to launch to reduce the background current and improve the sensor response time (i.e. the time it takes for the sensor electronics to respond to a change in ozone concentration) [Kohmyr, 1986; 1997]. Kohmyr and Harris [1971] show that the background current decreases after the ECC is stored for several days while charged with their working solutions; they call this process ‘self-cleaning’.
GRUAN protocols for measuring background current

GRUAN follows the WMO/GAW SOPs for background current measurement [Smit et al. 2014] requiring three background measurements as detailed below.

1. Initial conditioning, i.e. the conditioning procedures when the sensor is first taken out of the box, shall occur no less than 3 days before the ozonesonde flight. As this is the minimum acceptable period for the background current to decrease to within the thresholds defined below.

2. Day of flight preparations shall be made no more than 7 days after the initial conditioning. If more than 7 days have elapsed, then the cathode and anode chambers must be replaced with fresh solution and initial conditioning procedures must be repeated. Dates of repeated solution change shall be documented in the metadata for collection by the GRUAN RSLaunchClient (addressed in Section 3.6).

3. $I_{B0}$ is recorded when the calibration/ozonizer unit is used to run ozone-free air through the sensor, filled with fresh solution, for 10 minutes.
   a. Following BESOS procedures [Deshler et al., 2008] ozone-free air is run through the sensor until the background no longer drops or until the background current is less than 0.05 µA.
   b. If the background current does not drop below 0.05 µA after 20 minutes, the solutions must be changed and the background current measurement repeated. If, after another 20 minutes, the background does not fall below 0.05 µA the final value should be recorded in the metadata check list, regardless. Ideally, these steps should bring $I_{B0}$ below the 0.05 µA threshold value.

4. $I_{B1}$ is recorded after the response time measurement, i.e. the time required for the sensor current to drop from 4 µA to 1.5 µA, and after an additional 10 minutes of ozone-free air has been flushed through the cells. This value may be higher than $I_{B0}$.

5. $I_{B2}$ is recorded prior to launch with the ozonesonde intake tube fitted to an ozone destruction filter. This value may be higher than $I_{B0}$.

All three background currents shall be recorded by the GRUAN RSLaunchClient (see Section 3.6). Historically, operators have used $I_{B2}$ as the value for $I_B$ in Eqn. 1. In recent years other methods of applying background currents have been employed, such as the minimum of the three background currents [Ryan Stauffer/Penn State, personal communication], a laboratory determined $I_B$ [Holger Vömel/NCAR, personal communication], or $I_B$ set to an upper limit value for those background currents that exceed a maximum threshold based on average $I_B$ measured under optimal laboratory conditions [Bryan Johnson/NOAA, personal communication].

For the GRUAN central processing of ozonesonde flight data, $I_{B0}$ shall be used as the background current for the following reasons:

- The quality of the ozone destruction filter under launch conditions (non-laboratory controlled environment) used to measure $I_{B2}$ cannot be assured to be uniform between flights which introduces a source of random uncertainty which cannot be easily quantified [Reid et al., 1996]. This is particularly the case when ozonesondes are flown in
the tropics where high humidity affects the ozone removal efficiency of the filter [Newton et al., 2016].

- The use of $I_{B2}$ as the background current is likely an overestimate of the true background current which then leads to an underestimate of the ozone partial pressure. In particular, tropical and polar ozone profiles are strongly influenced by the magnitude of the background current [Reid et al., 1996; Vömel and Diaz, 2010; Newton et al.; 2016]. Under mid-latitude and tropical conditions, Smit et al. [2014] show that background currents ranging from 0.05 to 0.1 $\mu$A contribute 10-20% and 20-40%, respectively, to the measured cell current in the free troposphere.

- $I_{B1}$ is excluded as an option since it can be biased high. The 10-minute flow of ozone-free air after ozone exposure is arbitrary and likely not representative of the true background current [Thornton and Niazy, 1982; Vömel and Diaz, 2010; Bryan Johnson/NOAA, personal communication]. Laboratory experiments by Vömel and Diaz [2010] identified the decay of the cell current after exposure to ozone and showed that the current does not relax to pre-ozone values after 10 minutes of ozone-free air and that a much longer period of time (hours) is required to approach initial values. The BESOS field campaign [Deshler et al, 2008] found similar enhancements in the background current after ozone exposure. The elevated cell currents indicate a slower decay in the sensor response suggesting that the flushing of ozone-free air for 10 minutes through the cells is not long enough to reduce the cell current to pre-ozone exposure values.

- A field study conducted by Newton et al. [2016] found stable low background currents when the ozone exposure test during the day of flight preparations was ignored.

- Using $I_{B0}$ ensures that background currents are measured under stable, controlled laboratory conditions where uncertainties can be more robustly quantified.

When $I_{B0}$ exceeds 0.05 $\mu$A the following steps shall be taken:

1. If a solution change, followed by a reasonable length of time running zero ozone air does not bring $I_{B0}$ below 0.05 $\mu$A, then the minimum of $I_{B0}$, $I_{B1}$, and $I_{B2}$ shall be used as $I_B$.

2. If the minimum background current is still greater than 0.05 $\mu$A, then an $I_B$ value of 0.05 $\mu$A must be used. Smit et al. [2012] estimated that properly measured background currents since the mid-1990s should be less than 0.05 $\mu$A in the current generation of ECC sensors. Based on JOSIE results, 0.05 $\mu$A is an upper limit to $I_{B0}$ [Smit et al., 2007].

GRUAN will apply a constant background current correction following WMO/ASOPOS guidelines [Smit et al. 2012; 2014]. Thornton and Niazy [1982] showed that sensors in the early 1980s exhibited negligible sensitivity to $O_2$ allowing the background current to be treated as a constant. More recent studies support this finding [Smit et al., 1994; Reid et al. 1996; Newton et al., 2016]. Vömel and Diaz, [2010] introduced a modified ozone partial pressure equation that takes into account the excess ozone response due to the buffering of the solution. They measured uncertainties of 0.005 $\mu$A for a 1% full buffer solution and 0.009 $\mu$A for a 0.5% half buffered solution.

Any changes to the treatment of ozonesonde background currents to those described above must be founded on JOSIE-type experiments, followed by rigorous assessment.
2.3 Effects of different sensing solutions and ozonesonde type

While the fundamental chemistry and operating mechanics of the ECC sonde have remained largely unchanged, the KI solution concentrations have varied over the past decades in attempts to improve the measurement accuracy and stability. Inter-comparison campaigns and laboratory studies have been conducted to evaluate the ECC sonde performance using different sensing solution recipes with current sensor types [Hilsenrath et al., 1986; Boyd et al., 1998; Johnson et al., 2002; Smit et al., 2007; Deshler et al., 2008]. The JOSIE studies have shown that the precision and accuracy is strongly dependent on the ozonesonde type and solution [Smit et al., 2007]. JOSIE experiments reveal that differences in instrument construction between SPC and ENSCI significantly impacts the ozonesonde performance.

A variety of sensing solution concentrations and pH buffers are typically used in ECC sondes (see Table 2.3.1) The anode solutions are prepared by saturating the cathode solution with KI crystals.

Table 2.3.1

<table>
<thead>
<tr>
<th>Sensing Solution Type</th>
<th>KI, g/L</th>
<th>NaH$_2$PO$_4$•H$_2$O</th>
<th>Na$_2$HPO$_4$•12H$_2$O</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0% KI, full buffer</td>
<td>10</td>
<td>1.25</td>
<td>5.0</td>
</tr>
<tr>
<td>0.5% KI, half buffer</td>
<td>5</td>
<td>0.625</td>
<td>2.5</td>
</tr>
<tr>
<td>2.0% KI, no buffer*</td>
<td>20</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.0% KI, 1/10th buffer*</td>
<td>10</td>
<td>0.125</td>
<td>0.5</td>
</tr>
</tbody>
</table>

* Used at NOAA-led ozonesonde stations only.

The 1.0% KI with full pH-buffer is the conventional cathode sensing solution used for the ozonesonde types SPC-4A, -5A, and -6A [Science Pump Corporation manual, 1996]. Until 1996, ENSCI advocated using the 1.0% solution formula but then switched to recommending a 0.5% KI with half pH-buffer sensing solution formula after 1996 [ENSCI Corporation manual, 1996]. Johnson et al. [2002] introduced the 2.0% non-pH-buffered solution with no KBr that all NOAA-led ozonesonde stations used for a period of almost 10 years in the late-1990s to mid-2000s until switching to a modified 1.0% KI solution using a 1/10th buffer cathode sensing solution recipe. The 2.0% no-buffer solution formula is no longer recommended. The 1.0% KI with 1/10th buffer sensing solution is a relatively new formula and has yet to be included in JOSIE-led evaluation studies. Until that time, only the 0.5% half buffer and 1.0% full buffer sensing solutions shall be used in GRUAN, following WMO/GAW recommendations and as detailed in Table 2.3.2.

Table 2.3.2 Table of ECC sensors and solution pairing.

<table>
<thead>
<tr>
<th>Manufacturer/Model</th>
<th>Solution concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPC 6A</td>
<td>1%, full buffer</td>
</tr>
<tr>
<td>ENSCI Z, 2Z</td>
<td>0.5%, half buffer</td>
</tr>
</tbody>
</table>

The JOSIE-2000 experiment focused on combinations of ECC sensors and sensing solution types to determine the optimal pairing when compared with the world standard UV-photometer.
Results show a reduction in biases for SPC sondes when using the 1.0% KI solution with full buffer pair and for ENSCI sondes that use a 0.5% KI solution with half buffer solution. JOSIE results showed that the SPC/1% and Z/0.5% pairings behave similarly, i.e. measurement differences are within 1.0%.

Homogenizing records that use different sensing solutions

GRUAN recognizes that ECC sensor technology is constantly evolving as solution recipes are fine-tuned to optimize performance and that not all sites coming into GRUAN will operate with the same ECC sensor/solution pairing detailed in Table 2.3.2, e.g. an existing site may continue to use an obsolete sensing solution (e.g. 2% unbuffered) to avoid potentially introducing a discontinuity in the measurement time series, especially if transfer functions have not yet been tested and established.

Ideally, the ECC sensor and solution type should have a legacy of using one of the two combinations defined in Table 2.3.2. Sites using an ECC sensor/solution type outside of the SPC/1.0% or ENSCI/0.5% pairing should be homogenized with the application of transfer functions (see Section 7.2). Systematic biases between ozone measurements typically result from ECC sensors of the same manufacturing type being operated with different sensing solution concentrations. For ozonesonde sites performing long-term measurements, a change of the sensing solution concentration or ECC-sensor type can introduce a ±5% change, or more, in their ozone records, affecting the determination of ozone trends [Smit et al., 2014].

To support the homogenization of ozonesonde measurement series whose homogeneity is compromised by historical changes in sensing solutions, the ASOPOS working group, as part of the SPARC/IGACO-O3/IOC/NDACC initiative, has established transfer functions based on JOSIE experiments [Smit et al., 2007] for a variety of ECC sensor type and solution strength combinations. Their use allows homogenization of long-term records to conform to either an SPC/1.0% or ENSCI/0.5% sensor/solution pairing (Refer to Section 8.1.2, Table 3 of Smit et al. [O3S-DQA, 2012] for conversion factors). Section 7.2 provides further details and processing protocols involving transfer functions.

While GRUAN Ozonesonde Programmes should commit to using the same ECC sensor and solution type for the lifetime of the measurement programme, changes may be considered if

- Sufficient justification, as determined by the GRUAN Lead Centre and the centralized GRUAN ozonesonde data processing facility, is provided for the proposed change. A balance must be found between GRUAN Ozonesonde Programmes being responsive to the latest technological and scientific progress in ozonesonde measurement techniques and observational requirements, and the importance of avoiding discontinuities in the climate data record.

- A new model is developed or a new manufacturer enters the ECC market that recommends a new sensing solution recipe.

Changes in ozonesonde working solutions must be managed through an appropriate change management programme whereby the necessary tests, laboratory studies, and dual sonde launch
campaigns are conducted to characterize any systematic biases, and their uncertainties, in the stoichiometry and response times at all pressure altitudes (see Section 6 on the uncertainty budget). Sites undergoing such change management shall also participate in developing transfer functions required to maintain the homogeneity in the data record.

Ozonesonde expertise outside of GRUAN shall also be used to support the Lead Centre in guiding individual sites through changes in instrumentation without impacting long-term measurement time series.

### 2.4 Measuring pump flow rate

A common procedure in the ECC conditioning is to use the soap bubble flowmeter method to measure the volumetric flow rate of the pump, $\Phi$ [sec/100ml]. The required equipment and set-up are described in the ENSCI and SPC manuals [DMT manual, Appendix D, 2014; SPC manual Section 3.2.1, 1999]. While the ECC is charged with solution and the air pump is operating, the cathode outtake tube is connected to the flowmeter. The air flowing from the ECC pump into the burette allows soap bubbles to rise up the burette. As a single soap bubble rises, a handheld stopwatch is used to determine the time to displace that soap bubble 100 ml. Several flow rates are calculated and the mean is assigned as the final $\Phi$ applied in Equation 1. The uncertainty of the flow rate is small, generally within ±1% [Smit et al., 2014].

The GRUAN procedure for determining pump flow rate is as follows:

1. The flowmeter equipment provided by ENSCI and SPC is standard and reasonably identical. GRUAN will accept either.

2. GRUAN acknowledges that the soap bubble solution recipe varies among manuals and operators and requires only that the same recipe is used throughout the lifetime of the measurement record.

3. The measurement of the flow rate shall be made five times as required by WMO/GAW and implemented in most SOPs.
   - Flow rates that differ by 2 sec/100ml or more from the median after measuring the flow rate five times should be redone.
   - Mean $\Phi$ should be between 26 and 32 sec/100ml.
     - Lower and upper limits are chosen by consulting pump flow rate ranges found in the SPC manual [1999] and Smit et al., [2014].
     - If the mean $\Phi$ is not within the acceptable range, this must be reflected in the setting of an appropriate data QA/QC flag.

4. As recommended by WMO/GAW, flow rates must be measured on the day of the flight.

5. Lab temperature, relative humidity, and pressure should be recorded at the time the flow rate measurements are taken to correct for the evaporation of the soap bubble solution (see Komhyr et al. [1995], Johnson et al. [2002], and Smit et al., [2014] and Section 8.4).
GRUAN Ozone sonde Programmes must use equation 17 from Smit et al. [2012] to calculate the pump flow rate correction factor, $C_{PH}$. WMO/GAW defines $C_{PH}$ as

\[ C_{PH} = \left[1 - \frac{RH_{Lab}}{100}\right] \cdot \frac{P_{H2O,Sat}(T_{Lab})}{P_{Lab}} \]

where, $P_{H2O,Sat}$ is the saturation vapor pressure under laboratory conditions, i.e. $P_{Lab}$, $T_{Lab}$, and RH$_{Lab}$. $C_{PH}$ is applied to the mean $\Phi$ with the expectation that this has a negligible impact on the uncertainty calculations.

6. The pump flow rate must also be corrected for the temperature difference between the internal pump base temperature and the ambient room temperature. $C_{PL}$ is defined as

\[ C_{PL} = \frac{T_P - T_{Lab}}{T_{Lab}} \]

WMO/GAW reports ($T_p - T_{Lab}$) are on the order of +2K with an uncertainty of ±0.5K.

7. The corrected pump flow rate is then expressed as:

\[ \Phi_{Final} = [1 + C_{PL} - C_{PH}] \cdot \Phi \]

Section 6.3 addresses the flow rate uncertainty and its contribution to the ozone measurement uncertainty.

2.5 Estimating degradation in pump efficiency

It has been well documented that the efficiency of the ECC pump decreases at high altitudes [Komhyr, 1967; 1969; 1986; et al. 1995; Johnson et al., 2002; Smit et al., 2014]. Johnson et al. [2002], and references therein, cite pump leakage, dead volume in the piston pump, and back-pressure exerted on the pump by the cell solution as main causes of pump efficiency loss at low pressures. Experiments reveal that the pump flow rate, $\Phi$, measured at the ground is constant up to 100 hPa and decreases steadily to the top of the atmosphere. This is true for the pumps used in both SPC and ENSCI ozonesondes.

Calculated ozone partial pressures must therefore include a correction for the effects of pump efficiency loss. From Equation 1 (in Section 2.1), the pump flow conversion efficiency, $\Psi$ (1/pump correction factor), takes into account the efficiency loss in $\Phi$ as a function of pressure. Empirical averages obtained from various lab techniques have yielded pump correction factors (PCFs; Komhyr [1986]; Komhyr et al. [1995]). The two most widely used PCFs are shown in Table 2.5.1. Table 2.5.1 PCFs have been calculated based on SPC ECC type and models older than SPC 6A. The sample sizes are small (e.g. K95 N = 13) and it is recommended that laboratory studies be conducted to obtain much larger sample sizes of the various ECC models currently in use to verify or update the pump efficiency corrections and their uncertainties.
Table 2.5.1 Pump corrections factors (PCF) with 1-sigma uncertainties. PCF values are taken from the GAW Report No. 201, Table 3-3 [Smit et al., 2014].

Table 2.5.1 Pump corrections factors (PCF) with 1-sigma uncertainties. PCF values are taken from the GAW Report No. 201, Table 3-3 [Smit et al., 2014].

Following the recommendations of WMO/GAW report 201 [Smit et al., 2014], GRUAN Ozonesonde programmes shall use the K86 PCFs for SPC ozonesondes and K95 PCFs for ENSCI ozonesondes as listed in Table 2.5.1. PCFs between tabulated values must be interpolated on a log pressure scale with 2nd order polynomial interpolation. Ideally GRUAN should use PCFs derived individually for each sonde. As briefly mentioned above, obtaining PCFs for each sonde should result in smaller uncertainties on PCFs over using tabulated values which represent mean values across multiple samples. However, these measurements are time consuming, require additional hardware and, if made in a non-standard way, could introduce inhomogeneities across the network. See e.g. Figure 7 from Johnson et al. [2002] that shows a significant spread of PCF values that are based on different measurement techniques and different ECC types and models.

Methods for calculating PCFs are not standardized in the ENSCI and SPC manuals, nor considered in the WMO/ASOPOS recommendations. While it would be best practice for GRUAN to use PCFs specific to current models, i.e. SPC 6A or ENSCI Z ECC, based on statistically appropriate sample sizes, the resultant look-up tables do not currently exist. GRUAN therefore encourages peer-reviewed laboratory studies that will produce PCFs, with associated uncertainties, specific to manufacturer type and model. Until such results become available, GRUAN shall use the WMO/GAW recommended values tabulated above.

2.6 Measuring pump temperature

The temperature of the ozonesonde pump, $T_p$, is required in the calculation of the ozone partial pressure (see Equation 1., Section 2.1) to account for the temperature of the air flowing through the pump. Over time, the location of the thermister used to measure the pump temperature has changed, potentially introducing inhomogeneities into the sounding record [Smit et al., 2014]. Smit et al. [2014] has identified five configurations of $T_p$ measurements based on the placement of the thermister (see Table 2.6.1) and has characterized their uncertainty relative to the current placement of thermisters in modern ECC sondes which is inside the pump and is referred to as the internal pump temperature (see Case 5 in Table 2.6.1).
Table 2.6.1

<table>
<thead>
<tr>
<th>Case</th>
<th>Time Period</th>
<th>Location</th>
<th>Name</th>
<th>Sonde Types</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1960- end 1980s</td>
<td>Bottom of circuit board</td>
<td>Box Temperature</td>
<td>SPC 2A, 3A, 4A</td>
<td>Analog sondes</td>
</tr>
<tr>
<td>2</td>
<td>1990s</td>
<td>Suspended in the styrofoam box in the vicinity of the pump</td>
<td>Box Temperature</td>
<td>SPC 5A</td>
<td>Start of digital sounding systems. Behaves as in Case 3</td>
</tr>
<tr>
<td>3</td>
<td>1990s</td>
<td>Taped thermister at the pump base</td>
<td>External Pump Temperature</td>
<td>SPC 5A</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1990s</td>
<td>Epoxied at the pump base</td>
<td>External Pump Temperature</td>
<td>SPC 5A</td>
<td>Behaves like Case 1</td>
</tr>
<tr>
<td>5</td>
<td>&gt; 1995</td>
<td>Mounted inside the pump body, close to the piston</td>
<td>Internal Pump Temperature</td>
<td>ENSCI Z &amp; 2Z, SPC 6A</td>
<td>Current generation ECC soundings</td>
</tr>
</tbody>
</table>

Smit et al. [2014] considers the correct or 'true' $T_p$ as the pump temperature measured in the vicinity of the moving piston, $T_{\text{piston}}$. Based on Komhyr and Harris [1971] and JOSIE 2000 lab experiments [Smit et al., 2007], empirical pressure dependent equations have been formulated to adjust pump temperatures from Cases 1 through 4 to an internal pump based temperature (Case 5). Internal pump temperatures are considered to be the best approximation to the 'true' $T_p$.

Further, lab experiments that compare piston temperatures to internal pump, or pump-based, temperatures (the latter using the empirically derived equations) found a 1-3K difference, prompting an additional equation that corrects for this temperature bias [Smit et al., 2014]. The resultant pump temperature corrections required for each case listed in Table 2.6.1 are:

**Case 1: Equation 2.6.1**

(a) $T_{\text{case1}} = 7.43 - 0.393 \log_{10}(P)$ \hspace{1cm} $P \geq 40$ hPa
(b) $T_{\text{case1}} = 2.7 - 2.6 \log_{10}(P)$ \hspace{1cm} $6 < P < 40$ hPa
(b) $T_{\text{case1}} = 4.5$ \hspace{1cm} $P \leq 6$ hPa

**Case 2, 3: Equation 2.6.2**

(a) $T_{\text{case2,3}} = 20.6 - 6.7 \log_{10}(P)$ \hspace{1cm} $P > 70$ hPa
(b) $T_{\text{case2,3}} = 8.25$ \hspace{1cm} $15 \leq P \leq 70$ hPa
(c) $T_{\text{case2,3}} = 3.25 - 4.25 \log_{10}(P)$ \hspace{1cm} $5 \leq P < 15$ hPa

**Case 4: Equation 2.6.3**

(a) $T_{\text{case4}} = 6.4 - 2.14 \log_{10}(P)$ \hspace{1cm} $P > 40$ hPa
(b) $T_{\text{case4}} = 3.0$ \hspace{1cm} $3 \leq P \leq 40$ hPa

**Case 5: No adjustment, i.e. $T_{\text{case5}} = 0.0$**
The additional correction to account for differences between $T_{\text{piston}}$ and the internal pump, or pump based, temperatures is described as:

**Equation 2.6.4**

$$T_{\text{piston-internal}} = 3.9 - 0.8 \log_{10}(P)$$

It is recognized by GRUAN that equations 2.6.1 to 2.6.4 were derived from small statistical samples (Equation 2.6.4 from a sample of only three ECC sondes in the JOSIE chamber experiments; Figure 9 from Smit et al. [2007]). The adjustment formulae for Cases 2 and 3 were derived from a sample size of eight, while only three sondes were used to generate the Case 4 formula. Until GRUAN can conduct more detailed analyses of the biases related to different placements of the sonde thermistor, the uncertainties inherent in the small samples underlying equations 2.6.1 to 2.6.4 must be propagated through to uncertainties in the derived ozone partial pressures. Section 6.5 summarizes the pump temperature uncertainty parameters and equations and how these contribute to the ozone partial pressure uncertainty.

The ASOPOS panel recommends that the final adjusted pump temperature, $T_p$, used to calculate the ozone partial pressure, should be defined as:

**Equation 2.6.5**

$$T_p = T_{\text{measured}} + T_{\text{Pcase}_i} + T_{\text{piston-internal}}$$

where $T_{\text{measured}}$ is the pump temperature recorded by the sonde, $T_{\text{Pcase}_i}$ is the correction that depends on the case, and $T_{\text{piston-internal}}$ is the additional correction defined by equation 2.6.4.

### 2.7 Determining the partial ozone column above the top of flight

GRUAN's purpose for calculating total column ozone for each profile is to allow for comparisons against an independent spatially and temporally co-located total column ozone measurement to provide a means of validating the quality of the ozonesonde ozone profile. The standard technique for computing total column ozone from an ozonesonde measurement includes adding a climatological ozone partial column value above the balloon burst altitude. Most often, these partial columns are based on satellite and ozonesonde observations [McPeters et al., 1997, 2007, 2012; Labow et al., 2015], though some sites have developed their own monthly climatologies e.g. based on microwave radiometer-derived ozone profiles. Comparisons of the integrated ozonesonde ozone profile plus the partial column above the top of flight can then be made with ground-based and satellite measurements of total column ozone (e.g. Dobson spectrophotometer, Brewer spectrometer, OMI, GOME-2).

When integrating ozonesonde profiles within a GRUAN ozonesonde programme, that integration shall be truncated at 7 hPa since the ozone profile above 7 hPa has higher uncertainty due to the degradation of the pump efficiency (Section 2.5) and evaporative effects on the sensing solution at very low pressures [Bryan Johnson/NOAA, private communication]. It is preferable that GRUAN sites derive their own monthly climatologies of ozone partial columns above the top of the flight since these will be more relevant than the zonal mean climatologies provided by McPeters et al. [2012]. It is important that these climatologies include uncertainties so that these can be propagated through to the derived ozonesonde total column ozone uncertainty. Until site-
specific climatologies are available, the McPeters et al. climatologies may be used to derive the ozone partial column above the burst pressure. Where the balloon bursts at pressures higher than the McPeters et al. [2012] pressure limit of 32 hPa a total column ozone value cannot be derived and the flight total column ozone value should be recorded as a null value. It is recognized that there may be gaps in the profile measurements due to intermittent telemetry. Profiles with large data gaps shall be identified and evaluated on a case-by-case basis and the flight total column ozone value and, importantly, its uncertainty, calculated according. The GRUAN ozonesonde data product shall include the following ozone column-related metadata:

- The integrated ozone column amount (in DU) up to 7 hPa or balloon burst, whichever is lower.
- The pressure level at the top of the integration [hPa].
- The ozone partial column (in DU) above burst pressure either from the McPeters et al. [2012] climatology or from the site-specific climatology.
- If available, co-located ground-based or space-based measurements of total column ozone shall be included.

GRUAN encourages sites to include any ancillary measurements of surface and column ozone measurements in the metadata submitted to the centralized GRUAN ozonesonde data processing facility. Redundancy in ozone measurement systems provides a powerful tool for validating and evaluating the ozone measurements in any given time series.

### 2.8 Dependence on the radiosonde

Radiosonde pressure and temperature measurements are used to calculate the geopotential heights. Thus, radiosonde measurement errors will cause the measured ozone to be assigned incorrect altitudes and pressures. As with ozonesondes, there are a number of radiosonde manufacturers whose instruments have changed in model, material, and algorithm since the 1970's. There are measurable differences between manufacturers, i.e. Vaisala vs iMET, and between models, i.e. Vaisala RS-80 vs RS-92, that impact the ozonesonde measurement, particularly at low pressures [Smit et al., 2014; and references therein]. GRUAN shall document radiosonde manufacturer, model and type of interface so that appropriate calibrations and corrections to the pressure and temperature, as well as RH, can be made in the pre- and post-processing calculations of the geopotential height.

### GRUAN procedure protocol

- Calibration of the radiosonde surface pressure, temperature, RH and determination of any offset between geopotential and GPS height measurements, if and when available, shall follow the processing guidelines dictated by the GRUAN Radiosonde Technical Document (X.X.X).
- Handling biases in the geopotential height calculation in the absence of GPS measurements shall be the responsibility of the Radiosonde WG-GRUAN, task team, and Lead Centre.
- Radiosonde/Ozonesonde offsets in height and pressure, if any, shall be documented and geopotential heights shall be recalculated by the Lead Centre GOASS (refer to Section 3.7).
• Quantifying the contribution of the radiosonde uncertainty to the ozone measurements, if any, shall be the responsibility of the Radiosonde WG-GRUAN, task team, and Lead Centre.

2.9 Conversion efficiency

One of the terms in the ozone uncertainty calculation is the contribution of the uncertainty in the conversion efficiency. The conversion efficiency refers to the stoichiometric factor of 1:1 assumed in the I$_2$:O$_3$ relationship. Interferences with this one-to-one relationship can arise from the buffering of the solution [Johnson et al. 2002; Vömel and Diaz, 2010]. The cathode solution contains a buffer of sodium-hydrogen phosphate to maintain the solution concentration and a neutral pH of 7.0 during flight. GRUAN shall follow a half buffered cathode solution for ENSCI sensors and a full buffer for SPC, as recommended by WMO/ASOPOS [Smit et al., 2012; 2014]. Johnson et al. [2002] performed stoichiometric sensitivity and pH tests and measured excess ozone at low pressures due to the buffering effect. This would yield a I$_2$:O$_3$ relationship larger than unity. This offset in the stoichiometry has been documented by others (Smit et al., 2014, section 3.2.2 and references therein; Johnson et al., 2002, section 2.1 and references therein). In the ozone partial pressure equation, Equation 1, the conversion efficiency is assumed to be unity and is therefore excluded from the equation. However, the uncertainty of this unity assumption can be a significant contributor to the ozone uncertainty estimates and is addressed in Section 6.6.
3 GRUAN OZONESONDE PROGRAMMES

The GRUAN Guide (herein referred to as GCOS-171) states that the primary objective of GRUAN is to provide reference measurements for a range of upper-air climate variables. Reference quality observations are based on key concepts in metrology, in particular traceability. Metrological traceability is the process whereby a measurement and its uncertainty, can be related to a reference through a documented, unbroken chain of calibrations, each of which contributes to the measurement error.

To provide the best measurements of ozone and its uncertainty, a detailed understanding of the instrumentation, standard operating procedures (SOPs), and data processing is required. To lend confidence in the long-term stability of the data records for a single GRUAN OzoneSonde Programme and the entire network as a whole, the instrumentation, standard operating procedures, and data processing must produce datasets that are homogenized across the entire network.

For this reason, GRUAN ozonesonde certification applies to the overall infrastructure underlying the ozonesonde measurement and the subsequent production of a final GRUAN ozonesonde reference product. This infrastructure is defined in the present report as a GRUAN OzoneSonde Programme, and includes:

1. the SOPs that condition and calibrate each ozonesonde instrument prior to launch,
2. the mandatory collection of metadata used to characterize the singular features of each unique ozonesonde instrument,
3. the acquisition of the raw data and metadata to the RSLaunchClient utility for central processing,
4. the steps involved for create a final homogenized GRUAN ozonesonde product,
5. the handling of storage and dissemination of all pertinent levels of ozonesonde measurements.

In order to be GRUAN-certified each GRUAN OzoneSonde Programme must include the following three mandatory components:

1. The GRUAN OzoneSonde Instrumentation and Measurement Report (GOIMP): A dynamic document submitted to the GRUAN Lead Centre, via email, by the GRUAN ozonesonde programme representative describing their measurement program and capabilities, as well as documentation on the history of its ozonesonde data record, if any. The GOIMP shall include all aspects of the programme such as instrumentation inventory, SOPs, measurement schedule, and up-to-date data acquisition and archiving status. Further details of what should be included in the report are addressed in Section 3.2.

2. Proof of the ability to provide all essential metadata and raw data to the RSLaunchClient utility: An interactive JavaScript tool designed to compile all metadata associated with each ozonesonde instrument launched (i.e. those measurements collected by the ground station data acquisition system per launch). The essential metadata is described in Section 3.6 and is upload together with the raw data by the RSLaunchClient at a designated
GRUAN ozonesonde data handling centre for processing by the GRUAN Ozonesonde Analysis Software System (GOASS). All metadata uploaded by RSLaunchClient shall be consistent with the latest version of the GRUAN check list (found in Appendix A-1 and A-2 for refurbished sondes).

3. The GRUAN Ozonesonde Analysis Software System (GOASS): A centralized data processing software collecting and analyzing in a standardized manner the raw-data of all certified GRUAN ozonesonde instruments sent out through the RSLaunchClient utility. Before processing the raw data, the GOASS reconciles the metadata received from the RSLaunchClient with those contained in the GOIMP. Any inconsistency is immediately reported, thus providing a near-real-time check of the measurement traceability and stability, as well as a quick identification of change. The output of the GOASS consists of certified GRUAN ozonesonde products of various levels designed to be used by different communities for different science applications. Individual GRUAN Ozonesonde Programmes will be audited, as well as annually reviewed in compliance with the requirements and recommendations of GCOS-171 and this present document. GRUAN Ozonesonde Programmes not in compliance all three of the mandatory components listed above may lose their GRUAN certification.
3.1 Site assessment and certification considerations for GRUAN Ozonesonde Programs

Ozonesonde sites seeking to become a GRUAN Ozonesonde Programme will be subjected to the same assessment and certification process as all other sites in the network. This section provides pragmatic criteria for assessing and certifying existing and new sites. Ozonesonde sites will follow the specific requirements regarding site assessment and certification under Section 5.1 of GCOS-171.

GRUAN recognizes that sites will vary in infrastructure and financial support. In order to be compliant with the mandatory operating protocols defined in Sect. 5.3 of GCOS-171, each GRUAN Ozonesonde Programme should do the following:

1. Provide reference quality observations, i.e., observations characterized by a traceable calibration, a comprehensive uncertainty analysis, a readily accessible documentation, a validation through inter-comparison campaigns, and complete metadata availability.

2. Provide access to raw data and assure long-term storage of the raw data, as well as metadata, either at the site, at another GRUAN facility, or at another internationally accessible archive in accordance with the GRUAN Data Policy document (referred to in Section 8.2 GCOS-171).

3. Provide complete metadata for each measurement as defined in Section 3.6 of this document.

4. If available, and certainly encouraged, provide redundant reference observations of ozone from co-located ground-based instruments for independent evaluation and validation (refer to Sections 7.7 and 8.3 on parallel observations and validation, respectively).

5. Provide annual reports summarizing the ozonesonde operations at the site, including changes in instrumentation, how those changes were managed, and any improvements made.

6. Conduct the ozonesonde programme with an operational philosophy of continually striving to improve measurement accuracy (e.g., by working with other GRUAN Ozonesonde Programmes, or participating in field and laboratory experiments).

7. Manage change proactively as defined in Section 7 of this document.

8. Actively communicate with the GRUAN Lead Centre, WG-GRUAN and GRUAN Task Team for Sonde (TTS) through attendance at meetings and emails.

Specifically, GRUAN ozonesonde certification shall be assessed based on the following criteria:

1. The content and completeness of the GOIMP each ozonesonde candidate site is required to file at the designated GRUAN Lead Centre (refer to Section 3.2).

2. The level to which the ozonesonde candidate site conforms to GRUAN prescribed SOPs consistent with WMO GAW Report 201 to guarantee homogeneity of quality across the network. Determining whether the SOPs of an existing site meet the prescribed operating protocols will be done objectively against the standards outlined in Section 3.5.
   i. Sites that do not meet the WMO operating procedure standards can choose to adopt the prescribed SOPs in order to qualify to become a GRUAN site.
   ii. New sites shall be expected to adopt the GRUAN prescribed SOPs.
iii. Sites that launch refurbished ECC-sensors should follow the NOAA re-conditioning SOPs in Appendix A-2 or manufacturer SOPs (refer to Section 4.5).

3. The level to which the ozonesonde candidate site conforms to the GRUAN prescribed conditioning and pre-flight check list whose metadata will be collected by the RSLaunchClient. Metadata requirements from the check list are addressed in Section 3.6.

4. The schedule frequency where a minimum of twice monthly launches spaced bi-weekly is required. This is addressed in Section 5.2. A *fully* operating GRUAN Ozonesonde Programme shall perform weekly launches. Weight shall be given to the added value each candidate site brings to the network (see Section 3.2.1 below).

### 3.2 GRUAN Ozonesonde Programme assessment and certification process

A schematic of the site assessment and certification process is provided in Figure 2 of GCOS-171.

Once a site has been identified for possible inclusion in GRUAN, through either of the routes shown in Figure 2 of GCOS-171, the following sequence of events will be used to assess the site for potential GRUAN certification:

1. The candidate site will be given the GRUAN manual (GCOS-171) and this ozonesonde technical document, as well as documentation describing data submission protocols and the procedures that must be followed when data are submitted to the internal GRUAN archives via the RSLaunchClient (addressed in Section 3.6).

2. The response from the candidate site shall be given in the form of the GOIMP submitted to the designated GRUAN Lead centre and should include:

   1. If it is an established GRUAN site that proposes to add an ozonesonde measurements programme or a new GRUAN site that will include an ozonesonde measurement programme.

   2. A complete description of how the ozonesonde measurement programme will be conducted. Such information would include launch frequency and scheduling, detailed SOPs, a copy of the check list and metadata inventory, and data storage policies. This information must be sufficient to establish the ability of the site to meet the mandatory operating protocols outlined in Sections 3.5 – 3.7.

   3. Include any cooperative agreements with other sites and institutions already in the network. This is highly desirable to ensure that expertise is disseminated to similar measurement programmes in operation at other sites.

   4. The management structure of the site and a general description of the manner in which the site is operated. This would include a description of current and expected future funding levels for on-going operation of the site.
5. A description of which data centres the measurements have previously been submitted to and are currently being submitted to.

6. A description of how past ozonesonde measurements from the site have been processed. This will be used to assess whether the time series to date meet the standards for a GRUAN reference measurement. Particularly important in this regard will be detailed documentation around how changes in SOPs over the history of the measurement programmes have been managed to derive a homogeneous time series of measurements.

7. A description of past metadata data records and storage. This will be used to assess whether the time series to date meet the traceability standards for a GRUAN reference measurement.

8. A list of the ozonesonde experts employed at the site who would likely participate in the analyses of the data collected within GRUAN. This may include mention of experts at partnering scientific organizations.

3. There is likely to be some iteration between the Lead Centre and the candidate site to confirm specific details, fill in information gaps, and finalize the documentation from the candidate site.

4. Based on the documentation received from the candidate site, the Lead Centre will then write a short recommendation. This, together with the documentation from the candidate site, will then be submitted to the WG GRUAN who will evaluate the proposal within 6 calendar months against the requirements listed in Sections 3.5, 3.6, and 4. One or more visits to the site by members of the WG and/or Lead Centre within this 6-month period may be required to obtain specific additional information about the measurement programmes slated for inclusion in GRUAN at that site. If accepted, these measurement programmes will then be included in the GRUAN certification for the site.

5. Regardless of the outcome, the WG-GRUAN and Lead Centre will provide written constructive feedback to the candidate site outlining strengths and weaknesses of their programme for GRUAN purposes and suggestions as to future improvements for GRUAN operational purposes. This feedback is non-binding but rather intended to provide useful guidance and support to site capability development and retention of current capabilities.

6. Annual reports shall summarize GRUAN operations at the site identifying any changes in ECC or radiosonde instrumentation, scheduling, procedures, equipment, and improvements. The intent of the annual report is to ensure that SOPs developed for the network have been adhered to, and to identify changes that may require additional reprocessing that is not already taken into account or require re-assessment of GRUAN certification. These reports will be presented at annual GRUAN meetings.

**3.2.1 Criteria for assessing added value**

The GRUAN Ozonesonde Programme assessment and certification process follows closely the more general GRUAN site certification process described in Section 5.5 of the GCOS-171. Once
a site has committed to operating a set of measurement programmes under the protocols defined in Section 5.3 of GCOS-171, the added value that an ozonesonde site brings to the GRUAN network will be assessed according to:

- The extent to which the ozonesonde site can fulfill the measurement programme expected of a fully equipped GRUAN site (Section 3.1). Achieving all of the measurement programme requirements is not mandatory for the inclusion of a site in GRUAN. However, the extent to which a site can meet these requirements will determine, in part, the additional value that that site brings to the network. For example, ozonesonde sites located in a large region of the globe containing no other GRUAN Ozone Sonde Programmes and making the minimum required bi-weekly launches will be assessed as adding as much value to the network as a site making weekly reference quality measurements but located very close to another GRUAN ozonesonde site. These high priority measurement programmes will be refined as the research which forms their basis progresses. This documentation will be updated to reflect scientific requirements.

- The extent to which the ozonesonde site provides profiles measurements of ozone in regions of atmospheric phenomena which were not previously sampled. In this case, the added value will depend on the locations and capabilities of the sites already participating in the network.

- The extent to which the ozonesonde site brings unique observational and/or analysis capabilities aligned with GRUAN scientific objectives to the network as a whole and the likelihood of being able to propagate those capabilities across other sites in the network.

- The extent to which the ozonesonde site is prepared to forgo locally established operating procedures and adhere to the SOPs established by the Lead Centre and adopted by the majority of the sites already in the network. Unwillingness or inability to do this would count against a site in the assessment of the added value it would bring to the network.

- The availability of historical measurements that conform to the GRUAN standard. All else being equal, a candidate site that extends an existing multi-decadal time series of reference quality measurements will be assessed as adding more value to the network than a site that would initiate the same measurement programme starting at the present. Detailed documentation in the GOIMP would be required describing how changes in SOPs, instruments, calibration procedures, data processing algorithms and operators over the history of the measurement programmes have been managed to ensure that the historical measurements are reference quality. Where historical reference quality measurements are available, consideration will be given by the WG GRUAN and Lead Centre to providing these as GRUAN data through the GRUAN data archives.

- The extent to which the ozonesonde site can commit to a multi-decade programme of measurements. While it is recognized that a multi-decade programme of measurements cannot be guaranteed, a statement of intent with documented support (e.g. from the host institution or relevant funding agency) will add to the assessment of the value that the site brings to the network.

- The extent to which the ozonesonde site can provide redundant observations of the priority 1 and ECVs or can conduct periodic inter-comparisons and laboratory studies.
• The extent to which a site is capable of measuring other ECVs identified in GCOS 112 as being desired quantities.

• The level of institutional support for the site and commitment to maintaining long-term reference quality measurement programmes. If, in addition, a site can demonstrate that it is actively pursuing resources to enhance its capability, such as the addition of new measurement programmes, this would also enhance the added value the site would bring to the network. It is also desirable that there is full host institution commitment to GRUAN-related activities and that this commitment is not dependent on a single individual.

• The level of institutional support for the site (and any partner institutions) to undertake fundamental scientific research of the measurements from the site and other GRUAN sites. Because GRUAN includes aspects of both operational and research networks, a strong and ongoing science programme is required to ensure that GRUAN fulfills its role as a research network.

• The degree of historical or planned cooperation with other sites both within and outside the GRUAN network including other GRUAN-relevant networks e.g. NDACC, SHADOZ, GAW, and WOUDC.

Such assessments of added value shall rely on the expert judgement of the WG-GRUAN and Lead Centre, recognize the heterogeneity of the sites within the network, and facilitate a practical approach to expansion of the network following the 2009-2013 implementation phase for GRUAN (GCOS-134) and its amendments.

Determining optimal locations for GRUAN sites as part of added-value assessment to ensure that the needs of the user community are met shall consider the following:

1. Covers a major climate region.

2. Covers a region of large atmospheric modes, e.g. ENSO, SAM, QBO

3. Environment, e.g., tropics, mountainous, desert, island

4. Spatial co-location with other Ozonesonde Programmes

3.3 GRUAN Ozonesonde Training Programme

Operational uncertainty includes uncertainties related to instrument set-up and operation. To reduce operational uncertainty, and in line with Section 1.4 of GCOS-171, the Lead Centre and WG-GRUAN shall identify Ozonesonde Programmes where instrument operators need training on GRUAN ozonesonde SOPs, and shall organize cost-efficient training courses for those operators at appropriate locations to encourage uniformity of ozonesonde instrument operation between sites. At least one staff member of a GRUAN Ozonesonde Programme should be in attendance to an initial training session in which the GRUAN-specific ozonesonde best measurement practices and the use of RSLaunchClient are taught. The GRUAN Ozonesonde Programme representative shall be one of the trained staff.

In addition to training at the time of certification, training is required for any new measurement scientist joining the ozonesonde programme team. Though training may be done through other
existing members of staff, it is strongly recommended that a GRUAN training session be
provided at a GRUAN site where optimal standard operating procedures are kept up-to-date.

If WG members deem that a potential candidate requires training, or an existing GRUAN
Ozonesonde Programme requires re-training, GRUAN will try to partner the site organization
with an ozonesonde expert who can do a site visit for training or re-training. The Lead Centre
require that at least one member of the WG-GRUAN is an ozonesonde expert. An ozonesonde
expert includes operators of a GRUAN Ozone Programmes, members of ASOPOS, or other
ozonesonde experts that have participated in JOSIE studies and ozonesonde inter-comparison
field campaigns. Thus, although not required, re-training may be done by an ozonesonde expert
within the WG-GRUAN.

For those GRUAN Ozone Programmes already partnered with ozonesonde launch experts,
training and maintaining up-to-date practices shall be coordinated between the two partners.
Sites that require re-training will be determined by these means:

• A GRUAN site makes a formal written request for re-training to the Lead Centre.
• When the WG-GRUAN concludes that upon reviewing a sites annual report that re-
training is necessary to guarantee consistency of quality.
• An audit, addressed in Section 3.10, reveals deficiencies in the operating procedures that
necessitate re-training to maintain GRUAN certification.

3.4 GRUAN Ozone Programme data management

General considerations shall be drawn from Section 8 of GCOS-171.

3.4.1 Overview of the data flow

Refer to Figure 3 of GCOS-171 which shows a schematic representation of the flow of data in
GRUAN to the user community.

GRUAN data levels relevant to ozonesondes are based on the GRUAN Data Management
Manual:

• Level 0 (L0): Original primary raw data (PRD). This is the ‘rawest’ form of data
available before any processing has been applied, i.e., the raw data slices acquired by the
data acquisition electronics
• Level 1 (L1): Converted raw data (CRD). These data are stored in a common well-
described file format intended for long-term storage. They are pre-processed raw data and
might already represent parameters to be used in end-user’s application
• Level 2 (L2): Standard GRUAN product data (SGPD) resulting from all processing steps
associated with a single instrument.

Measurements and metadata are bound together in each of these data levels. PRD are ingested
from all GRUAN sites into the internal GRUAN data archive hosted at the Lead Centre. Direct
exchange of PRD between sites is discouraged since this circumvents the data versioning
protocols and reduction of the raw data to a common CRD file format. Similarly, direct exchange
of CRD between sites is discouraged since this circumvents network wide application of
corrections, re-processing, and homogenization techniques applied to convert CRD to SGDP that would be implemented at the Lead Centres' data processing facility.

From PRD data submission to processing, storing and dissemination of SGPD

1. Level 0 ozonesonde raw data (PRD) and metadata, listed in Section 3.6, shall be collected by the RSLaunchClient utility.
2. A complete list of the essential and desirable PRD is found in Table 3.1 of this section.
3. A complete list of the essential and desirable metadata is found in Table 3.4 of this section.
4. Each GRUAN site is responsible for storing the PRD and associated metadata in its original format and in digital format.
5. The PRD shall be saved as Level 1 converted raw data (CRD) via the RSLaunchClient.
6. Processing of the ozonesonde raw data will be held in the designated GRUAN internal data archive at the Lead Centre.
7. The Lead Centre GOASS will be responsible for using the CRD and essential metadata to create the final standard ozone products (SGPD), as outlined in Section 3.7.
8. A complete list of SGPD are found in Table 3.2 of this section.
9. A designated GRUAN Lead Centre storage facility shall be responsible for archiving and maintaining the ozonesonde metadata, CRD, and SGPD for all Ozonesonde Programmes.
10. The SGPD, including their metadata and documentation, will be provided to the user community through the external GRUAN data archive hosted at NCEI.

Processing of the CRD, held in the GRUAN internal data archive, to produce SGPD will occur at the designated Lead Centre central processing facility. This processing should include applying the necessary corrections, and uncertainty estimates in a consistent and traceable manner across identical instruments from other Ozonesonde Programmes. The SGPD, including their metadata and documentation, are provided to the user community through the external GRUAN data archive currently hosted at NCEI. A performance monitoring process (see Section 9 of GCOS-171), implemented at the Lead Centre, will provide feedback on performance to individual sites.

3.4.2 GRUAN data policy

Since GRUAN is co-sponsored by WMO, GRUAN ozonesonde data dissemination and use shall comply with WMO Resolution 40 (Cg-XII) which calls for free and unrestricted international exchange of data. Refer to Section 8.2 of GCOS-171 for further details on the data dissemination and exchange policy.

3.4.3 Collation of Metadata

Essential and desirable metadata are listed in Section 3.6.1. Metadata will be submitted via the RSLaunchClient utility and archived at the designated GRUAN Lead Centre and NCEI. “Desirable” metadata defined in Section 3.6.1 are not required and the RSLaunchClient will not reject profiles if these desirable variables are excluded.
Metadata should not preclude information derived from historical documents such as observing practices manuals, site inspection reports, government policies, resource and funding programmes.

Management and maintenance of metadata requires the investment of resources. Present day technology for database warehousing of digitized metadata has the added benefit that metadata can be accessed, linked to measurements, and easily transferred. To facilitate metadata collation, the RSLaunchClient utility will be responsible for ingesting as much metadata as possible to be saved and stored at a designated GRUAN archive. Ozonesonde Programmes are required to keep original copies of their metadata at their own storage facility, as secondary storage back-up.

Metadata documents related to historical operations at GRUAN sites and to historical data archives should be inventoried and properly conserved until such time as their information content can be transferred to a medium which supports multiple users’ access and conforms to GRUAN reference measurement guidelines.

Metadata needs to have the same level of commitment as observed data. Incomplete, outdated, or inaccurate metadata can be as detrimental, indeed in some cases worse, than no metadata at all. Regular reviews of metadata content for confirmation and accuracy should be part of regular GRUAN operations. Support to investigate new metadata sources, information management technologies and information sharing capabilities should be ongoing in an effort to make accessible and preserve the historical investment in the data collected.
3.4.4 Ozone Data Products

The Ozone Primary Raw Data (PRD)

Each ozonesonde launched generates an array of measurements captured by the ground station data acquisition system. The PRD generally measures, but is not limited in measuring, the following variables listed in Table 3.1. The essential data variables listed are the basic fundamental data variables that are to be collected by the RSLaunchClient. The RSLaunchClient will collect and manage uploaded ozonesonde PRD to the designated GRUAN Lead Centre. All the PRD shall be saved to a Level 1 converted raw data (CRD) file for archiving at the designated GRUAN Lead Centre storage facility and processing shall be done by the GOASS addressed in Section 3.7 to create the SGDP. Desirable PRD (in blue) is not required input to the RSLaunchClient and profile data will not reject if these desirable variables are excluded.

Table 3.1 Essential and Desirable Ozone Primary Raw Data (PRD) variables

<table>
<thead>
<tr>
<th>16. Time [min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>17. Time GMT [hh:mm:ss]</td>
</tr>
<tr>
<td>18. Pressure [hPa]</td>
</tr>
<tr>
<td>19. Geopotential height [gpm]</td>
</tr>
<tr>
<td>20. Temperature [K]</td>
</tr>
<tr>
<td>21. Relative Humidity [%]</td>
</tr>
<tr>
<td>22. Ozone Partial Pressure [mPa]</td>
</tr>
<tr>
<td>23. Ozone Mixing Ratio per volume [ppm]</td>
</tr>
<tr>
<td>24. Horizontal Wind Direction [decimal degrees] (range: 0:360)</td>
</tr>
<tr>
<td>25. Horizontal Wind Speed [m/s]</td>
</tr>
<tr>
<td>26. GPS Geometric Height [m]</td>
</tr>
<tr>
<td>27. GPS Longitude [decimal degrees] (range: -180:+180)</td>
</tr>
<tr>
<td>28. GPS Latitude [decimal degrees]</td>
</tr>
<tr>
<td>29. GPS Satellites</td>
</tr>
<tr>
<td>30. GPS Time GMT [hh:mm:ss]</td>
</tr>
<tr>
<td>31. GPS Pressure [hPa]</td>
</tr>
<tr>
<td>32. Internal Temperature [K] (box or pump)</td>
</tr>
<tr>
<td>33. Ozone Current [µA]</td>
</tr>
<tr>
<td>34. Battery Voltage [V]</td>
</tr>
<tr>
<td>35. Pump Current [µA]</td>
</tr>
<tr>
<td>36. Rise Rate [m/s]</td>
</tr>
</tbody>
</table>

The Ozone Standard GRUAN Data Product (SGDP)

Each PRD should be archived at the same vertical and temporal resolution. Thus, each ozonesonde profile shall archive SDPG at the same vertical and temporal resolution. The GOASS shall use the PRD, in conjunction with the metadata also collected from the RSLaunchClient, to generate the ozonesonde SGPD. Section 3.7 goes through the GOASS steps required to generate the ozonesonde SGPD from the CRD. The family of ozonesonde SGPD are
listed in Table 3.2. Apart from the uncertainty estimates, it is not mandatory for all variables under the ozonesonde SGDP family to be measured. For example, heritage ozonesonde measurements used radiosondes that did not have the means or capability of acquiring GPS information.

**Table 3.2 Collection of Ozonesonde SGPD**

<table>
<thead>
<tr>
<th>No.</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Time [min]</td>
</tr>
<tr>
<td>2.</td>
<td>Radiosonde Pressure [hPa]</td>
</tr>
<tr>
<td>3.</td>
<td>Radiosonde Pressure Offset [hPa]</td>
</tr>
<tr>
<td>4.</td>
<td>Geopotential height [gpm]</td>
</tr>
<tr>
<td>5.</td>
<td>Radiosonde Temperature [K]</td>
</tr>
<tr>
<td>6.</td>
<td>Radiosonde Temperature Offset [K]</td>
</tr>
<tr>
<td>7.</td>
<td>Radiosonde Relative Humidity [%]</td>
</tr>
<tr>
<td>8.</td>
<td>Radiosonde RH offset [%]</td>
</tr>
<tr>
<td>9.</td>
<td>Ozone Partial Pressure [mPa] using Equation 2.6.5</td>
</tr>
<tr>
<td>10.</td>
<td>Ozone Partial Pressure uncertainty [%] using Equation 6.5.2</td>
</tr>
<tr>
<td>11.</td>
<td>Ozone Partial Pressure [mPa] using Equation 2.6.6</td>
</tr>
<tr>
<td>12.</td>
<td>Ozone Partial Pressure uncertainty [%] using Equation 6.5.1</td>
</tr>
<tr>
<td>13.</td>
<td>Ozone Mixing Ratio per volume [ppm] using (9) of this list.</td>
</tr>
<tr>
<td>14.</td>
<td>Ozone Mixing Ratio per volume [ppm] using (11) of this list.</td>
</tr>
<tr>
<td>15.</td>
<td>Radiosonde Horizontal Wind Direction [decimal degrees] (range: 0:360)</td>
</tr>
<tr>
<td>16.</td>
<td>Radiosonde Horizontal Wind Speed [m/s]</td>
</tr>
<tr>
<td>17.</td>
<td>Radiosonde GPS Geometric Height [m]</td>
</tr>
<tr>
<td>18.</td>
<td>Radiosonde GPS Longitude [decimal degrees] (range: -180:+180)</td>
</tr>
<tr>
<td>19.</td>
<td>Radiosonde GPS Latitude [decimal degrees]</td>
</tr>
<tr>
<td>20.</td>
<td>Internal Temperature [K] (box or pump)</td>
</tr>
<tr>
<td>21.</td>
<td>Ozone Current [$\mu$A]</td>
</tr>
<tr>
<td>22.</td>
<td>Ozone Current and background contribution (Section 6.2)</td>
</tr>
<tr>
<td>23.</td>
<td>Ozone Partial Pressure, ( \Phi ) (Section 6.3).</td>
</tr>
<tr>
<td>24.</td>
<td>Ozone Mixing Ratio, ( \Psi ), (Section 6.4).</td>
</tr>
<tr>
<td>25.</td>
<td>Ozone Pump Temperature, ( T_P ) (Section 6.5).</td>
</tr>
<tr>
<td>26.</td>
<td>Ozone Conversion efficiency, ( \eta ) (Section 6.6).</td>
</tr>
<tr>
<td>27.</td>
<td>Radiosonde Pump and Temperature offset uncertainty [defined and addressed in the GRUAN Radiosonde Technical Report (X.X.X)]</td>
</tr>
<tr>
<td>28.</td>
<td>Total Column Ozone (TCO) [DU]</td>
</tr>
<tr>
<td>29.</td>
<td>Pressure above which the TCO is calculated [hPa]</td>
</tr>
<tr>
<td>30.</td>
<td>Partial column ozone above (29) [DU]</td>
</tr>
</tbody>
</table>

As seen from Table 3.2, uncertainty estimates shall form part of the ozonesonde SGDP collective. The Lead Centre GOASS shall be responsible for calculating these estimates addressed in detail in Section 6. The measurement uncertainty describes the current best knowledge of instrument performance under the conditions encountered during an observation and therefore merits its own separate listing in Table 3.3 below.

**Table 3.3 Uncertainty variables as part of the ozonesonde SGPD.**
1. Ozone partial pressure uncertainty (Section 6.1).
2. Ozone Current and background contribution (Section 6.2)
3. Pump Flow rate, $\Phi$ (Section 6.3).
4. Pump Correction Factor, $\Psi$, (Section 6.4).
5. Pump Temperature, $T_p$ (Section 6.5).
6. Conversion efficiency, $\eta$ (Section 6.6).
7. Radiosonde Pressure and Temperature uncertainty. These values will be calculated according to the GRUAN Radiosonde Technical Report (X.X.X)

3.4.5 File naming convention

The filename convention described here is taken from Section 2.1 of the Manual for the Data Management in GRUAN [GRUAN-TD-1 DRAFT v0.3v0.3 (2010-132010-07-13)] and will apply for metadata XML files and for the CRD and SGPD data files in the designated GRUAN Lead Centres file archive. The obligatory parts of the file names should be:

- Unique Station Identifier → GAW ID and station location name, i.e. NRB_Nairobi_Kenya
- Data level → number
- Data product level → CRD or SGPD (not used for metadata file naming)
- Version of data product → number
- Date / Time → in universal standard time (UTC)
- Date / Time of the creation of CRD and SGPD files
- Identification of the specific instrument → 'ECCSonde'
- Identification of central tracer → 'Ozone'

3.4.6 Data format

- Metadata will be provided to the end-user in XML format.
- CRD and SGPD will be stored in CSV ASCII format. SGPD will be provided to the NCEI in that format. ASCII format is an accepted standard output used by the leading ozonesonde archiving centers (SHADOZ, NDACC, and WOUDC).

3.4.7 Data dissemination

- Users of GRUAN data shall have access not only to the measurements and their uncertainties, but also to the metadata information which includes instrument specifications, operating procedures, data algorithms used, and when changes to any of these occurred through the complete time period of the data set.
- Users shall have access to previous versions of the ozonesonde SGDP.

3.4.8 Data archiving
• The ozonesonde metadata, CRD and SGPD are expected to be stored at the nominated GRUAN central data processing facility Lead Centre.

• A designated GRUAN storage facility should be established. This would:
  ◦ Allow the Lead Centre to maintain statistics on data usage. This would be useful when applying for funding to support GRUAN operations.
  ◦ Allow users of data to be informed if and when newer versions of the data become available.
  ◦ Facilitate reporting of potential errors, flags, and anomalies in the data by end-users.

• GRUAN sites shall be responsible for storing their PRD.

• The metadata and SGPD shall be made available at the NCEI.

• Ozonesonde data dissemination shall comply with the data policy guidelines in Section 8.2 of GCOS-171.

• It is important that the GRUAN archive includes all previous versions of any given data set so that analyses using previous versions of data can be repeated if required.

3.4.9 Data gaps

GRUAN recognizes that there may be gaps in the profile measurements due to telemetry interference.

1. Profiles should not be excluded if data gaps occur. There is useful data extending from the surface up to the lower stratosphere, i.e. around 35 km or 5 hPa, that satisfies the four key user groups of GRUAN data products. From Section 1.2 of GCOS-171 they are the (i) climate detection and attribution community, (ii) satellite community, (iii) The atmospheric process studies community, and (iv) numerical weather prediction (NWP) community. Depending on where the data gaps occur and the extent of these data gaps, there remains useable quality reference data that can still satisfy one or more of these four communities. However, the satellite community will be the most affected by data gaps.

1. Profiles with very large and intermittent data gaps should be identified and evaluated in the annual reports and periodic audits. Ultimately, it is up to the end-user to determine whether the data gaps should be excluded from their study.

3.5 The GRUAN Standard Operating Procedures

GRUAN seeks to ensure that all sites operate to the same reference quality standard to guarantee homogeneity of quality across the network. JOSIE and BESOS demonstrated that changes of an ozonesonde instrument (e.g. different manufacturers) or operating procedures (e.g. incorrect choice of sensing solutions, incomplete metadata, missing procedures) can have a large impact on sonde data quality and thus influence the trends derived from such records. ASOPOS demonstrated that after standardization and homogenization improvement of precision and accuracy by about factor 2 might be gained. The JOSIE-1996 results show that differences between the ECC ozone sensors types are largely due to differences in the preparation and correction procedures applied by the different sites [Smit et al., 2000]. The WMO/GAW SOPs are designed to reduce random errors by maintaining consistent and reproducible ozonesonde
measurements. Standardization of the SOPs has been shown to improve the precision and accuracy to less than ±5%, while non uniformity in SOPs will lead to inhomogeneities in the time series and between station data records [Smit et al, 2007, Deshler et al, 2008].

**GRUAN protocol**

GRUAN strongly recommends that Ozonesonde Programmes use the WMO/GAW ozonesonde conditioning and preparation procedures outlined in detail in Annex A of GAW Report No. 201. Associated with the SOPs is a check list to help ensure that the site operators follows the WMO/GAW ozonesonde conditioning and preparations procedures in a consistent manner. The GRUAN check list (Appendix A-1) has been designed to be a guide to certify that SOPs are being followed correctly. It is strongly recommended that potential site candidates use the GRUAN check list in place their own SOPs, but it is not required as long as sites can demonstrate that WMO/GAW SOPs are being followed and all essential metadata are recorded.

**Refurbished Sonde SOPs**

Refurbished sensors must follow more rigorous conditioning and testing. The ASOPOS panel concluded that at present it is not clear in how often recovered ozonesondes can be re-used after reconditioning. Currently there are no quality assurance standards for refurbished sensors and a number of ozonesonde sites fly refurbished sondes using their own set of SOPs. Sites risk potentially introducing artifacts in the data records if the re-conditioning procedures are not done properly. A basic set of SOPs for refurbished sensors can be found in Appendix A-2, although manufacturer SOPs should not be discounted. Further discussion on refurbished sensors can be found in Section 4.5. GRUAN strongly recommends and encourages that JOSIE studies, independent laboratory tests, and inter-comparison field measurements be conducted to establish SOPs for refurbished sondes that GRUAN can draw on to incorporate across the OzoneSonde Programme network.

**3.6 The RSLaunchClient Utility**

The RSLaunchClient utility will collect and manage uploaded metadata and ozonesonde PRD to the GRUAN Lead Centre. Specifically, GRUAN OzoneSonde Programmes will be required to provide essential metadata and PRD to the RSLaunchClient. GRUAN defines essential data as input requirements to the RSLaunchClient. If one of the basic essential metadata variables is missing a flag will be given or, in some cases, the entire profile will be rejected (e.g. if a metadata variable required to calculate an uncertainty estimate is missing). Because each ozonesonde ECC sensor is considered a new instrument it is essential that every singular feature of each sensor is documented. The metadata represents all the characteristics that define each unique ozonesonde and will be collected by the RSLaunchClient. Most of the metadata shall be taken from the check list that has been designed to follow the WMO/GAW SOPs. The GRUAN check lists for new and refurbished ozonesondes are provided in Appendix A-1 and A-2. The red font in the check lists indicates that it is essential RSLaunchClient metadata. It is strongly recommended that potential sites use the GRUAN check list in place of the manufacturer check list.
3.6.1 Metadata for RSLaunchClient

To provide the best evaluation for the ozonesonde measurement uncertainty, a detailed understanding of the instrumentation is required for the conditions under which it is used. The ozonesonde metadata summarizes the unique characteristics of each ozonesonde instrument in response to standard operational procedures, and it makes all factors that contribute to the measurements traceable. Following the WMO/GAW SOPs a list of essential and desirable metadata has been designed and is provided in Table 3.4 below. Desirable metadata (in blue) is not required input to the RSLaunchClient. Profiles shall not be discounted if desirable metadata is not included.

Table 3.4 Essential and Desirable metadata variables specific to ECC sensors

<table>
<thead>
<tr>
<th>Number</th>
<th>Metadata Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Station Name</td>
</tr>
<tr>
<td>2.</td>
<td>GAW Number</td>
</tr>
<tr>
<td>3.</td>
<td>Site Latitude [decimal deg (range -90:+90)]</td>
</tr>
<tr>
<td>4.</td>
<td>Site Longitude [decimal deg (range -180:+180)]</td>
</tr>
<tr>
<td>5.</td>
<td>Site Elevation [m]</td>
</tr>
<tr>
<td>6.</td>
<td>Re-conditioned Sonde: Y or N. If Y then the following information is required:</td>
</tr>
<tr>
<td>6.1</td>
<td>Date flown (YYYYMMDD)</td>
</tr>
<tr>
<td>6.2</td>
<td>Date found (YYYYMMDD)</td>
</tr>
<tr>
<td>6.3</td>
<td>Date returned (YYYYMMDD)</td>
</tr>
<tr>
<td>6.4</td>
<td>Date stored on shelf until ready for the 3-7 day pre-condition (YYYYMMDD)</td>
</tr>
<tr>
<td>6.5</td>
<td>Comments on overall ozonesonde/pump condition</td>
</tr>
<tr>
<td>6.6</td>
<td>100 ppbv calibrated source current [$\mu$A]</td>
</tr>
<tr>
<td>6.7</td>
<td>100 ppbv ECC-sensor current [$\mu$A]</td>
</tr>
<tr>
<td>6.8</td>
<td>Zero Ozone air calibrated source current [$\mu$A]</td>
</tr>
<tr>
<td>6.9</td>
<td>Zero Ozone air ECC-sensor current [$\mu$A]</td>
</tr>
<tr>
<td>6.10</td>
<td>Date of Initial Pre-conditioning or Re-conditioning (done at least 3 days prior to flight): YYYYMMDD</td>
</tr>
<tr>
<td>6.11</td>
<td>Date of Secondary Preconditioning (if done): YYYYMMDD</td>
</tr>
<tr>
<td>6.12</td>
<td>Launch Date: YYYYMMDD</td>
</tr>
<tr>
<td>6.13</td>
<td>Launch time [GMT]: HH:MM:SS</td>
</tr>
<tr>
<td>6.14</td>
<td>Sonde Type and Serial Number</td>
</tr>
<tr>
<td>6.15</td>
<td>Radiosonde Type and Serial Number</td>
</tr>
<tr>
<td>6.16</td>
<td>Interface Type and Serial Number</td>
</tr>
<tr>
<td>6.17</td>
<td>Ground station system and software version</td>
</tr>
<tr>
<td>6.18</td>
<td>Pump current [$\mu$A]</td>
</tr>
<tr>
<td>6.19</td>
<td>Pump Pressure [psi]</td>
</tr>
<tr>
<td>6.20</td>
<td>Pump Vacuum [in Hg]</td>
</tr>
<tr>
<td>6.21</td>
<td>Zero Ozone Source</td>
</tr>
<tr>
<td>6.22</td>
<td>KI Solution Strength [%]</td>
</tr>
<tr>
<td>6.23</td>
<td>Buffer amount</td>
</tr>
<tr>
<td>6.24</td>
<td>Volume of cathode sensing solution [cm$^3$]</td>
</tr>
<tr>
<td>6.25</td>
<td>IB0</td>
</tr>
<tr>
<td>6.26</td>
<td>IB1</td>
</tr>
</tbody>
</table>
24. IB2
25. Initial preparation Response Time [$\mu$A/sec] = Time for ozone to drop from 4-1.5 microA
26. Initial preparation current after Response Time [$\mu$A]
27. Flow rate: All 5 flow rates [sec/100ml]
28. Flow rate average [sec/100ml]
29. Lab Temperature during Flow rate test [degC]
30. Lab RH during Flow rate test [%]
31. Lab Pressure during Flow rate test [hPa]
32. Surface Pressure at launch site [hPa]
33. Surface Temperature at launch site [degC]
34. Surface RH at launch site [%]
35. Surface Wind Direction at launch site [deg]
36. Surface Wind Speed at launch site [m/s]
37. Inverse pump efficiencies factors
38. Balloon Brand
39. Balloon Pay-off Weight [grams]
40. Independent measurements of total column ozone.
41. Dobson or Brewer or other instrumentation to be defined in Section 8.3.

Variables specific to the radiosonde data stream, such as P-T-U calibrations, offsets, and uncertainty calculations, shall borrow from the Radiosonde Analysis Software in the GRUAN Radiosonde Technical Document (X.X.X).

### 3.7 The GRUAN OzoneSonde Analysis Software System (GOASS)

The GRUAN OzoneSonde Analysis Software System (GOASS) is the centralized data processing software that shall analyses the PRD of all certified GRUAN OzoneSonde Programmes sent out through the RSLaunchClient utility. Before processing the PRD, the GOASS reconciles the metadata received from the RSLaunchClient with those contained in the GOIMP. Any inconsistency is immediately reported, thus providing a near-real-time check of the measurement traceability and stability, as well as a quick identification of change. The GOASS must be transparent, i.e., must be developed and optimized in consultation with all GRUAN OzoneSonde Programme Representatives/investigators, as well as the GRUAN Lead Centre, WG-GRUAN, and TTS. These investigators shall meet regularly to discuss the implementation of updates to the GOASS, and whether processing changes pertain to one or all of the GRUAN OzoneSonde Programmes. The output of the GOASS consists of certified ozonesonde metadata, CRD, and SGDP defined in Sections 3.5 and 3.6.

The basic principles driving the technical programming of the GOASS are as follows:

1. Each GRUAN ozonesonde instrument shall be considered as a unique instrument within the network.
2. Each GRUAN ozonesonde may experience instrumentation change over time.
3. Each GRUAN ozonesonde shall use up-to-date SOPs recommended by WMO/GAW across the network.
The need for centralized processing therefore implies a very stringent data processing approach. The GOASS must integrate correction methods and associated uncertainties that are accepted by GRUAN and user communities as being appropriate for the science application foreseen. It is therefore the GRUAN Lead Centre, TTS, and GRUAN Ozonesonde Programme Representative’s joint responsibility to develop and maintain the operational GOASS. Failure of GRUAN Ozonesonde Programmes to use an operational version of the RSLaunchClient and GOASS will result in delivery delays of the ozonesonde SGDP, and therefore can result in the cancelation of the Programme’s certification at the time of its audit.

The PRD and associated metadata accepted by the RSLaunchClient will be processed by the Lead Centre using the GRUAN Ozonesonde Analysis Software System (GOASS). The GOASS shall perform the following steps to transform the PRD to the final Level 2 GRUAN standard ozonesonde product (SGDP) (defined in this Document as a collection of profile measurements of ozone, meteorological variables from the radiosonde and uncertainties):

1. Apply filtering criteria to test the performance of an individual ECC sensor, summarized in Table 3.5 below. Aspects of the conditioning process should fit within the following specific thresholds. GRUAN site operators shall use these threshold criteria to gauge the quality of the ECC sensor and perform repeat tests if necessary to bring the ECC sensor into compliance. Ideally, ozonesonde raw data should not be uploaded to the RSLaunchClient if certain threshold criteria are violated.
Table 3.5 Threshold criteria for ECC ozonesondes used by the RSLaunchClient to test the performance quality of each sensor. These are specifically for SPC and ENSCI sensor types.

<table>
<thead>
<tr>
<th>Test Indicator</th>
<th>Threshold Criteria</th>
<th>Action if violated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average pump flow rate</td>
<td>Within 26-36 sec/ml</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>Response Time</td>
<td>20-30 sec</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>Pump temperature</td>
<td>273-315 K (15 – 40°C)</td>
<td>Flag for ozonesonde datum exceeding threshold.</td>
</tr>
<tr>
<td>Background I&lt;sub&gt;B0&lt;/sub&gt;</td>
<td>0-0.05 µA</td>
<td>See 1.1</td>
</tr>
<tr>
<td>Background I&lt;sub&gt;B1&lt;/sub&gt;</td>
<td>0-0.1 µA</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>Background I&lt;sub&gt;B2&lt;/sub&gt;</td>
<td>0-0.1 µA</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>Background I&lt;sub&gt;B&lt;/sub&gt;</td>
<td>Should be I&lt;sub&gt;B0&lt;/sub&gt; or the minimum of I&lt;sub&gt;B0&lt;/sub&gt;, I&lt;sub&gt;B1&lt;/sub&gt;, and I&lt;sub&gt;B2&lt;/sub&gt; if I&lt;sub&gt;B0&lt;/sub&gt; &gt; 0.05 µA</td>
<td>See 1.1</td>
</tr>
<tr>
<td>Pump motor current</td>
<td>&gt; 100 µA for SPC, &gt; 90 µA for ENSCI</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>Pump pressure</td>
<td>&gt; 10 psi</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>Pump vacuum</td>
<td>&lt; 20 in Hg</td>
<td>Flag and record in metadata</td>
</tr>
<tr>
<td>KI Solution</td>
<td>0.5% buffered for ENSCI; 1.0% buffered for SPC</td>
<td>Should be always be correct for GRUAN certification. For historic data, where applicable, transfer functions shall be applied.</td>
</tr>
<tr>
<td>Pump Correction Factors (PCF)</td>
<td>Komhyr [1986] values for SPC-6A and Komhyr et al. [1995] values for ENSCI</td>
<td>Ozone values shall be recalculated using the correct (PCF)</td>
</tr>
</tbody>
</table>

1.1 I<sub>B0</sub> shall be used as the final background, I<sub>B</sub>, in the ozone equation (addressed in Section 2.2). For the case where I<sub>B0</sub> > 0.05 µA GOASS shall recalculate ozone using the minimum of I<sub>B0</sub>, I<sub>B1</sub>, and I<sub>B2</sub> as I<sub>B</sub>. If that minimum background current exceeds the 0.05 µA threshold then GOASS shall recalculate ozone using I<sub>B</sub>=0.05 µA shall be used and flagged in the metadata. It should be recorded in the metadata which background is used as I<sub>B</sub>.

2. GOASS shall apply the RH correction, C<sub>PH</sub>, explained in detail in Section 2.4. The final flow rate, Φ=(mean flow rate)•C<sub>PH</sub>, shall be used in Equation 2.1.1 to calculate the Level 2 ozone partial pressure product.

3. Radiosonde/Ozonesonde offsets in height and pressure, if any, shall be documented in the metadata and geopotential heights shall be recalculated, in accordance with the GRUAN Radiosonde Technical Document (X.X.X).

4. Adjusted pump temperatures using Equation 2.6.5 and sub-equations shall be calculated. That along with the measured pump temperatures shall be used to calculate two ozone partial pressures.
5. After the above corrections are applied ozone partial pressure shall be recalculated using Section 2.1 Equation 1 in two ways: (i) using the original measured pump temperature and (ii) the adjusted pump temperature based on bullet 4 above.

6. Uncertainties for each measured parameter in the ozone partial pressure equation shall be calculated and are defined in the subsections of Section 6.

7. The individual uncertainties shall be used to calculate the ozone partial pressure for each ozone datum, as defined in Section 6.1.

8. A total column product shall then be calculated based on the processing protocol defined in Section 2.7.

Flagged Data

Data that are not within threshold levels itemized in Table 3.5 shall not be rejected but must be flagged and documented in the final archived metadata. Flagged metadata shall be included as a diagnostic tool in each GRUAN Ozone Sonde Programmes annual report. Audits shall use the statistics gathered on flagged metadata and the SGDP to help evaluate the continuity of GRUAN Ozone Sonde Programmes.

3.8 GRUAN ozonesonde calibration management

Ozonesonde ground stations generally do not require calibration at the manufacturing, instrumentation, or operational levels. Calibration of the ECC sensor comes from adhering to the SOPs and completing the metadata check list requirements. The results of the conditioning procedures summarizes the unique responses of the individual sonde to a standard fixed set of operating procedures. At the time of this document, there is no precedent or standard rules that requires sites to test or calibrate aspects of the ground station equipment, nor is there a mechanism to ensure equipment standards and quality. It would ideal to establish guidelines by which a GRUAN Ozone Sonde Programme can calibrate its ground station equipment such that sources of error and uncertainty can be further identified, traced, and included as part of the uncertainty budget for ozonesondes.

World Calibration Facility for Ozonesondes (WCFOS)

The World Calibration Center for Ozonesondes (WCCOS) at the Forchungszentrum, Jülich, Germany periodically conducts inter-comparison experiments (JOSIE) to establish and maintain quality assurance of the ozonesonde sensors. JOSIE performs routine testing of existing and newly manufactured ECC ozone sensors to (i) check the instrument performance in a controlled environment, (ii) maintain up-to-date SOPs, (iii) test individual ECC sensor capabilities, and (iv) develop uncertainty estimates for the individual instrument parameters. The WG-GRUAN shall use findings from the JOSIE reports to evaluate current best practices and whether changes to the ozonesonde SOPs or processing procedures need to change. Members of the WG-GRUAN are encouraged to participate in JOSIE initiatives to keep abreast of new findings. It is highly desirable for GRUAN sites to endorse and participate in JOSIE-led activities.

Calibration of the ozonizer test unit
The ozonizer used to condition and prepare an ECC sensor does not generate a traceable amount of ozone. Comparisons against an independent calibrated reference, such as a TEI surface ozone monitor, to generate a known ozone amount would be very useful. It would be desirable for sites to provide traceable ground/instrument checks, such as a surface ozone monitor (e.g. TEI) at the time of each profile measurement, prior to launch and independent of the manufacturer. In the case of refurbished ECC sensors it is strongly recommended that a calibrated source of ozone be used and included as part of their SOPs.

### 3.9 OzoneSonde Programme versioning system

A system of traceable version numbers and dates for all GRUAN OzoneSonde Programmes shall be developed to allow for a full identification and tracking of changes in SOPs, and data processing since the initial certification. Every reprocessing of the metadata, CRD, and SGDP must be reflected in an increment in the data version and an update to the date of creation by the GOASS (see file naming convention in Section 3.4.5) as prescribed in the data versioning protocols developed by the GRUAN Lead Centre. Such data updates must also be communicated to users who have accessed earlier versions of the data and who have voluntarily registered to receive notifications of such data updates (see Section 8.6 of GCOS-171). For this reason it is also important that all older versions of any data set are always archived and made available through the GRUAN Lead Centre's archive.

### 3.10 GRUAN OzoneSonde Programme auditing

Certification of GRUAN sites will not be a single event. GRUAN sites will be audited by members of the WG-GRUAN at 3-4 year intervals to ensure that the programme continues to meet GRUAN standards.

The audit will involve:

1. A review of the sites annual reports.
2. An ozonesonde launch in front of WG-GRUAN auditors that demonstrates that the SOPs are being followed in accordance with Section 3.5.
3. Check lists will be reviewed against the GRUAN Check lists if not used.
4. Discussions with the scientists responsible for the measurement programmes at the site.
5. In the eventuality of identified site problems the following protocols shall be followed (taken from Section 5.6 of the GCOS-171):
   1. Should a measurement programme at an existing GRUAN site show significantly reduced observational capability over more than a year, as evaluated by the criteria listed above, the WG-GRUAN and Lead Centre shall investigate the circumstances at that site, and, if needed, exclude that programme from the GRUAN certification for that site. The WG-GRUAN and Lead Centre shall work proactively with sites to resurrect such programmes providing training, technical and in-kind support as practical and as needed.
   2. Should the overall contribution of a site be deemed sufficiently diminished to call into question its continued presence in the network, the site shall be informed immediately.
in writing. The site shall be given six months to form a capabilities recovery plan, in
consultation with the Lead Centre and WG GRUAN. Should this plan be accepted the
site will have no more than two calendar years from its acceptance to implement
agreed key aspects. In the eventuality that this is not achieved, the site shall be
suspended with an invitation to submit anew at such a time as problems are remedied.

3. An existing GRUAN site may also request the temporary suspension of some or all of
the measurement programmes at that site from GRUAN certification. This could
occur for example in cases of unforeseen budget limitations, non availability of
personnel or some other unavoidable circumstance affecting the measurement
programmes at the site. Such a request must be submitted in writing to the
WG-GRUAN and the Lead Centre. At some later time, should the site request
recertification of those measurement programmes previously suspended, the
procedure for certification as outlined in Figure 2 of GCOS-171 shall be followed.

4. A certified GRUAN Ozoneonde Programme may also request a temporary
suspension of its certification. This could occur, for example, in case of unforeseen
budget limitations, non-availability of personnel or some other unavoidable
circumstance affecting the measurement programme. Such a request must be
submitted in writing to the WG-GRUAN, Lead Centre, TTS. The normal procedure
for certification should be followed if re-certification is later requested.

Along with the cooperation and goodwill of participating sites, nations, and individuals, the
establishment of these GRUAN site assessment and certification guidelines provides one of the
main foundations for ensuring that GRUAN meets its goals as a climate observing network.
4 GRUAN OZONESONDE INSTRUMENTATION

As described in Section 2 (and elsewhere) of the GCOS-171, one key requirement of GRUAN instruments is to provide reference measurements, i.e., using principles based on key concepts in metrology such as (but not limited to) traceability. Traceability must apply at all levels of the data acquisition and processing chain, including instrumentation. Therefore to ensure full traceability, a complete and accurate description of each certified GRUAN Ozonesonde Programme system must be provided in GOIMP (defined in Section 3.2). An entire ozonesonde system comprises the following components:

1. Electrochemical concentration cell (ECC) ozonesonde which is encased in a molded polystyrene weatherproof box for ascent into the lower stratosphere

2. Radiosonde

3. Interface electronics, if applicable, to couple the ECC ozonesonde to the radiosonde.

4. A ground station for receiving data provided by the radiosonde manufacturer. The ground station consists of a portable, tripod mounted, antenna with built-in pre-amplifier, and a long coaxial cable that connects the antenna to a 403 MHz receiver.

5. A laptop with pre-installed data acquisition and processing software. This allows data to be received and processed during the balloon flight.

6. A 1200 baud modem that connects the laptop to the 403 MHz receiver.

Refer to the GRUAN Radiosonde Technical Report (X.X.X ) for instrument details pertaining to radiosondes and their ground stations and data acquisition systems. Refer to the ECC manuals for information pertaining to the materials and electronics of the ECC sensor mainframe, and type interface circuitry which couples the sensor to the particular type of meteorological radiosonde [e.g. DMT, 2014; SPC, 1999].

The requirements and recommendations on ozonesonde instrumentation provided in this section apply only to the ozonesonde techniques recognized to be mature enough to be providing reference measurements of ECVs of highest-enough priority for GRUAN. As of this document, these include the SPC and ENSCI instruments coupled with the Vaisala and iMET radiosondes and ground stations and associated data acquisition and processing software. Other radiosonde and ground station data acquisition system packages, addressed in Section 4.4, shall be included as they are assessed and recognized by the Lead Centre and WG-GRUAN to be providing products compliant with GRUAN measurement standards. It is important to mention that GRUAN shall not prescribe any instrumentation system and setup in particular. Rather, GRUAN shall provide simple and practical recommendations that encourage sites to use the best practices in full compliance with the requirements and recommendations detailed in this Guide.

4.1 General considerations from Section 6.1 of the GRUAN Guide to Operations (GCOS-171)

Periodic reviews of ozonesonde instrumentation likely to be of use within GRUAN shall be undertaken. It must also be recognized that not all Ozonesonde Programmes within GRUAN will
operate the same ozonesonde instrumentation and ground station system. GRUAN will not
prescribe the use of specific ozonesonde instruments and ground station systems in the network
since the emphasis is not on prescribing an instrument, but rather on prescribing the capabilities
required of an instrument and allowing individual sites to select an instrument that achieves those
capabilities. That selection will be influenced by the requirements and recommendations put
forth by this document, and other scientific, programmatic, and practical constraints on the site.
That said, the fewer the number of different types of instruments and measurement techniques
deployed within and among GRUAN Ozonesonde Programmes, the more likely network
homogeneity will be achieved.
A number of criteria should be considered when selecting ECC ozone sensor instruments for use
in GRUAN including: instrument heritage (i.e. maturity), sustainability, robustness of
measurement uncertainty, and manufacturer support.

Since 1996, the Forchungszentrum, Jülich, Germany has been the site of the WCCOS. The first
Jülich Ozone Sonde Inter-comparison Experiment (JOSIE) (1996) has shown that ECC ozone
sensors that performed with the best precision and accuracy were the Science Pump Corporation
(SPC) and ENSCI instrument manufacturers [Smit et al., 2000]. The 1996 experiment calculated
a precision to within ±(3-4)% and an accuracy to within ±(4-5)%. Subsequent JOSIE-led
activities have included both types of ECC sensors in their inter-comparisons.

GRUAN recognizes that ECC sensor technology is constantly evolving and that not all sites
within GRUAN will operate the same ECC sensor, e.g. a new site may decide to adopt a new
ECC-sensor that has not been yet been included in JOSIE studies, or an existing site may
continue to use an older manufacturing model or obsolete sensing solution (e.g. 2% unbuffered)
to avoid potentially introducing a discontinuity in the measurement time series.

### 4.1.1 Instrument Selection

As of this Document there are two ECC sensors on the market:

a. Science Pump Corporation (SPC)
b. ENSCI

1. Both manufacturer types are considered the leading industry standard for ECC
ozonesondes and have a long heritage of launches.
2. The commercial demand for SPC and ENSCI is sufficient to support the production and
use of the instrument for the expected multi-decade deployment within GRUAN.
3. There is no reason to suspect that both instrument manufacturers will stop production in
the foreseeable future, even if a newer (but not necessarily better) instrument is
developed and marketed.
4. All ozonesonde stations with long-term ECC records use one or both types and are
archived at SHADOZ, NDACC, and the WOUDC.
5. Finally, all WMO-supported ECC inter-comparison studies (JOSIE), campaigns
(BESOS) and other laboratory and field studies have included these two manufacturing
types. Thus, there is a substantial body of literature documenting its performance and
measurement uncertainty.
6. Through JOSIE and independent dual-launch studies, the precision and accuracy claims for both instruments and its resultant data is sufficiently robust and meets the uncertainty and stability standards under Section 4.1 of GCOS-171.

In the event that a new ECC ozone sensor is commercially developed, GRUAN expects the manufacturer to (i) actively participate in JOSIE and other instrument inter-comparisons, (ii) be willing to disclose the necessary information required to form a fully traceable chain of sources of measurement uncertainty in accordance with the GCOS-171 mandatory operating requirements, and (iii) make available the algorithms used for corrections within the data processing software to conduct uncertainty analysis. In accordance with GCOS-171 guidelines, it is a 'fundamental requirement that the information required to reprocess the data at any time in the future must be made available (though not necessarily publicly available').

4.2 Measurement Redundancy

"Having different instruments at GRUAN sites measuring the same atmospheric parameters will be invaluable for identifying, understanding and reducing systematic effects in measurements" - GCOS-171

Examples of redundant instruments that measure profile ozone are the ozone Lidar and Microwave Radiometer. Other ozone monitoring instruments to consider that can complement ozonesonde profile measurements are the TEI surface ozone monitor, and UV Vis instrumentation. All these instruments can provide uninterrupted hours of measurements at one given location. Unlike these fixed located instruments, balloon-borne ozonesondes provide in-situ measurements at varying locations and altitudes with time. The challenge therefore is to match the ozonesonde altitude and time with those other instruments with careful considerations about the geographic displacement from the ground-based instrument site. Section 6.4.2. of GCOS-171 provides an overview of the characteristics of Lidar and microwave instrumentation. Methods on resolving the time/altitude differences from these instruments shall draw on information found in the GRUAN technical documents for Lidar and Microwave Radiometers. GRUAN shall draw on methods developed by Calisesi et al. [2005], Bodeker et al. [2013], Hassler et al., [2008] and references therein, that create site atmospheric state best estimates (SASBE) of ozone profiles from combining ozone instrumentation of varying temporal and spacial resolutions to provide objective evaluation of ozonesonde performance. Ozonesonde measurements themselves may be part of SASBE.

4.3 The SCIENCE PUMP CORPORATION ozonesonde

The earliest Science Pump Corporation (SPC) ECC ozonesonde measurements occurred in the late 1960's [Komhyr, 1969]. Table 1 from Johnson et al. [2002] summarizes the model production dates and design changes from the earliest SPC design (SPC-1A). The first known operating guidelines for preparing ozonesondes for flight was created for the now retired SPC-4A model in the NOAA technical memorandum [Komhyr, 1986]. The current manual has been optimized for the SPC-6A model design [SPC Manual, 1999].
GRUAN protocol procedure

As of this document, the GOASS shall process PRD from SPC-4A models and higher to produce the ozonesonde SGDP using procedure protocols established in this document. All other historic SPC profiles from older SPC models should be inventoried and properly conserved until such time as their information content can be evaluated, assessed, and assigned uncertainty estimates that conform to GRUAN reference standards and guidelines.

While the SPC modifications over time improved ECC performance, error characterization in models older than SPC-4A are not as well known. The first SOP manual was conceived with the SPC-4A model design in mind and changed with model design as they were altered to optimize performance. Given that these older SPC models no longer exist and are no longer flown, JOSIE-type studies or campaigns are necessary to determine error estimates or empirical corrections to all historic instrumental parameters.

4.4 The ENSCI ozonesonde

ENSCI Corporation started in the late 1980's with similar ECC sensor instrument configuration to that of the SPC-5A model (refer to Table 1 of Johnson et al., [2002]). Komhyr [1997] published the first ENSCI operations handbook for the 2Z model. There is no significant instrumental differences between the Z and 2Z models [Bryan Johnson/NOAA, personal communication]. The Z model is configured to be compatible with interface boards of other ground station systems (e.g. Vaisala) while the 2Z has a built-in V7 interface board compatible with the iMET ground station.

Since the late 2000’s Droplet Measurement Technologies (DMT) took over the manufacturing of ENSCI ECCs. The model design has remained unaltered at the helm of DMT, thus GRUAN does not make a distinction between the two companies. As of this document, the most up to date ENSCI manual has been published by DMT [2014] and includes much of the WMO/GAW SOP recommendations and protocols. As of this Document, ENSCI has separated from DMT and is once again it's own manufacturing entity.

GRUAN protocol procedure

The GRUAN archive shall accept ENSCI Z, 2Z ozonesonde instrument profiles to produce the ozonesonde SGDP.

4.5 A typical GRUAN ozonesonde data acquisition systems

The ozonesonde is interfaced with a radiosonde and uses its data acquisition system to transmit and record the ozone current and other parameters that calculate the ozone partial pressure (see Equation 1 in Section 2.1). The ozonesonde/radiosonde equipment and data acquisition system shall also be referred to as the 'ozonesonde ground station'. From to Section 6.1 of GCOS-171

“GRUAN will not prescribe the use of specific instruments in the network since the emphasis is not on prescribing an instrument, but rather on prescribing the capabilities
required of an instrument and allowing individual sites to select an instrument that
achieves those capabilities.”

As of this Document, there are a number of ozonesonde/radiosonde ground station systems
operating with varying degree of publicly available documentation. These include Vaisala
(Finland), iMET (USA), Lockheed-Martin-Sippican (LMS, USA), Meisei (Japan), Modem
(France), and Chang Feng (China). The Vaisala type ground station system is the most
commonly used, having a heritage of long term records of ozonesonde and radiosonde
measurements. Specific to radiosondes there is a large body of literature that have characterized
the uncertainties and biases among the Vaisala models (Dirksen et al., [2014] and references
therein; Hurst et al. [2011]; Nash et al. [2006; 2011]; Steinbracht et al., [2008] and references
therein; and Vömel et al. [2007]). Hurst et al. [2011] and Stauffer et al [2014] were among the
first inter-comparison studies of iMET and Vaisala models. Both iMET and Vaisala adhere to the
instrument selection requirements addressed in Section 6.1 in GCOS-171. This includes, but is
not limited to, information content, instrument heritage (e.g., maturity), sustainability (e.g.
sufficient commercial demand), robustness of measurement uncertainty, and manufacturer
support. Both ozonesonde ground station systems are known to provide all the essential raw data
and metadata listed in Tables 3.1 and 3.4, respectively.

As of this Document, there is varying degree of documentation that is publicly available on the
other supporting ozonesonde/radiosonde ground station systems mentioned above. However,
meeting the GCOS-171 instrument selection criteria and GRUAN data quality assurance and
measurement standard policies can be assured provided that the manufacturer is:

- Committed to improving the performance of its instrument.
- Willing to provide essential GRUAN raw data and metadata listed in Tables 3.1 and 3.4,
  respectively.
- Prepared to actively participate in instrument inter-comparisons (e.g. JOSIE) and field
campaigns (e.g. BESOS).
- Willing to disclose the necessary information required to form a fully traceable chain of
sources of measurement uncertainty (e.g. releasing SOPs and algorithms used for any
corrections within its data processing software).

**GRUAN procedure protocol**

1. At a minimum, GRUAN requires that candidate sites use ground stations that provide the
essential metadata (Table 3.4) and raw data (Table 3.1). These parameters are critical to
characterizing each individual ozonesonde.

2. GRUAN shall encourage all ozonesonde/radiosonde ground station manufacturers to
participate in JOSIE-led activities.

3. GRUAN shall encourage ozonesonde/radiosonde ground station manufacturers to provide
documentation on laboratory and dual sonde launches to demonstrate that the precision
and accuracy fits within ±(3-4)% and ±(4-5)% of the JOSIE results, respectively. These
results have been determined by Smit et al. [2000] using the leading SPC and ENSCI
ECC sensors (see Section 4.1.1).
4.6 Refurbished Ozonesondes

The ASOPOS panel concluded that at present it is not clear in how often recovered ozonesondes can be re-used after reconditioning. The general recommendation by the ASOPOS panel is not to fly re-used ECC-sondes, however, for a number of ozonesonde sites it is the most cost-effective way to the ensure financial stability of their programme and maintain their ozonesonde launch schedule. GRUAN shall (i) encourage sites at unique locations (refer to Section 3.2.1 on added-value criteria) that regularly launch re-used sondes to apply to become a GRUAN site and (ii) not prohibit existing Ozonesonde Programmes from including data from refurbished ozonesondes, provided that all operating conditions set forth by this Document are met.

Refurbished sensors falls under one of the “9 items” under managing changes in Section 7 of this report. Thus, established GRUAN Ozonesonde Programmes that wish to include refurbished sensors falls under the guidelines of a “change event” and programmes shall follow steps in Section 7.1 to include refurbished ozonesondes into their programme. For new candidate sites seeking to become a GRUAN site this information should be included as part of their GOIMP.

For individual GRUAN Ozonesonde Programmes re-using ECC-sensors, the re-conditioning SOPs of recovered sondes should be done by well-skilled and trained personnel and be done in such a way that the resulting metadata is always within the threshold criteria defined in Table 3.5 and does not introduce artifacts in their long term ozone records. For refurbished ozonesondes it is recommended that Ozonesonde Programmes following the modified NOAA prescribed re-conditioning instructions found in Appendix A-2 or re-conditioning procedures as given by the sensor-specific manufacturer.

In recognition of the heterogeneity of the GRUAN ozonesonde network, the WG-GRUAN and GRUAN Lead Centre shall evaluate individual candidate sites ability to launch refurbished sondes based on the following:

- Sites seeking to become a GRUAN site will first be assessed according to their ability to meet the mandatory operating protocols defined in Section 5.3 of GCOS-171 and specifically 3.1 of this report, and then according to the added value they bring to the network, as defined in Section 3.2.1 of this document. This will enable candidate sites to operate their ozonesonde programme to GRUAN standards.

- In assessing the value a specific site adds to the network, the WG GRUAN and Lead Centre will base decisions on sound scientific research while exercising its discretion in evaluating the proposal against the criteria defined in value-added assessment in Section 3.2.1 of this document. Consideration shall be given to, but not be limited to, the following:
  - Body of peer-reviewed literature using refurbished sondes.
  - Historical data – sites with long term homogenous data records is a desirable factor.
  - Operation set-up
  - The ability and skill of site operators to re-condition sensors following re-conditioning operating protocols (Appendix A-2 or manufacturer specific).
○ The availability of an ozone calibrator to assess the performance of each re-used sensor.
○ Funding constraints.
○ Launch schedule which is a defining factor in assessing the extent to which the candidate site can become a fully operational GRUAN Ozonesonde Programme.

GRUAN Ozonesonde Programmes shall be responsible for conducting tests to ensure that the continuity of the data record is not compromised. Sites must clearly demonstrate that each refurbished ozonesonde is measuring ozone with an accuracy and uncertainty similar to that of a new ozonesonde. This can be done using calibrated ozone instrumentation, e.g. TEI, that tests the sensor performance against known quantities of ozone, and through duel sonde inter-comparisons.
As detailed in Section 5.2.1 of GCOS-171, a fully equipped GRUAN site is required to make weekly ozone profile measurements. While it is not stipulated whether such measurements should be made using ozonesondes, lidar or microwave radiometer, the expectation is that an ozonesonde measurement programme would be a staple of an GRUAN vertical ozone profile measurement programme.

Scientifically, measurement scheduling for GRUAN ozonesonde programmes is likely to be driven by:

1. The needs of the stratospheric ozone change detection community. Ozonesonde flights need to be made sufficiently frequently to provide ozone time series suitable for detecting trends in the vertical distribution of ozone.
2. The needs of the air quality assessment community. Because ozone is a component of urban air quality, ozonesonde measurements need to be made sufficiently frequently to support air quality process studies.
3. The needs of the satellite validation community. To the extent possible ozonesonde launches should be timed to coincide with overpasses of satellite which are also making measurements of the vertical profile of ozone.

Ozonesonde protocols will continue to develop over time and, in the case of conflict between GCOS-171 guidelines and this Ozone Technical Document, the schedule outlined in this Document shall take precedence (see Section 7.5 of GCOS-171).

5.1 General considerations from Section 7 of the GRUAN Guide

Responsibilities

- The candidate site shall work with the WG-GRUAN and assigned TTS to define measurement schedule that allow the resultant ozone data products to best capture all important scales of temporal variability, both for trend analysis and for process understanding.
- In designing the Ozone Programmes measurement schedule it will be necessary for the TTS and WG-GRUAN to work closely with individual sites since scheduling is likely to be site specific. For example, some sites are more likely to (i) experience specific or unique atmospheric conditions related to the understanding of associated processes compared to other sites, (ii) be more financially constrained compared to other sites, and (iii) experience limit operating capabilities compared to other sites.
- These schedules should be conservative in the early stages of GRUAN because schedules will vary and depend on both the system being sampled (e.g. greater sampling being required in seasons of greater variability) and financial constraints (e.g. the costs of expendables). Thus, it is important to consider the added value of a site to the GRUAN ozonesonde network (see Section 3.2.1).
- Given that task teams have a finite operating life, should the TTS no longer exist, this scheduling guidance responsibility shall fall to selected members of the WG-GRUAN who may include participants from the wider GRUAN community to assist with revising measurement scheduling protocols.
Guiding Principles

- Where available, scientific and statistical studies shall inform the process for establishing ozonesonde measurement schedules. However, a sound scientific basis for the measurement schedules discussed in this Document and in the GRUAN Guide to Operations may not always be available and until they become available, the measurement schedules must be considered to be preliminary.
- The timing of an ozonesonde launch may be shifted to coincide with a satellite overpass and in this way provide valuable high quality data for satellite validation. This will serve the high priority satellite community.
- Where possible, measurement schedules for redundant systems should be synchronized so as to avoid sampling biases when combining the measurements into a single data product.
- Required measurement schedules may vary regionally and seasonally. In places and seasons where the parameter being measured is more variable, measurements should ideally be made more frequently.
- Factors affecting trend detection: The magnitude of the variability, the autocorrelation, the random error on the measurements, and the size and seasonality of the expected ozone trends are the factors influencing the quality of trend detection that should guide the development of measurement schedules.
- Measurement scheduling shall remain stable unless there is a clear requirement for change, which would then have to be agreed with the relevant GRUAN sites.

Amendments to the GRUAN measurement scheduling protocol shall follow guidelines outlined in Section 7.1 of this report.

Ozonesonde sites vary in levels of maturity (length of operation), resource (launch frequency), and possess varying levels of infrastructure (air-conditioned versus ambient laboratory conditions) and financial support (piece-meal, intermittent, or core funding). Consideration will be given to sites with limited funding to operate at the optimal launch frequency determined by the task team.

5.2 GRUAN ozonesonde measurement scheduling

Ozonesondes are classified as ancillary measurements that provide complementary priority 1 ECV measurements of temperature, pressure and water vapor, and priority 2 ECV measurements of ozone in the troposphere and lower stratosphere. All ECC-sensors considered in this report are considered to be research-grade instruments. To date, measuring ozone at a fixed high vertical resolutions with high precision can only be done by ozonesondes. Thus, it is highly desirable to include GRUAN ozonesonde data records to service end-user communities defined in Section 1.2.

Measurement scheduling for GRUAN ozonesondes is driven by one main factor: financial support for expendables which include the ozonesonde, interface electronics, and the balloon payload. Each ozonesonde is considered a unique instrument and generally, once an ozonesonde is launched it is lost. It is not common for sites to retrieve, re-condition, and re-launch the same sensor. Geography, land restrictions, weather, and additional resources can prohibit such rescue attempts. Schedules will depend upon available expendables and so there cannot be a “one-size fits all” solution.
In seeking a practical balance between sites with funding constraints and GRUAN scientific goals, GRUAN shall accept a minimum requirement of two times per month launches to be spaced every other week. Sites seeking to become GRUAN sites shall first be assessed according to their ability to meet the mandatory operating protocols defined in Section 5.3 of GCOS-171 and then according to the added value they bring to the network, as defined in Section 3.2.1.

1. **A fully** equipped GRUAN ozonesonde site shall make weekly launches. If and when possible, GRUAN shall encourage candidate or newly certified sites to become a fully equipped GRUAN site.

2. Sites shall upload metadata and PRD to the RSLaunchClient as soon as the launch is complete and that site has successfully archived their metadata and PRD.

3. Sites shall commit to launching at around the same time of day. This is to maintain the representativeness and homogeneity of the data record. Variable ozonesonde launch times may affect the accuracy of trend assessments [Thompson et al., 2014].

4. To the extent possible, ozonesonde launches should be timed to coincide with satellite overpass times that measure total column ozone and/or vertical profiles of ozone.

5. Weather permitting, GRUAN advises launching the same day for bi-monthly to weekly sounding schedules. Altering a planned launch date due to inclement weather such as a natural disaster, strong winds, heavy rains, and storms that would impede a successful launch is expected. Altered scheduled launches shall be included as part of the annual report summaries.

6. Where possible, measurement schedules for redundant systems should be synchronized so as to avoid sampling biases when combining the measurements into a single data product.

### 5.3 Raw data acquisition and archiving

The rawest form of ozonesonde data (PRD) acquired within a certified GRUAN ozonesonde programme and leading to the production of certified GRUAN data products is subject to all articles of the GRUAN data management policy described in Section 8 of GCOS-171, and adapted specifically for the ozonesondes in Section 3.4.

The ozonesonde PRD acquisition procedure should follow the optimal SOPs defined in Section 3.5. The essential raw data and metadata per ozonesonde launch shall then be uploaded to the RSLaunchClient (See Tables 3.4 and 3.1 for the lists of essential and metadata and PRD, respectively).

The raw data (PRD) format and metadata shall be in ASCII text and the RSLaunchClient shall be responsible for converting the PRD to Level 1 converted raw data files (CRD) for processing by the GOASS described in Section 3.7 to create the GRUAN standard product (SGDP).

Raw data (PRD) sampling
Vertical range: 1-2 second raw data with no averaging.

Temporal range: As defined in Section 5.2 a minimum of bi-weekly launches will be accepted, although weekly launches are the ideal and encouraged.

GRUAN Ozonesonde Programmes PRD are expected to be archived in perpetuity at the site where the measurements took place, and must be uploaded as soon as the launch cycle is complete onto the designated centralized GRUAN ozonesonde data handling facility. The upload procedure must be performed using the mandatory RSLaunchClient utility. No PRD data shall be accepted if they are not uploaded through the RSLaunchClient utility. If one or several changes of instrumentation or operating procedure occurred during a given 24 hours cycle, the PRD must be uploaded separately for each of the multiple uninterrupted data acquisition periods, each of these periods shall be considered as a separate GRUAN ozonesonde observation. Each GRUAN Ozonesonde Programme should have included in their certification application a full description of the local storing location and an overview of the raw data format.
6 DATA PROCESSING AND UNCERTAINTY BUDGET

The measurement uncertainty of the ozonesonde system describes the current best knowledge of instrument performance under the conditions encountered during an observation. This section summarizes how the centralized GRUAN Ozonesonde Analysis Software System (GOASS) processes the raw ozonesonde data (PRD/CRD) to produce a GRUAN ozonesonde standard data product (SGDP).

The assessment of the uncertainty budget of ozone measured from ozonesondes is a complex task. Measurement uncertainties in ozonesondes should, in the first instance, be characterized in the laboratory. In the past, JOSIE (Jülich Ozonesonde Inter-comparison Experiment) has played a key role in describing/analyzing all sources of measurement uncertainty to the extent possible, quantifying/synthesizing the contribution of each source of uncertainty to the total measurement uncertainty, and verifying that the derived net uncertainty is a faithful representation of the true uncertainty and is in agreement with the required (expected) target uncertainty. However, results from laboratory studies should be corroborated with field campaigns which are likely to test the sondes in an environment closer to their standard operating environment e.g. the BESOS (Balloon Experiment on Standards for Ozonesondes) campaign (Deshler et al., 2008). While it may be necessary to GRUAN to conduct laboratory studies and/or field campaigns to resolve operational issues specific to the use of ozonesondes within GRUAN, the GRUAN ozonesonde community must, wherever possible, collaborate with other international ozonesonde communities such as GAW, NDACC and SHADOZ whenever they are conducting laboratory studies and/or field campaigns.

With regards to the BM and CI type sondes it shall be the responsibility of the Lead Centre and the WG-GRUAN to evaluate the appropriateness of uncertainty estimates and determine if BM and CI data records are of sufficient quality to meet the GRUAN reference measurement standards (see Section 8 on Quality Management).

6.1 The Ozone uncertainty equation: Principles and rationale

Since the 1990's tests conducted by JOSIE-led experiments, campaigns such as BESOS, and dual flight experiments have clearly demonstrated the need to characterize singular features of the ECC ozone sensors and standardize measurements. These activities have lead to the creation of the ASOPOS panel whose goals are to (i) standardizing the ozonesonde conditioning and preparation procedures, (ii) establishing guidelines for the reprocessing and homogenization of ozonesonde data records, and (iii) determining the contributions of the individual uncertainties of the different instrumental parameters to the ozone measurement. The WMO/GAW Report 201 is a comprehensive summary of the ASOPOS findings and is the foundation on which GRUAN has used to established this technical report. The treatment of uncertainty in the GRUAN ozonesonde data processing will follow the recommendations and definitions of the WMO/GAW Report 201. These uncertainty parameters are part of the ozonesonde SGPD.
The Ozone Uncertainty Equation

GRUAN shall adopt the WMO/GAW ozone uncertainty equation taken from Equation E-3-2 in Smit et al, [2014]). It is written as follows:

Eqn. 6.1.1

$$\frac{\Delta P_{O3}}{P_{O3}} = \sqrt{\left(\frac{\Delta I_M}{I_M + I_B}\right)^2 + \left(\frac{\Delta I_B}{I_M + I_B}\right)^2 + \left(\frac{\Delta \eta_c}{\eta_c}\right)^2 + \left(\frac{\Delta \Phi_p}{\Phi_p}\right)^2 + \left(\frac{\Delta T_p}{T_p}\right)^2 + \left(\frac{\Delta \Psi}{\Psi}\right)^2}$$

where the term, $$\left[\left(\frac{\Delta I_M}{I_M + I_B}\right)^2 + \left(\frac{\Delta I_B}{I_M + I_B}\right)^2\right]$$ is the contribution of the uncertainty in background current, where $$\Delta I_M$$ is the uncertainty in the measured current, $$I_M$$, and $$\Delta I_B$$ is the uncertainty in the background current, $$I_B$$.

Contribution of the uncertainty in background current

The term $$\left[\left(\frac{\Delta I_M}{I_M + I_B}\right)^2 + \left(\frac{\Delta I_B}{I_M + I_B}\right)^2\right]$$ from equation 6.1.1 is the contribution of the uncertainty in background current, where $$\Delta I_M$$ is the uncertainty in the measured current, $$I_M$$, and $$\Delta I_B$$ is the uncertainty in the background current, $$I_B$$.

Based on the JOSIE results above, GRUAN will adopt a ±0.02 µA background current uncertainty, $$\Delta I_B$$, for ENSCI 0.5% half buffer KI solution and ±0.013 µA for Science Pump ECC 1.0% full buffer KI solution because there are no other uncertainty estimates for $$I_B$$ in the literature. Furthermore, there is the added complication that this is a single measurement per unique ECC sensor so uncertainties cannot be be directly ascertained.
The uncertainty in the ozone current, $\Delta I_M$, shall be set to 0.1 $\mu$A which is the resolution of the digital interface board (Terry Deshler/UWy and Herman Smit/Forchungszentrum, personal communication).

The uncertainty constants are summarized in Table 6.2.1 below.

Table 6.2.1 Constants in the ozone current uncertainties

<table>
<thead>
<tr>
<th>ECC Sensor</th>
<th>$\Delta I_M$</th>
<th>$\Delta I_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENSCI/0.5%</td>
<td>$\pm 1%$ of measured currents above 1 $\mu$A, and $\pm 0.01$ $\mu$A for currents below 1 $\mu$A.</td>
<td>$\pm 0.02$ $\mu$A</td>
</tr>
<tr>
<td>SPC/1.0%</td>
<td></td>
<td>$\pm 0.013$ $\mu$A</td>
</tr>
</tbody>
</table>

Background uncertainties outside the ENSCI/0.5% and SCP/1% pairing shall have to undergo similar rigorous testing to establish uncertainty estimates. In this case, profiles shall be stored in CRD format until such time as background uncertainties can be established and applied to create the ozonesonde SGDP. SGDP cannot be generated unless all uncertainty contributions to ozone in Equation 6.1 are known.

### 6.3 Contribution of the uncertainty in pump flow rate

From Section 2.4 Equation 2.4.1 the final mean flow rate is corrected for the humidification effect, $C_{PH}$, and differences between the internal pump temperature and the ambient air, $C_{PL}$.

The uncertainty associated with the determination of the mean flow rate is the ratio of the standard deviation of the five flow rates to the square root of the sample population, which in this case is five. The equation is expressed as

Equation 6.3.1 $\Delta T_{100} = \frac{\sigma_{T_{100}}}{\sqrt{N}}$ where $N=5$

This equation is based on error analysis by Bevington and Robinson [1992] (Chapters 3 and 4).

The uncertainty in $C_{PH}$ and $C_{PL}$ are site specific. For existing sites that have established at least one year’s worth of ozonesonde launches, i.e. a minimum of 24 total launches, relative uncertainties, $\Delta C_{PH}$ and $\Delta C_{PL}$, shall be calculated in the following way

Equation 6.3.2 $\Delta C_{PH} = \frac{\sigma_{C_{PH}}}{\sqrt{N_{C_{PH}}}}$, $\Delta C_{PL} = \frac{\sigma_{C_{PL}}}{\sqrt{N_{C_{PL}}}}$

where $N_{C_{PH}}$ and $N_{C_{PL}}$ are a minimum of 24 and $\sigma_{C_{PH}}$ and $\sigma_{C_{PL}}$ are the 1-sigma standard deviation of the $C_{PH}$, $C_{PL}$, respectively, as defined in Section 2.4.
For new GRUAN Ozonesonde Programmes with no launch history it is impossible to estimate $\Delta C_{PH}$ and $\Delta C_{PL}$. In this case, the term shall not be used in the ozone uncertainty equation until after one year's worth of ozonesonde launches have been processed by the GRUAN Lead Centre. Until such time, profiles shall be stored in CRD format until $\Delta C_{PH}$ and $\Delta C_{PL}$ can be calculated and then used to create the ozonesonde SGDP.

Table 6.3.1 Uncertainty estimates for the pump flow rate

<table>
<thead>
<tr>
<th>$\Delta T_{100}$</th>
<th>Use Equation 6.3.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta C_{PL}$</td>
<td>Use Equation 6.3.2</td>
</tr>
<tr>
<td>$\Delta C_{PH}$</td>
<td>Use Equation 6.3.2</td>
</tr>
</tbody>
</table>

Thus, the full equation to calculate the pump flow rate uncertainty shall be expressed in the following equation:

$$\frac{\Delta \Phi}{\Phi} = \sqrt{\left(\frac{\Delta T_{100}}{T_{100}}\right)^2 + \left(\Delta C_{PL}\right)^2 + \left(\Delta C_{PH}\right)^2}$$

This term may change as the data record expands, thus $\Delta C_{PH}$ and $\Delta C_{PL}$ should be continually evaluated by the Ozonesonde Programmes annually to check for large deviations from its constant value and assess whether and how fluctuations in the uncertainty terms affect the ozone uncertainty significantly. It may be that re-processing of the entire data record of a given site is required if $\Delta C_{PH}$ and $\Delta C_{PL}$ statistics changes significantly over time.

### 6.4 Contribution of the uncertainty in pump correction factor (PCF)

The uncertainty in the pump correction factors (PCF), $\Delta \Psi$, shall be taken from Table 2.5.1 and are re-iterated in Table 6.4.1 below.

Table 6.4.1 Pump correction factor uncertainties

<table>
<thead>
<tr>
<th>Pressure [hPa]</th>
<th>K86 $\Delta \Psi$</th>
<th>K95 $\Delta \Psi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sfc-100</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>100</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>50</td>
<td>0.006</td>
<td>0.005</td>
</tr>
<tr>
<td>30</td>
<td>0.008</td>
<td>0.008</td>
</tr>
<tr>
<td>20</td>
<td>0.009</td>
<td>0.012</td>
</tr>
<tr>
<td>10</td>
<td>0.010</td>
<td>0.023</td>
</tr>
<tr>
<td>7</td>
<td>0.012</td>
<td>0.024</td>
</tr>
<tr>
<td>5</td>
<td>0.014</td>
<td>0.024</td>
</tr>
</tbody>
</table>
Calculating $\Delta \Psi$ between data points shall be done on a log pressure scale with polynomial interpolation.

From Table 6.4.1 the GRUAN GOASS shall use the following PCF uncertainties to the following ECC sensors:

(i) K86 $\Delta \Psi$ for SPC ECCs
(ii) K95 $\Delta \Psi$ for ENSCI ECCs.

New ECC sensors shall have to undergo similar JOSIE testing, laboratory and field tests to establish and validate their PCF values and uncertainties. GRUAN protocols for managing a change in sensor technology shall follow guidelines put forth in Section 7.1.

### 6.5 Contribution of the uncertainty in pump temperature

Calculating the adjusted pump temperature is discussed in detail in Section 2.6 and the associated uncertainties are summarized in Table 6.5.1 below.

<table>
<thead>
<tr>
<th>Case</th>
<th>Location</th>
<th>Sonde Type</th>
<th>$\Delta T_P$</th>
<th>$\Delta T_{P\text{Case}}$</th>
<th>$\Delta T_{\text{Piston-internal}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Bottom of circuit board</td>
<td>SPC 2A, 3A, 4A</td>
<td>$\pm 1.0K$</td>
<td>$\pm 1.0K$</td>
<td>$\pm 0.5K$</td>
</tr>
<tr>
<td>2</td>
<td>Suspended in the styrofoam box in the vicinity of the pump</td>
<td>SPC 5A</td>
<td>$\pm 0.5K$</td>
<td>3.9–$1.13 \log_{10}(P)$ for $P &gt; 70\text{hPa}$ 3.0–$1.13 \log_{10}(P)$ for $P \leq 70\text{hPa}$</td>
<td>$\pm 0.5K$</td>
</tr>
<tr>
<td>3</td>
<td>Taped thermister at the pump base</td>
<td>SPC 5A</td>
<td>$\pm 0.5K$</td>
<td>Same as Case 2</td>
<td>$\pm 0.5K$</td>
</tr>
<tr>
<td>4</td>
<td>Epoxied at the pump base</td>
<td>SPC 5A</td>
<td>$\pm 0.5K$</td>
<td>$\pm 0.5K$</td>
<td>$\pm 0.5K$</td>
</tr>
<tr>
<td>5</td>
<td>Mounted inside the pump body, close to the piston</td>
<td>EnSci Z &amp; 2Z, SPC 6A</td>
<td>$\pm 0.5K$</td>
<td>No uncertainty</td>
<td>$\pm 0.5K$</td>
</tr>
</tbody>
</table>

The additional correction to account for differences between moving piston, $T_{\text{piston}}$, and the internal pump, or pump based, temperatures is defined as $\Delta T_{\text{piston-internal}} = \pm 0.5K$ and is true for all cases.

The full contribution of the measured pump temperature to the ozone uncertainty includes the uncertainty of the additional corrections defined in Section 2.6 and summarized in Table 6.5.1. This equation is expressed as
Equation 6.5.1

\[ \frac{\Delta T_p}{T_p} = \sqrt{\left( \frac{\Delta T_p}{T_p} \right)^2 + \left( \frac{\Delta T_{\text{Case} - i}}{T_p} \right)^2 + \left( \frac{\Delta T_{\text{piston} - \text{int error}}}{T_p} \right)^2} \]

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6.6 Contribution of the uncertainty in the conversion efficiency

GRUAN shall adopt the WMO/GAW uncertainty calculation for the conversion efficiency [Smit et al., 2014, Equation E-3-4], written as

Equation 6.6.1

\[ \frac{\Delta \eta_C}{\eta_C} = \sqrt{\left( \frac{\Delta \alpha_{O_3}}{\alpha_{O_3}} \right)^2 + \left( \frac{\Delta S_{O_3: I_2}}{S_{O_3: I_2}} \right)^2} \]

where,

\[ \Delta \eta_C/\eta_C = \text{conversion efficiency uncertainty term to be used in the ozone uncertainty equation} \]

6.1.1

\[ \alpha_{O_3} = \text{absorption efficiency from the gas into liquid phase of the sensing solution} = 1.0 \]

\[ \Delta \alpha_{O_3} = \text{\( \alpha_{O_3} \) uncertainty} = \pm 0.01 \]

\[ S_{O_3: I_2} = \text{stoichiometry of the conversion of O}_3\text{ to I}_2 = 1.0 \]

\[ \Delta S_{O_3: I_2} = S_{O_3: I_2} \text{ uncertainty} = \pm 0.02 \text{ at } Z=0\text{km with a linear increase to } \pm 0.05 \text{ at } Z=35\text{km. This translates to the linear equation,} \]

Equation 6.6.2

\[ \Delta S_{O_3: I_2}(Z) = 0.000857143*Z + 0.02 \]

Setting the absorption efficiency (\( \alpha_{O_3} \)) equal to one are for cases where the volume of the cathode solution is 3.0 cm\(^3\). GRUAN will use the following WMO/GAW equations to calculate \( \alpha_{O_3} \) for a 2.5 cm\(^3\) volume, as follows

Equation 6.6.3

\[ \alpha_{O_3}(P) = 1.0044 - 4.4 \times 10^{-5} \times P \] \( 100 \text{ hPa} < P < 1050 \text{ hPa} \]

Equation 6.6.4

\[ \alpha_{O_3}(P) = 1.0 \] \( P \leq 100 \text{ hPa} \]

\[ \Delta \alpha_{O_3} \text{ is } \pm 0.01 \text{ for both cathode volumes.} \]

GRUAN shall require new candidate sites to use 3.0 cm\(^3\) volume cathode sensing solution to reduce added uncertainty in the ozone uncertainty equation and maintain a constant absorption efficiency throughout the profile measurements.

6.7 Contribution of the uncertainty in the radiosonde temperature and pressure to ozone uncertainty

The designated GRUAN Ozonesonde Lead Centre shall adopt the GRUAN Radiosonde Technical Report (X.X.X) processing procedures for calculating the uncertainties associated with the radiosonde measurements. Handling biases in the geopotential height calculation in the
absence of GPS measurements shall be the responsibility of the Radiosonde WG-GRUAN, assigned task team, and responsible Lead Centre.
7 MANAGING CHANGES

Changes in instrumentation, operating procedures, and data processing algorithms are likely to introduce sources of operational uncertainty into the ozone profiles measured within GRUAN Ozonesonde Programmes. The primary goals are to (i) avoid unnecessary changes, i.e. those changes that have no scientific, financial or operational benefit, and (ii) where changes are beneficial and/or necessary, to manage those changes in a way that the homogeneity of the ozonesonde data record is maintained across the transition and that the change does not compromise the integrity of the long-term record.

Ozonesondes have gone through several modifications since they were first introduced in the 1960's and there is no reason to believe that those modifications will cease. Without such modifications there would be no opportunity to improve the performance of the instruments. Therefore, while GRUAN encourages ozonesonde manufacturers to improve the performance of the instruments, GRUAN also recognizes that managing such changes in instrument design or function is essential for determining long-term stability of the ozonesonde data products.

Factors influencing trends in an ozonesonde dataset to consider include the following changes (termed as “9 items” hereinafter):

1. SOPs
2. GOASS data processing algorithms
3. ECC-sensor manufacturer
4. Solution concentration
5. Location of launch site
6. Operating environment of the ozonesonde
7. Ground station system
8. Radiosonde manufacturer
9. Including refurbished ECC-sensors

They are all likely to introduce inhomogeneities into ozonesonde SGDP. This section describes the protocols for managing changes in the ozonesonde SGDP. This section is developed based on the section “Managing change” of the GCOS-171 GRUAN Guideline.

7.1 Guiding principles

The GCOS climate monitoring principles relevant to guiding principles for managing changes in GRUAN Ozonesonde Programme include:

- The impact of new ozonesonde systems or changes to existing systems should be assessed prior to implementation.
- A suitable period of overlap for new and old items is required. This will be dictated by the GCOS-171 guidelines and is addressed further in Section 7.7.
Embracing change: GRUAN Ozonesonde Programmes must not be resistant to change but must actively encourage carefully managed changes. However, the advantages of making any change must always be weighed against the inherent disadvantages of making a change.

Change event notification: A change event begins with the start of change of any one of the above “9 items”.

A change event notification is first issued by the GRUAN site by email to the GRUAN Lead Centre.

The Lead Centre, a GRUAN Ozonesonde Programme, an ozonesonde instrument manufacturer, or another member of the GRUAN community can initiate a proposal for changes.

A change event ends with the official acceptance of the change that has been made after a careful and rigorous assessment. Proposed changes in (1) and (2) of the “9 items” will likely be initiated by the Lead Centre.

Justification of change: Any change to the “9 items” above in a GRUAN Ozonesonde Programme must be fully justified before the change is enacted. An assessment report must be submitted in which advantages and disadvantages of making the change must be carefully assessed. Laboratory tests of old and new items (anyone of the “9 items” listed above) should be included in the assessment report.

The Lead Centre must act as a clearinghouse for all proposed changes to (a) assure high stability and (b) decide when an improvement merits a change to the GRUAN ozonesonde procedures.

- The Lead Centre, in consultation with ozonesonde experts, makes an initial evaluation of the proposed change.
- If considered to be worth pursuing, the Lead Centre assesses the advantages, disadvantages, and potential impacts of the proposed change.

The information and data required to manage the change are captured in a “change evaluation report” that will become a key component of the metadata associated with the change.

Preparing for change: A quantitative assessment of the impacts of any planned change must be undertaken before the implementation of the change.

- The assessment must cover a sufficient period of time, not just covering the change period.
- If the knowledge needed for quantitatively assessing the impact of changes exists, it should be immediately encapsulated in the metadata associated with the change event. Official acceptance of the change should be expedited so that there is no disruption to the launch schedule.
- Some changes have already been anticipated and assessed in this Document with a change implementation process as part of the GOASS (e.g. changing from SPC to
ENSCI, or changing solution strength (See Section 7.2)). In this case, official acceptance of the change should be expedited so that there is no disruption to the launch schedule.

- If additional laboratory studies or dual ozonesonde launches are required, such studies must be undertaken by either the Lead Centre, a task force commissioned by the Lead Centre, the GRUAN site scientists, members of the ASOPOS panel, or other ozonesonde experts. Any relevant results in the peer-reviewed literature should be included in any change assessment.

- The impact on the ozonesonde SGDP product and its uncertainty needs to be assessed in such a way that (1) knowledge of the newly changed item is at least as detailed as knowledge of the old one, (2) tests are, or have been, conducted (e.g. processing a large number of common datasets by both new and old algorithms if a change in algorithm is proposed), (3) the resulting ozonesonde SGDP after the change are either unchanged or an improvement to those prior to change, in terms of continuity, accuracy or integrity. If continuity, accuracy and integrity cannot be improved at the same time, at least they should not be worse than before. If a considerable improvement in one aspect (e.g. accuracy) is gained, at the cost of a slight degradation of the other aspects, it might be still justifiable to propose a change.

- When laboratory studies and dual ozonesonde launches are proposed to be conducted, regular observations schedule must not be interrupted. In the case when laboratory or field studies cannot be reconciled, this must be noted as part of the metadata. In this case, a proposal of how to resolve the discrepancy should be developed by the Lead Centre WG-GRUAN.

- If the GRUAN site decides to proceed and implement the change, any data and metadata collected as part of the change process, as well as a full report on how the change is managed and implemented, must be submitted to the Lead Centre within 3 months of the completion of the change. This information will then be archived as part of the metadata record for the ozonesonde data series from that GRUAN site.

- Validating impacts: No discontinuities in the measurement series should occur if a change has been properly managed. This is done through the justification (5) and preparing for change (6) items. Validation of the process can be achieved by subjecting the entire measurement series to homogenization tests, or may require a reprocessing of historical data. Impacts of changes must be assessed in light of the different intended uses of GRUAN ozonesonde data products.

- Change and uncertainty: Knowledge of an ozonesonde measurement system can never be complete or perfect. Transitioning from an old to a new measurement system always introduces an additional source of uncertainty which must be captured in the uncertainty estimate on the measurements.

- Supporting reprocessing: As new and more in-depth knowledge of ozonesonde instrumentation and processing is gained, and in particular following change events (see #4), reprocessing of historical data may be necessary. Such reprocessing may require revision of the homogenization procedures applied at each previous change.
event to produce a homogenized data record. It is essential, therefore, that raw data, as was well as detailed metadata collected during change events, are archived so that such reprocessing can be easily achieved.

- **Single changes**: Whenever a measurement system is changed, as many similarities as possible between the old and new systems should be maintained e.g. both the ozonesonde and ground-station should not be simultaneously changed. Multiple simultaneous changes must be avoided so that the quantitative assessment of the impact of the change on the measurement and its uncertainty is not confounded with other, simultaneous, assessments.

- **Monitoring changes**: Most changes are planned and therefore can be managed. However, some changes may be unplanned (e.g. natural disaster, changes in funding). Under these circumstances, GRUAN sites shall be placed on hold until the site can be re-established. It may be that re-certification is required. This shall be determined by a site visit from members of the Lead Centre (see Section 3.2).

- **Use of independent, redundant measurements**: Redundancy in ozone measurement systems provides a powerful tool for validating the management of changes in any one of those systems. To take advantage of measurement system redundancy, it is essential that these independent systems are not changed simultaneously.

- **Use of models**: Where changes in an historical measurement record have not been adequately managed, and where physical or statistical models can faithfully reproduce the key characteristics of the measurement record, the model time series can provide a means of detecting and correcting for systematic biases between old and new measurement systems. In GRUAN, where all changes are managed changes, the use of models for this purpose should not be necessary.

- **Manufacturer involvement**: Efforts must be undertaken to avoid unknown changes e.g. the instrument manufacturer making unannounced changes. GRUAN needs to establish close working relationships with instrument manufacturers so that any changes implemented in the manufacturing of an instrument are made know to the GRUAN ozonesonde community.

7.2 **Transfer Functions**

There have been a number of studies that have used laboratory, dual-sonde, and multi-sonde payloads to derive methods of calculating transfer functions that characterize differences in instrument and solution concentration [Smit et al., 2007; Kivi et al., 2007; Deshler et al., 2008; Stubi et al., 2008; Mercer et al., 2008].

As part of the SPARC-IGACO-IOC-NDACC (SI2N) initiative, the Assessment of Standard Operating Procedures for Ozone Sondes (ASOPOS) working group established empirical transfer functions specifically for the SPC and ENSCI type ozonesondes using either the 1% full buffer or 0.5% half buffer solutions [Smit et al., 2012]. This work uses all data taken from the above cited studies. Their aim is to homogenize long term ozonesonde records, that use these

These transfer functions represent the quantitative differences of the ozonesonde response based on changes in instrumentation and stoichiometry of the conversion of O₃ to I₂ with a change in solution concentration. They are not a reflection of changes in SOPs. Smit et al. [2007] and Thompson et al. [2007] showed that there are discontinuities in the time series of a single site that have used a variety of instruments and solution strength, citing the need to homogenize the long term records of individual ozonesonde sites.

The conversion relationship is summarized in Table 3 of Smit et al. [2012].

**GRUAN processing protocol**

1. Where applicable, transfer functions taken from Smit et al. [2012] shall be applied and shall be part of the ozonesonde SGDP.

2. Data records where transfer functions should be applied but do not yet exist shall remain in the Level 2 stage but shall not be considered as part of the ozonesonde SGDP.

3. Transfer functions for time series that use a combination of BM and ECC shall follow WMO/GAW #201 Report guidelines found in Section 4.3 and subsections. It shall be the responsibility of the Lead Centre and the WG-GRUAN to evaluate the appropriateness of the transfer functions and determine if BM data records are of sufficient quality to meet the GRUAN reference measurement standards.

4. As of this document, there are no transfer functions for time series that use a combination of CI and ECC sondes. However, dual sonde launches have been conducted by Nakamura et al., [2008] and have the potential to be used to develop transfer functions. The Lead Centre and WG-GRUAN shall work with the manufacturer (Japanese Meteorological Agency) to determine the extent to which uncertainties estimates have been established and validated and the status of deriving transfer functions between CI and ECC sondes by the group. It shall be the responsibility of the Lead Centre and the WG-GRUAN to evaluate the appropriateness of the transfer functions and determine if the historic CI data records are of sufficient quality to meet the GRUAN reference measurement standards.

### 7.3 Managing changes in instrumentation

GRUAN Ozonesonde Programme is characterized by the fact that every ozone profile is measured with a different instrument. Managing changes in instrumentation therefore extends to managing changes in sondes between flights. Efforts must be undertaken to avoid unknown changes e.g. the instrument manufacturer making unannounced changes to the material or configuration of the ECC sensor, or a ground station software update. Late response to changes or upgrade announcements may result in discrepancies in the measurement time series. One way to ensure that instrument changes are identified, characterized, and recorded such that there is no discontinuity in the network, as a whole, is for mandatory GRUAN representation at future
JOSIE studies. This will not only safeguard the homogeneity of datasets due to instrumentation changes but will also ensure that GRUAN:

1. Follows retractions or addendum's to the original GAW Report No. 201 recommendations and SOP protocols.
2. Be informed of changes in manufacturer design and materials, and how these affect ozonesonde performance.
3. Be aware of changes in the processing software.
4. Be advised of additional concerns in the SOPs.

All of the above will impact GRUAN processing procedures. Therefore, GRUAN participation should be mandatory.

GRUAN Lead Centre needs to establish close working relationships with ozonesonde instrument manufacturers (e.g. SPC and ENSCI) and ozonesonde/radiosonde ground station manufacturers (e.g. Vaisala, Modem, Chang Feng, etc) so that any changes to be implemented or having been implemented are known to them. Preferably the changes can be known substantially in advance of deployment, allowing sufficient time to investigate, understand, prepare for and document the change and its likely impacts. Links to instrument manufacturers: Dealing with changes in instrumentation will require GRUAN task team to establish close two-way links to instrument and ground station manufacturers. Inclusion of ASOPOS panel members, other ozonesonde experts, and other ozonesonde archives (e.g. SHADOZ and NDACC) in discussions of instrument change would be advantageous.

7.4 Managing changes in SOP and operating environment

Currently, there are multiple variations in ozonesonde preparation procedures since the first manual was written [Komhyr, 1986]. Besides modifications in the manufacturer’s instructions in past the decades, scientific institutions have established their own modified operating procedures. There is also a number of ozonesonde processing software that applies their own treatment of the variables that go into Equation 1. Testing of the ozonesondes under laboratory conditions has showed the need to standardize the operating procedures and provide guidelines to homogenize the data based on community consensus [Smit et al., 2014]. Smit et al., [2007] reports that maintaining SOPs improves the precision of the overall measurements better than ±3-5%. GRUAN recommends that each station maintain the GRUAN Lead Centre certified set SOPs for pre-flight and day of flight conditioning established by WMO/GAW to ensure consistency and homogeneity in operating practices. The goal here is not to disrupt the continuity of the long-term practices.

As described in Section 3.5, while implementing these SOPs is not mandatory, sites are required to document where they have deviated from the GRUAN certified SOPs and, when audited, are assessed for their ability and willingness to adhere to the SOPs within GRUAN.

Some changes in the operating environment may be unplanned, such as in the event of a natural disaster, erosion of the field site or land-use changes that necessitates moving the operating environment. Under these circumstances, a GRUAN site shall be placed on hold until the
physical site can be re-established. It may be that the new location is far enough away from the original location that a new GRUAN site needs to be established in place of the old site. This shall be determined by the task team assigned by the Lead Centre. In this case, re-certification will be required because the new location and operating conditions will need to be re-assessed. The process of re-certification shall follow the guidelines addressed in Section 3.2.

In their annual report, each site shall document any changes to their current certified SOPs and operating environment and include (1) why those changes occurred, (2) how those changes were managed, and (3) the impact, if any, on the homogeneity, accuracy, and integrity of their measurements.

GRUAN sites shall follow the change protocol outlined in Section 7.1 if changes to items (1) and (6) of the “9 items” occur.

GRUAN representation at future JOSIE studies is strongly recommended to follow (1) retractions or addendum's to the original WMO/GAW Report No. 201, (2) recommendations and SOP protocols, and (3) be advised of additional concerns in the SOPs.

7.5 Managing changes in data processing algorithms

As in any data processing situation, there will be occasional re-processing of the ozonesonde converted raw data (CRD) after updates/upgrades of the GRUAN GOASS, addressed in Section 3.7. The GOASS must be transparent, i.e., developed and optimized in consultation with WG-GRUAN members. WG-GRUAN shall meet regularly to discuss the implementation of updates to the GOASS, whether they pertain to one site or the entire ozonesonde network. Planned changes in data processing algorithms should be dealt with in a fashion similar to planned changes in SOPs (Section 7.4).

Changes in the GOASS may be due to the following:

1. New or modified transfer functions (Section 7.2)
2. Updated uncertainty calculations (Section 6)
3. Changes in the pump efficiency factors (Section 2.5)
4. Changes in the partial ozone column calculation above balloon burst (Section 2.7)
5. Changes in the Metadata (Section 3.6)

Changes resulting in (2) – (5) will likely result in the complete reprocessing of entire data sets across the network. Since there is a time and administrative cost associated with the reprocessing of a record, such reprocessing should only be undertaken when justified. Protocols must be established by the designated Lead Centre ozonesonde data processing facility to indicate when reprocessing of the full measurement record at any site is justified or required.

Traceability is a leading component of GRUAN. Every single GOASS update must be associated with an increment of the data processing version. A system of traceable version numbers for all ozonesonde level products has been developed to allow for a full identification and tracking of the data processing changes made since the initial product delivery. This product versioning system shall be determined by the Lead Centre task team.
Data processing updates must be communicated to users who have accessed earlier versions of the data and who have voluntarily registered to receive notifications of such data updates (see Section 8.6 of the GRUAN Guide). Therefore, all older product versions must be made available through the GRUAN archives.
7.6 Managing changes in calibration

When ozonesondes are calibrated to fundamental calibration standards as part of the pre-flight ground-check, changes in sonde performance can be more easily managed. If possible, the impacts of a change in calibration should be quantified through traceability of the calibration standard. For example, the WCFOS in JOSIE studies satisfies the protocols for maintaining ozonesonde continuity, accuracy and integrity through periodic quality checks of instrumental performance of ozonesonde from different manufacturers, and establishing up-to-date SOPs. It would ideal to establish guidelines by which a GRUAN Ozonesonde Programme can calibrate its ground station equipment such that sources of error and uncertainty can be further identified, traced, and included as part of the uncertainty budget for ozonesondes. Metadata provides a traceable source from which a change in the essential characteristics of each unique ozonesonde sensor can be identified, measured, and recorded (essential metadata are addressed in Section 3.6).

7.7 Validating changes using parallel observations

Cases where parallel observations are applicable to the ozonesonde programme are the following (hereafter called “4 cases”):

- A new ECC sensor is developed
- A new sensing solution recipe is developed
- Change in SOPs
- Change in radiosonde manufacturer and/or model

If any of the above changes occur, a combination of JOSIE studies, other laboratory inter-comparisons, and dual sonde launches must be made to establish (1) new precision and accuracy estimates, if any, (2) changes in uncertainties, and (3) new transfer functions to maintain homogeneity within a time series of a single site and within the network. While these studies are proposed and conducted, the regular observations schedule must not be interrupted. In the case when laboratory studies cannot be reconciled, this must be noted as part of the metadata. In this case, a proposal of how to resolve the discrepancy should be developed by the Lead Centre or a task force commissioned by the Lead Centre.

Measurement redundancy: Measurement redundancy (see Section 6.2 of GCOS-171) highlights the benefits for managing instrumentation change. If parallel observations of the above four changes are not feasible, the availability of additional redundant measurements with similar sampling attributes (vertical resolution, temporal sampling frequency etc.) is essential for validating a managed change. In such cases, an evaluation of the redundant system(s) with the old and new systems over an overlap period of at least 12-months must be undertaken to validate the robustness of change management.

Inter-comparisons: Formal measurement inter-comparisons, in the form of dual ozonesonde launches are essential for developing the in depth understanding required to manage changes in the “four cases”. For this reason, participation in inter-comparisons is expected. Outcomes from
such inter-comparisons must form an important component of the metadata archived at the
GRUAN Lead Centre. GRUAN Ozonesonde Programme should participate in, or leverage from
WMO and partner networks (e.g. SHADOZ and NDACC) instrument inter-comparison
campaigns.
7.8 Implementation of Network-wide changes

Considering the critical importance of change management and that GRUAN sites must not act unilaterally in implementing changes, a procedure for implementing network-wide changes has been described in Section 2.3.11 of the GRUAN Guide to Operations.

Managing change is essential to maintaining network homogeneity. Changes in ozonesonde measurement systems, i.e. the “9 items”, at GRUAN sites should therefore be conducted in such a way that the homogeneity of the resultant GRUAN ozone data products across the network is not compromised. The Lead Centre shall play a key role in ensuring such smooth transitions. In particular changes in (1) and (2) of the “9 items” will require network-side changes to ensure homogeneity.

The Lead Centre should consult with ozonesonde experts (e.g. members of the ASOPOS panel), science experts from the four key user communities, and other ozonesonde archive centres such as SHADOZ and NDACC to thoroughly evaluate the potential implications of network-wide implementation of the proposed change. If the proposed change is approved, the Lead Centre, in consultation with the nominated central processing facility, will develop a formal change plan for implementation across the network. The formal change plan is then communicated to all GRUAN ozonesonde sites within the network. Any changes or deviations from the documented approvals must be considered a new change and must be reassessed by the Lead Centre.

However, changes are not necessarily always network-wide. In some circumstances, changes to an individual site are allowed which do not compromise network homogeneity, for instance changes in instrument or solution concentration, a change in instrument operators, or change of operating environment. Documentation of these site changes in the form of metadata is essential. Sites will be audited on the completeness of their metadata submitted to GRUAN archives as part of the site assessment and certification process. Also see #9 in Section 7.1 Supporting reprocessing.

7.9 Data and metadata traceability

It is essential that metadata associated with the site and each ozonesonde instrument launched, and in particular change events (see Section 7.1) that may cause discontinuities in the measurement time series, are captured. Sufficient metadata must be available to tie the new SGDP via a comparable traceability chain, back to the same recognized standard as the old SGDP.

Storage: It is essential that a secondary back-up storage of raw data (L0 PRD) be maintained at each GRUAN site. Metadata on written on check lists should be digitized and stored similarly with the raw data. Each sites data storage policy shall be evaluated by the WG-GRUAN as part of the site assessment and certification process (Section 3.2), and re-evaluated in audits and annual reports.
Launch scheduling: Measurement scheduling shall remain stable unless there is a clear requirement for change. Amendments to the GRUAN measurement scheduling protocol shall be submitted by the WG-GRUAN before being distributed to GRUAN sites for implementation. In recognition of the heterogeneity of the network, the scheduling protocols defined in this Document may not apply at every GRUAN site, but any deviation from the measurement schedule must be agreed by the GRUAN Lead centre and then accepted by WG-GRUAN.

Metadata changes from the GRUAN check list: As described in Section 3.6, while using the GRUAN check list is not mandatory, sites are required to document where they have deviated from the prescribed check list and, when audited, are assessed for their ability and willingness to adhere to them within GRUAN.

Importance of Metadata: Metadata is a critical component when documenting network changes. Complete metadata should include a full account of the ozonesonde operation from the time the sensor is taken out of its' box to the time of launch release. Detailed archiving of instrument metadata will be vital to managing changes in instrumentation. This will allow later reprocessing of the raw data as thoroughly as possible (see Section 2.3.4 of GCOS-171). A detailed description of how each change in a measurement system was managed can be found in the GRUAN check list (Appendix A-1) and a complete list of the essential metadata components is in Section 3.6. These metadata lists include everything related to the quantitative assessment of the impact of the change on the measurement and its uncertainty.
8 QUALITY MANAGEMENT

This section defines the principles and the methodological framework for GRUAN operations, and details how activities will be coordinated to manage and control data quality within GRUAN. This section draws heavily from Section 10 of GCOS-171 and reiterates much of the data management policies central to all GRUAN measurement programmes.

Quality management within GRUAN consists of quality assurance and quality control:

Quality assurance (QA): The purpose of quality assurance is to provide confidence that the requirements for achieving quality will be fulfilled. QA includes all the planned and systematic activities that will be implemented such that quality requirements for a product or service will be fulfilled.

Quality control (QC): The purpose of quality control is to ensure that the expectations created by QA are fulfilled. QC is associated with those operational methods, techniques and activities used to ensure that the quality requirements (as defined by QA) are fulfilled.

The GRUAN quality management policy is to achieve a level of data quality that allows the primary goals of GRUAN to be met for all potential users of GRUAN data products. Quality assurance i.e. implementing systems to ensure quality, and quality control i.e. monitoring the results to ensure that the systems implemented are adequate to the task, are both required at all stages of the GRUAN ozonesonde data production. Because GRUAN ozonesonde data products are intended to be used for long-term trend detection, quality assurance and control are further extended to data re-processing and to the management of long-term consistency and stability (addressed in Section 7 of this Document).

Methods by which QA for Ozonesonde Programmes can be achieve is through the following:

1. The use of redundant measurements, as described in Section 4.1.2, serves to assure the quality of the GRUAN data products. Agreement of two independent measurements (e.g. Lidar and Microwave Radiometer), preferably based on different measurement principles, provides a high degree of confidence that no significant systematic effect was disregarded and uncertainties were not underestimated.

2. Laboratory tests are fundamental methods for establishing and confirming uncertainty estimates and transfer functions for GRUAN data products. Laboratory tests provide an opportunity to investigate in detail the performance of instruments under controlled conditions and to measure differences against certified references or other standards (e.g. JOSIE). Data from these experiments can be used to detect biases that may be corrected for and to determine calibration uncertainties.

3. Field inter-comparisons (dual or multi sonde launches on a single payload) allow multiple in-situ sensors to be directly compared under the actual atmospheric conditions of the required measurement, including the complex environmental conditions (temperature, humidity, pressure, wind/flow rate, radiation, and chemical composition) that cannot be fully reproduced in the laboratory. These complementary activities increase confidence...
that measurements are subject to neither unanticipated effects nor undiscovered systematic uncertainties. Therefore field experiments are particularly useful for assuring the quality of GRUAN data products.

QC will be achieved through the application of the various measurement protocols defined in this Document and in related measurement system documents (e.g. Lidar, Radiosonde technical documents). To the extent possible, visual inspection of all data by science/instrument experts will be required for ozonesondes to minimize anomalies that slip through automated routines. The Lead Centre shall coordinate this effort, which shall be distributed across different GRUAN sites and other interested parties as deemed appropriate including task teams and members of WG GRUAN. Vertically resolved uncertainty estimates, calculated by the GOASS for each site, will be used as a metric to compare the site to site quality of the observations.

Quality management is required at all points in the measurement process from network planning and training, through installation and site operations to data transmission and archiving. This quality management must include feedback and follow-up provisions across a range of timescales from sonde conditioning to annual reviews. Because of the emphasis on the provision of robust measurement uncertainties and the associated requirement for in-depth quality management, the resources required within GRUAN to undertake quality management will likely be a significant proportion of the cost of operating the network, and very likely more than the few percent of overall operating costs typical of many observational networks. However, without this expenditure, the quality of the data will be unknown, and their usefulness diminished.

A key aspect of quality management within GRUAN will be fulfilling customer requirements. To this end systems shall be developed to:

1. Inform users of GRUAN products of changes in measurements systems at specific sites.
2. Provide an incident reporting system that can flag data anomalies to users.
3. Inform users of the availability of updates to previously accessed data products.
4. Provide “help desk” support to users of GRUAN data products.
5. Establishing close working relationships with instrument manufacturers will also be central to quality assurance within GRUAN.

8.1 Assuring the quality of GRUAN Ozonesonde Programmes

The purpose of quality management is to ensure that GRUAN data meet the requirements in terms of uncertainty, resolution, continuity, homogeneity, representativeness, timeliness, format etc. for their intended use, at a minimum practicable cost. GRUAN recognizes that all measurements are imperfect, but, if their quality is known and demonstrable, they can be used appropriately. Minimizing cost without compromising quality is also an implied or explicit requirement for measurements made within GRUAN.

Five critical components are required to assure the long-term quality of GRUAN Ozonesonde Programmes include:
1. Maintaining consistent, up-to-date SOPs to minimize systematic errors and lend confidence in the observed trends.

2. GRUAN-specific training of the representative and ozonesonde technicians of candidate ozonesonde sites, the purpose of which is to ensure that the latest GRUAN-recommended best practices for ozonesonde operations are observed.

3. The RSLaunchClient utility, the purpose of which is to upload, the raw measurement data and metadata to the GRUAN central ozonesonde data processing facility.

4. The GOASS, the purpose of which is to analyses in a consistent manner the converted raw ozonesonde data (CRD) through the RSLaunchClient, and to calculate the ozonesonde SGDP and their uncertainties.

5. Maintaining documentation and statistics on flagged metadata (addressed in Section 3.7), and missing raw data to be used as a diagnostic tool as part of the quality control assessment and to ensure the continuity of individual GRUAN Ozonesonde Programmes.

Routine testing of newly manufactured ozonesondes, changes in instrument design or solution recipes will help to ensure confidence in observed trends in the future. Therefore, as part of the quality assurance (QA) for ozonesondes that are in routine use, GRUAN shall follow protocols established by the Forschungszentrum Jülich which houses the World Calibration Center for Ozone Sondes (WCCOS) [http://www.fz-juelich.de/iek-8/EN/Expertise/Infrastructure/WCCOS/WCCOS.html?nn=865134]. The simulation facility enables control of pressure, temperature and ozone concentration and can simulate flight conditions of ozone soundings up to an altitude of 35 km, whereby a UV photometer serves as a reference [Smit et al., 1998]. The long term objective of WCCOS is to ensure the major QA-tasks:

1. QA-Procedures: Establishment and up-date of SOPs of different sonde types.
2. QA-Manufacturers: Performance check of ozonesondes from different manufacturers
3. QA-Operation: Evaluation of ozonesonde operating practice of difference sounding laboratories

8.2 Raw data validation

Quality control at the raw data level is performed in two steps, first through uploads of the most recently acquired raw data and associated metadata through the RSLaunchClient utility, then through the threshold quality checks at the early processing stage of the GOASS (selection criteria are addressed in Table 3.7.1 of Section 3.7). The suitability check of the raw data and metadata to be accepted as part of the GOASS processed stream serves as a means to verify the completeness of the information required by the RSLaunchClient.

8.3 Ozonesonde data product validation

Ozone profiles derived from GRUAN Ozonesonde Programmes will, in the first instance, be validated against available redundant ozone profile measurements made at GRUAN sites (refer to Section 4.1.2). Multiple measurements of ozone will be invaluable for identifying, understanding and reducing systematic effects in ozonesonde measurements. One important factor for GRUAN is that redundant measurements of the same (or related) variables should be
reported in a consistent way. The cross checking of redundant measurements for consistency should be an essential part of the GRUAN quality assurance procedures. Since all data are to be reported with uncertainties, a consistency check should, in principle, be a straight forward task.

Satellite-based measurements of total column ozone (e.g. OMI, GOME-2) and profiles of ozone in the lower stratosphere (e.g. Aura/MLS) are common reference measurements that can be used to assess the quality of ozonesonde observations. GRUAN shall, where practical, schedule ozonesonde launches in near real-time (i.e. within 2 hours of a satellite overpass) to fulfill the requirement of providing a reference to satellite measurements.

In addition, GRUAN Ozonesonde Programmes are encouraged to participate in field campaigns involving non-GRUAN instruments. All comparisons should be made between measurements independent from each other. If two measurements are known to be dependent, the degree of this dependence as well as its consequences must be specifically described and taken into account in the product assessment. As stated in Section 10 of the GCOS-171, “Agreement of two independent measurements, preferably based on different measurement principles, provides a high degree of confidence that no significant systematic effect was disregarded and uncertainties were not underestimated”.

### 8.4 Performance monitoring system

Applying the principles described in Section 10 of the GCOS-171 to GRUAN Ozonesonde Programmes, performance monitoring is a non-real-time activity in which the performance of an individual GRUAN Ozonesonde Programme, or of an ensemble of GRUAN Ozonesonde Programmes, is examined for trends and systematic deficiencies. Performance monitoring within GRUAN Ozonesonde Programmes is primarily the responsibility of the Lead Centre and the TTS.

Certification and re-certification of GRUAN Ozonesonde Programmes is an essential component of performance monitoring. Examples of quantitative performance indicators are:

1. **Ozonesonde SGDP downloads**
2. **Number of candidate sites wishing to become a GRUAN Ozonesonde Programme.**
3. **Number of GRUAN sites participating in JOSIE and inter-comparison field campaigns, and conducting laboratory studies whose results appear in peer reviewed journals.**
4. **The number of peer reviewed publications in which GRUAN ozonesonde data products have been used.**
5. **The number of GRUAN Ozonesonde Programmes funded through national or international funding agencies.**

All above indicators serve to provide a year-to-year traceability of GRUAN ozonesonde programmes' impact within the climate community.
<table>
<thead>
<tr>
<th>ACRONYMS</th>
<th>Definition</th>
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<tr>
<td>ASOPOS</td>
<td>Assessment of Standard Operating Procedures for Ozone Sondes</td>
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<td>BESOS</td>
<td>Balloon Experiment on Standards for Ozone Sondes</td>
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<tr>
<td>CRD</td>
<td>Converted Raw Data</td>
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<tr>
<td>DMT</td>
<td>Droplet Measurement Technologies</td>
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<tr>
<td>ECC</td>
<td>Electrochemical concentration cell</td>
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<td>ECV</td>
<td>Essential Climate Variable</td>
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<tr>
<td>GATNDOR</td>
<td>GRUAN Analysis Team for Network Design and Operations Research</td>
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<tr>
<td>GAW</td>
<td>Global Atmosphere Watch</td>
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<tr>
<td>GCOS</td>
<td>Global Climate Observing System</td>
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<td>GOASS</td>
<td>Ozonesonde Analysis Software System</td>
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<td>IGACO</td>
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<td>IGPD</td>
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<td>Intergovernmental Oceanographic Commission</td>
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<td>JOSIE</td>
<td>Jülich Ozone Sonde Inter-comparison Experiment</td>
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<tr>
<td>LMS</td>
<td>Lockheed Martin Sippican</td>
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<tr>
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<td>Network for the Detection of Atmospheric Composition Change</td>
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<td>National Center for Atmospheric Research</td>
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<td>WOUDC</td>
<td>World Ozone and Ultraviolet Data Centre</td>
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Appendix A.1: GRUAN STANDARD OPERATING
PROCEDURES CHECK LIST

Follows the WMO GAW Report #201 SOPs

INITIAL PREPARATION - NO LESS THAN 3 DAYS BEFORE FLIGHT.

OPERATOR INITIALS: _____
FLT # ____________
DATE (YYYYMMDD): ________________________
O₃ PUMP SERIAL #: ____________________

1. Run 10 minutes on no O₃ air: ____ (√)
2. PUMP CURRENT: __________ (µA)
3. PUMP PRESSURE: __________ (psi)
4. PUMP VACUUM: __________ (in Hg)
5. Run 30 minutes on HIGH O₃: ____ (√)
6. Run 5 minutes on no O₃: ____ (√)
7. ADD 3.0 CC FRESH CATHODE (Wait 2 min): ____ (√)
8. ADD 1.5 CC ANODE SOLUTION: ____ (√)
9. Run 10 minutes on no O₃: ____ (√)
10. RECORD O₃ CURRENT: _______ µA
11. Run 5 minutes at 5µA O₃ ____ (√) - then switch to no O₃ air.
12. RECORD TIME TO DROP FROM 4 TO 1.5 µA: ____ sec.
13. Run 10 minutes on no O₃: ____ (√)
14. RECORD O₃ CURRENT: _______ uA

For refurbished sensors, follow calibration procedures.

15. Add additional 2.5 cc of CATHODE: ____ (√)
16. Short the cell leads: ____ (√)
17. Intake tube stored in sonde frame: ____ (√)
18. Store inside Styrofoam flight box: ____ (√)

IF DORMANT AFTER 1 WEEK REPLACE SOLUTIONS.

DATE (YYYYMMDD) : ____________________

1. CHANGE CATHODE SOLUTION (3cc): ____ (√)
2. CHANGE ANODE SOLUTION (1.5cc): ____ (√)
3. Run 5 minutes on no O₃: ____ (√)
4. RECORD O₃ CURRENT: _______ μA
5. Run 5 minutes on 5µA O₃: ____ (√)
6. Switch to no O₃: ____ (√)
7. RECORD TIME TO DROP FROM 4 TO 1.5 µA: _____ sec
8. Run 10 minutes on no O₃ – RECORD CURRENT: _____ uA
9. Short cell leads and Store in Styrofoam flight: ____ (√)
IF DORMANT AFTER ANOTHER WEEKS REPLACE SOLUTIONS.

DATE (YYYYMMDD) : _____________

1. CHANGE CATHODE SOLUTION (3cc): _____ (√)
2. CHANGE ANODE SOLUTION (1.5cc): _____ (√)
3. Run 5 minutes on no O₃: _____ (√)
4. RECORD O₃ CURRENT: _______ µA
5. Run 5 minutes on 5µA O₃: _____ (√)
6. Switch to no O₃: _____ (√)
7. RECORD TIME TO DROP FROM 4 TO 1.5 µA: _____ sec
8. Run 10 minutes on no O₃ – RECORD CURRENT: ______ uA
9. Short cell leads and Store in Styrofoam flight: _____ (√)

DAY OF FLIGHT PREPARATION IN LAB:

DATE (YYYYMMDD): _____________
OPERATOR INITIALS: _____

1. CHANGE CATHODE SOLUTION (3cc): _____ (√)
2. CHANGE ANODE SOLUTION (1.5cc): _____ (√)
3. Run 10 minutes on no O₃: _____ (√)
4. RECORD O₃ CURRENT: BG#0 = _______ µA
5. Run 10 minutes at 5µA O₃: _____ (√)
6. Switch to no O₃: _____ (√)
7. RECORD CURRENT AFTER 30 Sec ______ µA, 1min______ µA, 2min______ µA
8. 3min______ µA, 5min______ µA, 10min______ µA
9. RECORD O₃ CURRENT: BG#1 = _______ µA
10. ROOM TEMP (C): _______ , ROOM RH (%): _______,
     ROOM Pressure (hPa)__________
11. RECORD T100 FLOWRATE TIMES:
     FLOWRATE #1: _______ sec
     FLOWRATE #1: _______ sec
     FLOWRATE #1: _______ sec
     FLOWRATE #1: _______ sec
     FLOWRATE #1: _______ sec
     AVERAGE T100:__________ sec

DAY OF FLIGHT AT THE LAUNCH SITE:

FLT #: __________________
OPERATOR INITIALS: _____

Dobson (if available): _______________(DU)
Brewer (if available): _______________(DU)
Other (if available): _______________(DU)

RADIOSONDE SERIAL #: ___________________
O<sub>3</sub> BACKGROUND CURRENT BEFORE FLIGHT BG#2: __________ µA

GMT Date (YYYYMMDD): ______________________

GMT Launch Time (HH:MM:SS): _______________

LOCAL date (YYYYMMDD): ____________________

LOCAL Launch time (HH:MM:SS): ______________

BALLOON SIZE: ___________ Grams:

TYPE: TOTEX ____ Hwoyee ____ PAWAN ____ (√ one)

SURFACE PRESS: ___________ (hPa)  SURFACE WIND SPEED: _________ (m/s)

SURFACE TEMP: _____________ (C)  SURFACE WIND DIR: ___________ (deg)

SURFACE RH: _________________ (%)

Sky Conditions and General Remarks:
Appendix A.2: RECOVERED OZONESONDE CHECKLIST

Follows the NOAA/ESRL/GMD Check list

DATE (YYYYMMD): ______________
OPERATOR INITIALS: ________

Was this a GPS Sonde recovered on day of flight? _____ Yes/No
If No, how many days between launch and recovery? ___ days

HISTORY:
O$_3$ PUMP SERIAL #: ______________
FORMER FLIGHT #: ______________
DATE FLOWN (YYYYMMDD): ______________
DATE FOUND (YYYYMMDD): ______________
DATE RETURNED (YYYYMMDD): ______________

COMMENTS: OVERALL SONDE/PUMP CONDITION: (looks new, dirt or coloring around pump present, signs of corrosion anywhere, 0-ring condition, pump noisy?, etc.)

INITIAL RINSE/RECONDITIONING – SOON AFTER DELIVERY:

Check that the cam that drives the piston is not turning off-center, loose or rubbing too close to the metal frame. If it is too close or has come loose then the sonde will be noisy and run with a high current. Sonde should not be flown in this case.

Rinse off outside of cells with warm tap water. ____ (√)
Squirt De-ionized water (DIW) through running pump inlet (2 or 3 times for about 5 seconds). ____ (√)
Rinse cells and tubing with DIW. ____ (√)
Fill cells about ¾ full of DIW. ____ (√)
Store sheet and ozonesonde until ready for the 3-7 day pre-condition. ____ (√)
Date stored on shelf until ready for the 3-7 day pre-condition (YYYYMMDD):
______________
During normal pre-conditioning preparations, an ozone calibrator, e.g. TEI, is strongly recommended to test the performance of the refurbished sonde. Re-conditioned sondes should not be flown if the sonde values are ±5% of calibrated source.

PRE-CONDITIONING CALIBRATION PROCEDURES:

DATE (YYYYMMDD): ______________________
Operator Initials: ______

Calibration Instrument/Model:_____________________________
Calibration Serial Number: _________________________

1. Run 50 ppbv O$_3$ for 10 minutes: _____ (√)
2. Record: CALIBRATOR: ______ ppbv OZONESONDE: ______ ppbv % Difference: ___
3. Run 100 ppbv O$_3$ for 10 minutes: ____ (√)
4. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: __
5. Run 150 ppbv O$_3$ for 10 minutes: ____ (√)
6. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ___
7. Run 200 ppbv O$_3$ for 10 minutes: ____ (√)
8. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ___
9. Run 50 ppbv O$_3$ for 10 minutes: ____ (√)
10. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ___
11. Run no ozone air for 10 minutes: ____ (√)
12. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ___

If the percentage differences for the 100 ppbv and ozone-free air exceeds ±5% do not fly re-used sonde.

FINAL COMMENTS:
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Komhyr, W. D. (1986), Operations handbook – Ozone measurements to 40-km altitude with model 4A electrochemical concentration cell (ECC) ozonesonde (used with 1680 MHz radiosondes), NOAA Tech. Memo. ERL ARL-149, Air Resources Lab., Boulder, CO.


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