

GRUAN OZONESONDE TECHNICAL DOCUMENT

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Purpose of this Guide

This Document of 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 traceable 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 atmospheric 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

45 random and systematic uncertainty and long-term stability for the operations of all ozonesonde
46 instruments in use at GRUAN sites. This Document establishes the philosophy under which
47 GRUAN ozonesondes shall operate. It informs current and future GRUAN sites of the expected
48 *modus operandi* for ozonesonde operations at GRUAN sites. The overall framework under
49 which an ozonesonde will operate in GRUAN is hereafter referred to as the ‘GRUAN
50 Ozonesonde Programme’.

51 The GRUAN community is not the international authority on ozonesonde operations. This
52 Document has been developed in close collaboration with international leaders in the
53 development of ozonesonde standard operating procedures (SOP). These are the principles in the
54 WMO ozonesonde community (Dr. H. Smit/Research Centre Jülich GmbH, and collaborators
55 who developed ASOPOS), the Network for Detection of Atmospheric Composition Change
56 (NDACC) working group, and the principles in the Southern Hemisphere Additional
57 OZonesondes (SHADOZ) network.

58
59 Relevant information from this GRUAN Ozonesonde Technical Document is expected to be
60 incorporated into the WMO Manual on the Global Observing System (WMO-No. 544) and the
61 Guide on the Global Observing System (WMO-No. 488). This Guide may be additionally
62 supported by a series of technical documents listed on the GRUAN web site at
63 <http://www.gruan.org>.

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147 1. INTRODUCTION

148 1.1. Ozonesonde heritage

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

159
160 The effects of ozone are not always positive. Ozone is a key component of photochemical smog
161 and high levels of ozone are associated with poor air quality. The common saying is that ozone is
162 'nice from far but far from nice'. Ozone in the troposphere also acts as a strong oxidizer and this
163 removes many compounds, including toxic substances, from the air. Ozone levels therefore play
164 a role in determining the tropospheric lifetimes of many compounds. Ozone is also a greenhouse
165 gas, absorbing outgoing infrared radiation from Earth's atmosphere. Because of its importance
166 both as an absorber of incoming solar UV radiation, and as an absorber of outgoing infrared
167 radiation, it is essential that changes in ozone concentrations throughout the atmosphere are
168 carefully monitored.

169
170 The vertical distribution of ozone in the atmosphere can be monitored using a range of different
171 techniques including satellite-based (solar occultation, limb-sounding, nadir viewing)
172 instruments, balloon-borne *in situ* instruments (ozonesondes, dropsondes), and ground-based
173 remote sensing systems (lidars and microwave radiometers). Ozonesondes fulfil an important
174 role in this suite of techniques by providing very high vertical resolution ozone profiles from the
175 surface to the middle stratosphere (30-35 km) with small measurement uncertainties, capable of
176 making measurements during periods of no sunlight, and can be easily deployed from remote
177 locations such as ships or small islands.

178
179 A number of quasi-independent ozonesonde measurement programmes have been established
180 globally to monitor changes in the vertical distribution of ozone. The WMO/GAW¹, NDACC,
181 and SHADOZ communities have established an expert panel, ASOPOS (Assessment of Standard
182 Operating Procedures for Ozonesondes), to develop standard operating procedures for
183 ozonesonde measurement programmes. This Document builds considerably on the large body of
184 material already developed by ASOPOS [Smit et al., 2012].

185
186 Because long-term satellite-based measurements of ozone in the troposphere and upper
187 troposphere/lower stratosphere (UTLS) are not currently available, the ozonesonde record
188 provides the primary source for deriving ozone trends in the troposphere and UTLS, especially in
189 the climate sensitive region around the tropopause. When combined with satellite-based

1 A complete list of all acronyms appearing in this Document is provided at the end of the document.

190 measurements of ozone, ozonesondes can provide a global, multi-decadal data set extending
191 from the surface to the mesosphere for long-term ozone trend detection (Bodeker et al., 2012).

192
193 There are challenges in making ozonesonde measurements such that they will meet the needs of
194 GRUAN users (see Section 1.2). Most ozonesondes are only flown once, making re-calibration
195 of the hardware impossible. Pre-flight calibration and quality checks of the hardware are
196 essential. Ensuring inter-instrument calibration in an environment where instruments from
197 different manufacturing batches may show systematic biases (Smit et al., 2007), presents a
198 challenge.

199 **1.2. The purpose of ozonesondes within GRUAN**

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

- 201 i) Provide long-term high quality climate records;
- 202 ii) Constrain and calibrate data from more spatially-comprehensive global observing systems
203 (including satellites and current radiosonde networks); and
- 204 iii) Fully characterize the properties of the atmospheric column.

205 To achieve these goals with respect to ozone, sites within the network should provide vertical
206 profiles of reference measurements of ozone for reliably detecting changes in global and regional
207 climate, on multi-decadal time scales, for major climatically distinct regions of the globe.

208 Changes in ozone, both in the stratosphere and troposphere are known to drive changes in global
209 and regional climate. Reference within GRUAN means that, at a minimum, the observations are
210 tied to a traceable standard, that the uncertainty of the measurement has been determined, and
211 that the entire measurement procedure and set of processing algorithms are properly documented
212 and accessible (Immler et al., 2010).

213
214 Potential uses of such ozonesonde measurements include:

- 215
216 i) Providing measurements at GRUAN sites that complement the priority 1 measurements of
217 temperature, pressure and water vapour and priority 2 measurements of ozone.
218 Understanding changes in the vertical distribution of ozone is required to understand
219 changes in the vertical distribution of temperature.
- 220 ii) Providing high-resolution profile measurements of ozone that are not possible with current
221 satellite-based measurements.

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

- 224 i) The climate detection and attribution community. Understanding changes in the vertical
225 distribution of ozone is essential to understanding changes in the thermal structure of the
226 atmospheric column.
- 227 ii) The satellite community. Validating satellite-based measurements of ozone is recognized as
228 an essential requirement of the GRUAN ozonesonde programme.
- 229 iii) The atmospheric process studies community. High vertical resolution measurements of the
230 ozone profile, with well-resolved measurement uncertainties, provide key data for

231 understanding atmospheric processes. Many aspects of stratospheric dynamics and the
232 dynamics associated with stratosphere-troposphere exchange can be studied using ozone
233 profiles from ozonesondes. Ozonesonde measurements have played a key role in
234 determining ozone loss rates in the Arctic vortex (Rex et al., 1998).

235 iv) The numerical weather prediction (NWP) community.

236 **1.3. Organization and design of the GRUAN Ozonesonde Programme**

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

240 **1.3.1. Terminology**

241 *A GRUAN Ozonesonde Programme* is an ozonesonde measurement programme implemented at
242 a site and having been assessed and certified as defined in Sections 4.1 and 4.2.

243
244 *A GRUAN Ozonesonde instrument* is one of the instruments employed in a GRUAN ozonesonde
245 programme. These are balloon-borne electrochemical concentration cell (ECC) ozone sensors
246 that measure high vertical resolution profiles of ozone, pressure, temperature, and relative
247 humidity. ECC ozone sensors are described in Section 2.1

248
249 *A GRUAN Ozonesonde Product* is an ozone product resulting from the measurements made
250 within a GRUAN ozonesonde programme. A GRUAN Ozonesonde Product is always produced
251 by the GRUAN Ozonesonde Analysis Software System (GOASS, see Section 4.7) designed to
252 implement the requirements and recommendations defined in this document.

253 **1.3.2. Responsibilities**

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

259
260 GRUAN sites hosting a GRUAN Ozonesonde Programme shall use a designated system of
261 methods, techniques and facilities in full compliance with the requirements and
262 recommendations detailed in this document. For any given GRUAN Ozonesonde Programme,
263 this system will not be changed without advanced notice to the TTR and GRUAN Lead Centre.
264 GRUAN Ozonesonde Programmes incorporate a programme to validate the stability and
265 uncertainty of the measurements, agreed with WG-GRUAN, and managed in detail by the
266 GRUAN TTR and GRUAN Lead Centre. This assurance programme comprises three mandatory
267 components, which are the GRUAN *Standard Operating Procedures* (SOP) for all GRUAN
268 ozonesonde instrument calibration (described in Section 4.5), the RSLaunchClient (described in
269 Section 4.6), and the GOASS (described in Section 4.7).

270
271 The design of GRUAN Ozonesonde Programmes shall recognize the heterogeneity of the
272 network of sites, many of which will have primary responsibility to networks other than

273 GRUAN. GRUAN Ozonesonde Programmes shall integrate, where possible and when feasible,
274 with other international long-term monitoring programmes.

275
276 GRUAN Ozonesonde Programmes shall be responsive to the latest technological and scientific
277 progress in ozonesonde measurement techniques and observational requirements. Non-GRUAN
278 ozonesonde development work can continue at a GRUAN site in collaboration with the TTR
279 until mature and validated, at which point any improvements can be introduced into GRUAN
280 operations with the agreement of the TTR and GRUAN Lead Centre.

281
282 WG-GRUAN, the GRUAN Lead Centre and TTR will act as the interfaces between GRUAN
283 and the community of users of GRUAN ozonesonde products.

284 **1.4. Implementation of GRUAN Ozonesonde Programmes**

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

289
290 The WG-GRUAN and TTR shall use this Document which establishes standard operational
291 procedures (SOP) and metadata requirements for all GRUAN Ozonesonde Programmes. The
292 TTR shall evaluate the appropriateness of uncertainty estimates, the usefulness of particular
293 measurements and operational procedures, synthesize the available knowledge, and develop
294 recommendations to improve GRUAN measurements and operations. The TTR and WG-
295 GRUAN shall confer regularly to evaluate the current status of GRUAN observations, to identify
296 weaknesses, and to incorporate new scientific understanding into GRUAN. The expertise of
297 these teams shall also be used to support the Lead Centre in guiding individual sites through
298 changes in instrumentation and operating procedures without impacting long-term measurement
299 time series.

300
301 The GRUAN Lead Centre shall identify sites where instrument operators need training, re-
302 training, and organise cost-efficient training courses for the network at appropriate locations, as
303 advised by the appropriate TTR, to encourage uniformity of instrument operation between sites.
304 The Lead Centre may liaise with National Metrological Institutes in this regard.

305
306 All activities associated with the implementation of GRUAN are the responsibility of the
307 institution/organization hosting the GRUAN site and should, as far as possible, be met through
308 national funding. To best serve the needs of the climate monitoring and research communities, it
309 is essential that GRUAN is cognizant of the evolving science that drives the measurements and
310 accuracy of the GRUAN data. The ozonesonde instrumentation deployed and the observing
311 schedules may differ among sites, as agreed with WG-GRUAN as part of the site assessment and
312 certification process, but the practices are expected to be uniform among all GRUAN sites.

313 **1.5. Links to partner networks and satellite-based measurement**
314 **programmes**

315 In the original charter for GRUAN (GCOS-92) it is stated that ‘where feasible, the GRUAN sites
316 should be co-located and consolidated with other climate monitoring instrumentation’. GRUAN
317 Ozonesonde Programmes shall not be run in isolation of existing ozonesonde networks and
318 GRUAN is not intended to replace existing networks. GRUAN Ozonesonde Programmes are
319 likely to operate within the framework of existing networks such as the Network for the
320 Detection of Atmospheric Composition Change (NDACC) and SHADOZ (Southern Hemisphere
321 Additional OZonesondes), and to leverage off the expertise available in these networks and e.g.
322 through the GAW (Global Atmosphere Watch²) scientific advisory group for ozone. As a result,
323 close and regular coordination between the governing bodies of these networks and with the
324 WG-GRUAN and GRUAN TTR+AM is required. This coordination can be achieved by having
325 members of the WG-GRUAN and TTR+AM attend steering group meetings of partner networks
326 and by inviting co-chairs or steering group members from partner networks to attend WG-
327 GRUAN and GRUAN TTR+AM meetings.

328 **1.5.1. NDACC (Network for the Detection of Atmospheric Composition Change)**

329 NDACC comprises more than 70 remote-sensing research sites for observing and understanding
330 the physical and chemical state of the stratosphere and upper troposphere and for assessing the
331 impact of stratospheric changes on the underlying troposphere and on global climate. A number
332 of NDACC sites fly ozonesondes and NDACC has a standing Sonde Working Group on
333 ozonesondes, water vapor sondes, and aerosol sondes.

334 **1.5.2. GAW (Global Atmosphere Watch)**

335 GAW is a coordinated network of observing stations, associated facilities, and related scientific
336 assessment activities that supply basic information to be used by policy-makers [Global
337 Atmosphere Watch Guide, GAW Report No.86, 1993]. GAW does not provide or archive
338 observations, but serves an important link between end users and high quality data networks that
339 include world data centres, such as the WOUDC (World Ozone Ultraviolet Data Centre) and
340 other archives, such as SHADOZ.

341 **1.5.3. Atmospheric Radiation Measurement (ARM) Programme**

342 The goal of the U.S. Department of Energy ARM programme is to study changes in climate, land
343 productivity, oceans or other water resources, atmospheric chemistry, and ecological systems
344 that may alter the capacity of the Earth to sustain life. This includes improving the atmospheric
345 data sets used in regional and global climate models. A primary objective of the ARM user
346 facility is to improve scientific understanding of the fundamental physics related to interactions
347 between clouds and radiative processes in the atmosphere.

348

349 A dedicated Data Quality (DQ) Office provides ARM with a number of tools to ensure the high
350 quality of the collected data. The potential use of these tools in GRUAN must be explored to
351 ensure network-wide homogeneity of the GRUAN ozonesonde measurements. The ARM DQ

² http://www.wmo.ch/web/arep/gaw/gaw_home.html

352 Office has developed a suite of sophisticated data quality visualization tools that may be of
353 interest to GRUAN Ozonesonde Programmes.

354 **1.5.4. SHADOZ (Southern Hemisphere ADditional OZonesondes)**

355 SHADOZ (Southern Hemisphere ADditional OZonesonde) is a project to augment and archive
356 ozonesonde data from over a dozen tropical and sub-tropical sites and has become the central
357 repository for vertical profiles of ozone in the tropics/sub-tropics. Prior to the creation of
358 SHADOZ, tropical ozonesonde data were accessible via campaigns or collaborative associations
359 with specific operating site representatives. Started in 1998 by NASA's Goddard Space Flight
360 Center, and other US and international co-investigators, SHADOZ is an important tool for
361 equatorial tropospheric ozone research. The rationale for SHADOZ is to: (1) validate and
362 improve model and remote sensing techniques for estimating tropical ozone, (2) contribute to
363 climatology and trend analyses of tropical ozone and (3) provide research topics to scientists and
364 educate students, especially in participating countries [Thompson et al., 2003a; 2003b, 2004,
365 2007, 2012]. SHADOZ functions as a data service to the global scientific community by
366 providing a central public archive location via the internet: <http://tropo.gsfc.nasa.gov/shadoz>.
367 SHADOZ data are mirrored at the Aura Validation Data Center (AVDC) and are deposited to
368 WOUDC. While the SHADOZ website maintains a standard data format for the archive, it also
369 informs data users of the differing sites' preparation techniques and data treatment. Data from
370 launches from various related field campaigns, such as, the Indian Ocean Experiment
371 (INDOEX), Sounding of Ozone and Water in the Equatorial Region (SOWER) and Aerosols99
372 Atlantic Cruise are also available.

373 **1.5.5. Satellite-based measurement programmes**

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

388 2. GRUAN OZONESONDE TECHNIQUES AND 389 MEASUREMENT PRINCIPLES

390 This section provides the GRUAN Ozonesonde Programmes and user community with essential
391 knowledge of the way ozonesondes measure profiles of ozone. For further comprehensive
392 reviews of the ozonesonde measurement technique, the reader should refer to the publications
393 mentioned in this section.
394

395 Ozonesondes are small, lightweight balloon-borne instruments that use an electro-chemical
396 technique to make in situ measurements of ozone from the surface of the Earth to an altitude
397 determined by balloon burst, typically 30 to 35 km [Smit et al., 2002]. The ozonesonde is
398 interfaced to a standard meteorological radiosonde for transmission of the data to the ground and
399 is usually flown together with the radiosonde as part of the same package. The package is carried
400 aloft by a rubber balloon similar to that used for radiosonde measurements, though in this case a
401 1000-1500 g balloon is typically used rather than the standard 300 g meteorological balloon. The
402 package ascends through the atmosphere at $\sim 5\text{-}7\text{ m.s}^{-1}$ and, with a measurement frequency of ~ 1
403 second, results in a vertical measurement resolution of less than 10 m (however, sensor time-
404 constants expand this, typically by a factor of 10). Ozonesondes constitute the most important
405 data source with long term-data coverage for the derivation of ozone trends with sufficient
406 vertical resolution, particularly in the important, climate sensitive, altitude region around the
407 tropopause.
408

409 As defined in GCOS-171:

410 “A reference measurement result typically arises from a defined measurement procedure
411 that involves standards traceable to national or international standards as maintained at National
412 Metrological Institutes (NMIs). For GRUAN, a reference measurement is one where the
413 uncertainty of the calibration and the measurement itself is carefully assessed. This includes the
414 requirement that all known biases have been identified and corrected, and, furthermore, that the
415 uncertainty on these bias corrections has also been determined and reported. An additional
416 requirement for a reference measurement is that the measurement method and associated
417 uncertainties should be accepted by the user community as being appropriate for the
418 application.”
419

420 To produce GRUAN ozonesonde reference measurements, mandatory and recommended
421 processing procedures have been established such that the ozonesonde data products derived
422 shall be reproducible at any time in the future. Section 2 describes the data processing procedures
423 required for each component of the ozonesonde measurement technique. The GRUAN
424 Ozonesonde Programmes and centralized ozonesonde data processing facility shall apply these
425 procedures to create the standard reference GRUAN ozonesonde data product (see Sections 4.5 -
426 4.7).
427

428 As of the time of the development of this Technical Document, the Electrochemical
429 Concentration Cell (ECC) sonde (Komhyr, 1969) is the dominant type of ozonesonde being
430 flown world-wide and therefore this document focusses solely on SOP for the ECC sonde type.
431 Brewer-Mast (BM) type sondes (Brewer and Milford, 1960) are flown operationally only at the
432 Hohenpeissenberg, Germany station. ECCs have replaced the Japanese manufactured Carbon

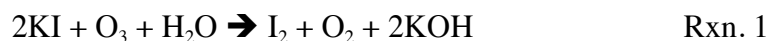
433 Iodide (CI) sonde (Kobayashi and Toyama, 1966). Little is known about the Indian-sondes
 434 which are flown exclusively in India. The homogenization of time series that have used BM and
 435 ECC sondes at the Uccle, Belgium, site has been first undertaken by De Backer [1999] using
 436 results from dual BM/ECC sonde launches [De Backer et al., 1998], then recently by Van
 437 Malderen et al. [2016] – see also Section 7.2 on the use of transfer functions for homogenizing
 438 time series that include BM and ECC sondes. Dual flight campaigns at the Payerne, Switzerland,
 439 site showed no detectable differences between their BM and ECC sondes [Stübi et al., 2008].
 440 Since the late 2000s, Japanese sites have switched from using CI sondes to using ECC sondes.
 441 Although Nakamura et al. [2008] conducted inter-comparison studies for CI and ECC sondes,
 442 transfer functions between the two sensors have not yet been derived.

443 **2.1. The ozonesonde measurement**

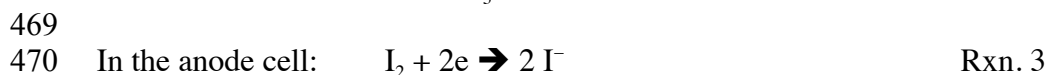
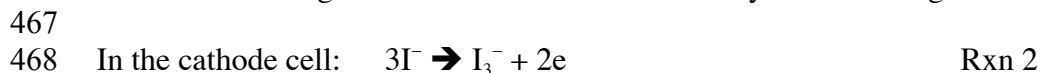
444 The ECC instrument consists of a non-reactive teflon gas-sampling pump connected to an ECC
 445 ozone sensor, and an electronic interface that connects the ozone sensor to a radiosonde for data
 446 telemetry (see Figure 1 of Komhyr, 1995). The instrument is encased in a polystyrene
 447 weatherproof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

451
 452 The ECC sensor measures ozone using iodine/iodide electrode reactions [Vetter, 1967]. Two
 453 platinum electrodes are immersed in separate cathode and anode chambers made of Teflon, also
 454 called half cells, of differing concentrations of potassium iodide (KI) solution. The anode cell
 455 contains a solution saturated with KI. Both cells contain an equal concentration of potassium
 456 bromide (KBr) and a phosphate buffer to maintain a neutral pH. An ion bridge connecting the
 457 two chambers allows ions to flow between the two cells but prevents mixing, thereby preserving
 458 their respective concentrations.

459
 460 Ambient air containing ozone (O_3) is pumped into the cathode cell and reacts with iodide (I^-) to
 461 form iodine (I_2) based on the aqueous reaction:



464
 465 To maintain electrochemical equilibrium iodine is converted back to iodide on the platinum
 466 electrode resulting in the release of two electrons by the following reactions:



473
 474 Rxn 2 and 3 are rate determining reactions and result in the transfer of ion to the electrode
 475 surfaces. An equilibrium exists between I_2 and I_3^- (tri-iodide) when the concentrations of I^- are
 476 kept constant.

477

478 As a result of the reactions detailed above, each ozone molecule entering the sensor causes two
479 electrons to flow through the ECC's external circuit, which are measured as a current. The
480 resulting electrical current is linearly proportional to the concentration of ozone in the sampled
481 air. The electrochemical technique assumes no secondary reactions take place and a 1:1
482 stoichiometric relationship of the I₂:O₃ ratio is maintained. The relationship between ozone and
483 the electrical current (measured in μA) is computed using:

$$484 \quad P_{O_3} = 4.307 \times 10^{-4} (I_M - I_{BG}) T_p \Phi_{Ground} \psi \quad \text{Eqn. 1}$$

485 where,

486 P_{O_3} = Ozone partial pressure (mPa)

487 I_M = Cell current (μA)

488 I_{BG} = Cell background current (μA)

489 T_p = Ozonesonde pump temperature (K)

490 Φ_{Ground} = Pump flow rate at the ground (s/100cm⁻³)

491 ψ = Pump flow conversion efficiency (1/pump flow correction factor, unitless)

492 The constant, 4.307×10^{-4} , is the half ratio of the ideal gas constant to Faraday's constant.
493 Measurement techniques and uncertainty estimates for each variable in Eqn. 1 are reviewed
494 below. The cell current, I_M , and pump temperature, T_p , are in situ measurements while the cell
495 background current, I_B , and flow rate, Φ_{Ground} , are measured during pre-flight preparations under
496 ambient laboratory conditions and are assumed to remain constant throughout the flight. While it
497 is preferable that the conversion efficiency, ψ , be determined for each flight, unless automated,
498 this can be very time consuming and as a result ψ values are usually taken from a table of pump
499 flow measurements made at varying low pressures to account for the decrease in pump efficiency
500 at low pressures. Uncertainties on ψ are expected to be smaller if they are determined
501 individually for each flight rather than taken from a table (which needs to also provide the
502 statistical uncertainty on the ψ values). ψ values vary with ECC sensor type and are further
503 explained in Section 2.5.

504 **2.2. Measuring the background current**

505 The background current (I_B) is the residual current measured by the sonde when sampling ozone-
506 free air. Conventional processing of the sonde telemetry assumes that the background current
507 remains constant during flight and the same assumption is made when processing ozonesonde
508 data within GRUAN. As seen in Equation 1, the background current is subtracted from the ECC
509 sensor current to infer the ozone partial pressure. In the initial conditioning procedure, both
510 cathode and anode cells are filled with sensing solution and stored for no less than 3 days prior to
511 launch to reduce the background current and improve the sensor response time (i.e. the time it
512 takes for the sensor electronics to respond to a change in ozone concentration) [Kohmyr, 1986;
513 1997]. Kohmyr and Harris [1971] show that the background current decreases after the ECC is
514 stored for several days while charged with their working solutions; they call this process 'self-
515 cleaning'.

516 **GRUAN protocols for measuring background current**

517

523 GRUAN follows the WMO/GAW SOP for background current measurement [Smit et al. 2014]
524 requiring three background measurements as detailed below.
525

- 526 • Initial conditioning, i.e. the conditioning procedures when the sensor is first taken out of the
527 box, shall occur no less than 3 days before the ozonesonde flight because this is the minimum
528 acceptable period for the background current to decrease to within the thresholds defined
529 below.
530
- 531 • Day of flight preparations shall be made no more than 7 days after the initial conditioning. If
532 more than 7 days have elapsed, then the cathode and anode chambers should be replaced with
533 fresh solution and a repeat of the response time test steps should be done.
534
- 535 • I_{B0} is recorded when the calibration/ozonizer unit is used to run ozone-free air through the
536 sensor, filled with fresh solution, after 10 minutes.
 - 537 ○ Following BESOS procedures [Deshler et al, 2008] ozone-free air is run through the
538 sensor until the background no longer drops or until the background current is less
539 than $0.05 \mu\text{A}$.
 - 540 ○ If the background current does not drop below $0.05 \mu\text{A}$ after 20 minutes, the solutions
541 must be changed and the background current measurement repeated. If, after another
542 20 minutes, the background does not fall below $0.05 \mu\text{A}$ the final value should be
543 recorded in the metadata check list, regardless. Ideally, these steps should bring I_{B0}
544 below the $0.05 \mu\text{A}$ threshold value.
545
- 546 • I_{B1} is recorded after the response time measurement, i.e. the time required for the sensor
547 current to drop from $4 \mu\text{A}$ to $1.5 \mu\text{A}$, and after an additional 10 minutes of ozone-free air has
548 been pumped into the cathode cell. This value may be higher than I_{B0} .
549
- 550 • I_{B2} is recorded prior to launch with the ozonesonde intake tube receiving ozone-free air from
551 the ozoniser or ozone destruction filter. This value may be higher than I_{B0} .
552

553 All three background currents shall be recorded by the GRUAN RSLaunchClient (see Section
554 3.6). Historically, operators have used I_{B2} as the value for I_B in Eqn. 1. In recent years other
555 methods of applying background currents have been employed, such as the minimum of the three
556 background currents [Ryan Stauffer/Penn State, personal communication], a laboratory
557 determined I_B [Holger Vömel/NCAR, personal communication], or I_B set to an upper limit value
558 for those background currents that exceed a maximum threshold based on average I_B measured
559 under optimal laboratory conditions [Bryan Johnson/NOAA, personal communication].
560

561 For the GRUAN central processing of ozonesonde flight data, operators should specify which
562 final I_B has been applied.
563

564 For stations that have on-going issues recording $I_{B2} < 0.05 \mu\text{A}$, GRUAN recommends using I_{B0}
565 as the final background current for the following reasons:
566

- 567 • The quality of the ozone destruction filter under launch conditions (non-laboratory
568 controlled environment) used to measure I_{B2} cannot be assured to be uniform between

569 flights which introduces a source of random uncertainty which cannot be easily
570 quantified [Reid et al., 1996]. This is particularly the case when ozonesondes are flown in
571 the tropics where high humidity affects the ozone removal efficiency of the filter
572 [Newton et al., 2016].

- 573 • The use of I_{B2} as the background current is likely an overestimate of the true background
574 current which then leads to an underestimate of the ozone partial pressure. In particular,
575 tropical and polar ozone profiles are strongly influenced by the magnitude of the
576 background current [Reid et al, 1996; Vömel and Diaz, 2010; Newton et al.; 2016].
577 Under mid-latitude and tropical conditions, Smit et al. [2014] show that background
578 currents ranging from 0.05 to 0.1 μA contribute 10-20% and 20-40%, respectively, to the
579 measured cell current in the free troposphere.
- 580 • I_{B1} is excluded as an option since it can be biased high. The 10-minute flow of ozone-free
581 air after ozone exposure is arbitrary and likely not representative of the true background
582 current [Thornton and Niazy, 1982; Vömel and Diaz, 2010; Bryan Johnson/NOAA,
583 personal communication]. Laboratory experiments by Vömel and Diaz [2010] identified
584 the decay of the cell current after exposure to ozone and showed that the current does not
585 relax to pre-ozone values after 10 minutes of ozone-free air and that a much longer period
586 of time (hours) is required to approach initial values. The BESOS field campaign
587 [Deshler et al, 2008] found similar enhancements in the background current after ozone
588 exposure. The elevated cell currents indicate a slower decay in the sensor response
589 suggesting that the flushing of ozone-free air for 10 minutes through the cells is not long
590 enough to reduce the cell current to pre-ozone exposure values.
- 591 • A field study conducted by Newton et al. [2016] found stable low background currents
592 when the ozone exposure test during the day of flight preparations was ignored.

593
594 Using I_{B0} ensures that background currents are measured under stable, controlled laboratory
595 conditions where uncertainties can be more robustly quantified.

596
597 When I_{B0} exceeds 0.05 μA the following steps shall be taken:

- 598 1. If a solution change, followed by a reasonable length of time running zero ozone air does
599 not bring I_{B0} below 0.05 μA , then the minimum of I_{B0} , I_{B1} , and I_{B2} shall be used as I_B .
- 600 2. If the minimum background current is still greater than 0.05 μA , then the profile data
601 shall not be accepted and zero-air from the ozonizer and destruct filter should be checked
602 and possibly replaced.

603
604
605 GRUAN will apply a constant background current correction following WMO/ASOPOS
606 guidelines [Smit et al. 2012; 2014]. Thornton and Niazy [1982] showed that sensors in the early
607 1980s exhibited negligible sensitivity to O_2 allowing the background current to be treated as a
608 constant. More recent studies support this finding [Smit et al, 1994; Reid et al. 1996; Newton et
609 al., 2016]. Vömel and Diaz, [2010] introduced a modified ozone partial pressure equation that
610 takes into account the excess ozone response due to the buffering of the solution. They measured
611 uncertainties of 0.005 μA for a 1% full buffer solution and 0.009 μA for a 0.5% half buffered
612 solution.

613

614 Any changes to the treatment of ozonesonde background currents to those described above must
 615 be founded on JOSIE-type experiments, followed by rigorous assessment and peer-reviewed
 616 publication.

617 **2.3. Effects of different sensing solutions and ozonesonde type**

618 While the fundamental chemistry and operating mechanics of the ECC sonde have remained
 619 largely unchanged, the KI solution concentrations have varied over the past decades in attempts
 620 to improve the measurement accuracy and stability. Inter-comparison campaigns and laboratory
 621 studies have been conducted to evaluate the ECC sonde performance using different sensing
 622 solution recipes with current sensor types [Hilsenrath et al., 1986; Boyd et al., 1998; Johnson et
 623 al., 2002; Smit et al., 2007; Deshler et al, 2008]. The JOSIE studies have shown that the
 624 precision and accuracy is strongly dependent on the ozonesonde type and solution [Smit et al.,
 625 2007]. JOSIE experiments reveal that differences in instrument construction between Science
 626 Pump Corporation (SPC) and EN-SCI ECC's significantly impacts the ozonesonde performance.

627
 628 There are a variety of sensing solution concentrations and pH buffers used in ECC sondes (see
 629 Table 2.3.1) The anode solutions are prepared by saturating the cathode solution with KI
 630 crystals.

631
 632 Table 2.3.1

Sensing Solution Type	KI, g/L	pH Buffer, g/L	
		NaH ₂ PO ₄ •H ₂ O	Na ₂ HPO ₄ •12H ₂ O
1.0% KI, full buffer	10	1.25	5.0
0.5% KI, half buffer	5	0.625	2.5
2.0% KI, no buffer*	20	0	0
1.0% KI, 1/10 th buffer*	10	0.125	0.5

633 * Used at some NOAA-supplied ozonesonde stations only.

634
 635 The 1.0% KI with full pH-buffer is the conventional cathode sensing solution used for the
 636 ozonesonde types SPC-4A, -5A, and -6A [Science Pump Corporation manual, 1996]. Until
 637 1996, ENSCI advocated using the 1.0% solution formula but then switched to recommending a
 638 0.5% KI with half pH-buffer sensing solution formula after 1996 [ENSCI Corporation manual,
 639 1996]. Johnson et al. [2002] introduced the 2.0% non-pH-buffered solution with no KBr that all
 640 NOAA-led ozonesonde stations used for a period of almost 10 years in the late-1990s to mid-
 641 2000s. This was followed by a switch to a modified 1.0% KI solution using a 1/10th buffer
 642 cathode sensing solution recipe. The 2.0% no-buffer solution formula is no longer recommended.
 643 The 1.0% KI with 1/10th buffer sensing solution is a relatively new formula and has yet to be
 644 included in JOSIE-led evaluation studies. Thus, until the latter solution is fully evaluated, only
 645 the 0.5% half buffer and 1.0% full buffer sensing solutions shall be used in GRUAN, following
 646 WMO/GAW recommendations and as detailed in Table 2.3.2.

647
 648 Table 2.3.2 Table of ECC sensors and solution pairing.

Manufacturer/Model	Solution concentration
SPC 6A	1%, full buffer
ENSCI Z, 2Z	0.5%, half buffer

649
650 The JOSIE-2000 experiment focused on combinations of ECC sensors and sensing solution
651 types to determine the optimal pairing when compared with the calibration standard UV-
652 photometer. Results show a reduction in biases for SPC sondes when using the 1.0% KI solution
653 with full buffer pair and for ENSCI sondes that use a 0.5% KI solution with half buffer solution.
654 JOSIE results showed that the SPC/1.0% and ENSCI/0.5% pairings behave similarly, i.e.
655 measurement differences are within 1.0%.

656

657 **Homogenizing records that use different sensing solutions**

658

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

665

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

674

675 To support the homogenization of ozonesonde measurement series whose homogeneity is
676 compromised by historical changes in sensing solutions, the ASOPOS working group, as part of
677 the SPARC/IGACO-O3/IOC/NDACC (see Acronyms) initiative, has established transfer
678 functions based on JOSIE experiments [Smit et al., 2007] for a variety of ECC sensor type and
679 solution strength combinations. Their use allows homogenization of long-term records to
680 conform to either an SPC/1.0% or ENSCI/0.5% sensor/solution pairing (Refer to Section 8.1.2,
681 Table 3 of Smit et al. [O3S-DQA, 2012] for conversion factors). Section 7.2 provides further
682 details and processing protocols involving transfer functions. Deshler et al. [2017] provides a
683 detailed description on the derivation of the transfer functions for the standard pairings, i.e.
684 SPC/1.0%, ENSCI/0.5%.

685

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

688

689

690

691

692

693

- 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.

- 694 • A new model is developed or a new manufacturer enters the ECC market that
- 695 recommends a new sensing solution recipe.
- 696 • An existing model is discontinued, forcing transition to a different model.

697
 698 Changes in ozonesonde working solutions must be managed through an appropriate change
 699 management programme whereby the necessary tests, laboratory studies, and dual sonde launch
 700 campaigns are conducted to characterize any systematic biases, and their uncertainties, in the
 701 stoichiometry and response times at all pressure altitudes (see Section 6 on the uncertainty
 702 budget). Sites undergoing such change management shall also participate in developing transfer
 703 functions required to maintain the homogeneity in the data record.

704
 705 Ozonesonde expertise outside of GRUAN shall also be used to support the Lead Centre in
 706 guiding individual sites through changes in instrumentation without impacting long-term
 707 measurement time series.

708 **2.4. Measuring pump flow rate**

709 A common procedure in the ECC conditioning is to use the soap bubble flowmeter method to
 710 measure the volumetric flow rate of the pump [sec/100ml]. The required equipment and set-up
 711 are described in the ENSCI and SPC manuals [DMT manual, Appendix D, 2014; SPC manual
 712 Section 3.2.1, 1999]. Several flow rates are measured and the mean is assigned as the measured
 713 flowrate, Φ_{Measured} , applied in Equation 1. The uncertainty of the flow rate is small, generally
 714 within $\pm 1\%$ [Smit et al., 2014].

715
 716 The GRUAN procedure for determining pump flow rate is as follows:

- 717 1. The flowmeter equipment provided by ENSCI and SPC is standard and reasonably identical.
 718 GRUAN will accept either.
- 719 2. GRUAN acknowledges that the soap bubble solution recipe varies among manuals and
 720 operators and requires only that the same recipe is used throughout the lifetime of the
 721 measurement record.
- 722 3. The measurement of the flow rate shall be made five times as required by WMO/GAW and
 723 implemented in most SOP.
 - 724 i. Flow rates that differ by ± 2 sec/100ml or more from the median after measuring the
 725 flow rate five times should be repeated.
 - 726 ii. Mean Φ_{Measured} should be between 26 and 32 sec/100ml.
 - 727 • Lower and upper limits are chosen by consulting pump flow rate ranges
 728 found in the SPC manual [1999] and Smit et al., [2014].
 - 729 • If the mean Φ_{Measured} is not within the acceptable range, this must be recorded
 730 in an appropriate data QA/QC flag.
- 731 4. The corrected pump flow rate at the ground is expressed as:

732
 733
 734 Eqn 2.4.1 $\Phi_{\text{Ground}} = [1 + C_{\text{PL}} - C_{\text{PH}}] \cdot \Phi_{\text{Measured}}$

735

736 Where C_{PL} is the correction for the temperature difference between the internal pump base
 737 temperature and the ambient room temperature, and C_{PH} corrects for the evaporation of the soap
 738 bubble solution (see Komhyr et al. [1995], Johnson et al. [2002], and Smit et al., [2014]).
 739 GRUAN shall follow ASOPOS equations to determine C_{PL} and C_{PH} .
 740
 741 Section 6.3 addresses the flow rate uncertainty and its contribution to the ozone measurement
 742 uncertainty.

743 **2.5. Estimating degradation in pump efficiency**

744 It has been well documented that the efficiency of the ECC pump decreases at high altitudes
 745 [Komhyr, 1967; 1969; 1986; et al. 1995; Johnson et al., 2002; Smit et al., 2014]. Johnson et al.
 746 [2002], and references therein, cite pump leakage, dead volume in the piston pump, and back-
 747 pressure exerted on the pump by the cell solution as main causes of pump efficiency loss at low
 748 pressures. Experiments reveal that the pump flow rate, Φ , measured at the ground is constant up
 749 to 100 hPa and decreases steadily to the top of the atmosphere. This is true for the pumps used in
 750 both SPC and ENSCI ozonesondes.

751
 752 Calculated ozone partial pressures must therefore include a correction for the effects of pump
 753 efficiency loss. From Equation 1 (in Section 2.1), the pump flow conversion efficiency, Ψ
 754 (1/pump correction factor), takes into account the efficiency loss in Φ as a function of pressure.
 755 Empirical averages obtained from various lab techniques have yielded pump correction factors
 756 (PCF; Komhyr [1986]; Komhyr et al. [1995]). The two most widely used PCF are shown in
 757 Table 2.5.1. However, both PCF have been calculated based on SPC ECC type and models older
 758 than SPC 6A and the sample sizes are small (e.g. K95 N = 13). GRUAN recommends laboratory
 759 studies with statistically significant sample sizes of the standard ECC types/models currently in
 760 use to verify or update these PCF and their uncertainties.
 761

Pressure [hPa]	Komhyr, 1986 (K86)	K86 uncertainty, $\Delta\Psi$	Komhyr et al., 1995 (K95)	K95 uncertainty, $\Delta\Psi$
Sfc-100	1.000	1.000	1.000	1.000
100	1.007	± 0.005	1.007	± 0.005
50	1.018	± 0.006	1.018	± 0.005
30	1.022	± 0.008	1.029	± 0.008
20	1.032	± 0.009	1.041	± 0.012
10	1.055	± 0.010	1.066	± 0.023
7	1.070	± 0.012	1.087	± 0.024
5	1.092	± 0.014	1.124	± 0.025
3	1.124	± 0.025	1.241	± 0.043

762 Table 2.5.1 Pump corrections factors (PCF) with 1-sigma uncertainties. PCF values are taken
 763 from the GAW Report No. 201, Table 3-3 [Smit et al., 2014].
 764

765 Following the recommendations of WMO/GAW report 201 [Smit et al., 2014], GRUAN
 766 Ozonesonde programmes shall use the K86 PCF for SPC ozonesondes and K95 PCF for ENSCI
 767 ozonesondes as listed in Table 2.5.1. PCF between tabulated values must be interpolated on a log
 768 pressure scale with 2nd order polynomial interpolation.

769 **2.6. Measuring pump temperature**

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

778
 779 Table 2.6.1

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

780
 781 Smit et al. [2014] considers the correct or 'true' T_p as the pump temperature measured in the
 782 vicinity of the moving piston, T_{piston} . Based on Komhyr and Harris [1971] and JOSIE 2000 lab
 783 experiments [Smit et al., 2007], empirical pressure dependent equations have been formulated to
 784 adjust pump temperatures from Cases 1 through 4 to an internal pump based temperature (Case
 785 5). Internal pump temperatures are considered to be the best approximation to the 'true' T_p .

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

790 Case 1: Equation 2.6.1

- 791 (a) $T_{P_{case1}} = 7.43 - 0.393\text{Log}_{10}(P)$ $P \geq 40$ hPa
 792 (b) $T_{P_{case1}} = 2.7 - 2.6\text{Log}_{10}(P)$ $6 < P < 40$ hPa
 793 (b) $T_{P_{case1}} = 4.5$ $P \leq 6$ hPa

794

795 Case 2, 3: Equation 2.6.2
 796 (a) $T_{P_{\text{case}2,3}} = 20.6 - 6.7\text{Log}_{10}(P)$ $P > 70$ hPa
 797 (b) $T_{P_{\text{case}2,3}} = 8.25$ $15 \leq P \leq 70$ hPa
 798 (c) $T_{P_{\text{case}2,3}} = 3.25 - 4.25\text{Log}_{10}(P)$ $5 \leq P < 15$ hPa
 799

800 Case 4: Equation 2.6.3
 801 (a) $T_{P_{\text{case}4}} = 6.4 - 2.14\text{Log}_{10}(P)$ $P > 40$ hPa
 802 (b) $T_{P_{\text{case}4}} = 3.0$ $3 \leq P \leq 40$ hPa
 803

804 Case 5: No adjustment, i.e. $T_{P_{\text{case}5}}=0.0$
 805

806 The additional correction to account for differences between T_{piston} and the internal pump, or
 807 pump based, temperatures is described as:
 808

809 Equation 2.6.4 $T_{\text{piston-internal}} = 3.9 - 0.8\text{Log}_{10}(P)$
 810

811 Note that equations 2.6.1 to 2.6.4 were derived from small statistical samples (Equation 2.6.4
 812 from a sample of only three ECC sondes in the JOSIE chamber experiments; Figure 9 from Smit
 813 et al. [2007]). The adjustment formulae for Cases 2 and 3 were derived from a sample size of
 814 eight, while only three sondes were used to generate the Case 4 formula. The uncertainties
 815 inherent in the small samples underlying equations 2.6.1 to 2.6.4 must be propagated through to
 816 the uncertainties in the derived ozone partial pressures. Section 6.5 summarizes the pump
 817 temperature uncertainty parameters and equations and how these contribute to the ozone partial
 818 pressure uncertainty.
 819

820 The ASOPOS panel recommends that the final adjusted pump temperature, T_p , be used to
 821 calculate the ozone partial pressure, should be defined as:
 822

823 Equation 2.6.5 $T_p = T_{\text{measured}} + T_{P_{\text{case}_i}} + T_{\text{piston-internal}}$
 824

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

827 **2.7. Determining the partial ozone column above the top of flight**

828 GRUAN's purpose for calculating total column ozone for each profile is to allow for
 829 comparisons against an independent spatially and temporally co-located total column ozone
 830 measurement to provide a means of validating the quality of the ozonesonde ozone profile. The
 831 standard technique for computing total column ozone from an ozonesonde measurement includes
 832 adding a climatological ozone partial column value above the balloon burst altitude. Most often,
 833 these partial columns are based on satellite and ozonesonde observations [McPeters et al, 1997,
 834 2007, 2012; Labow et al., 2015], although some sites have developed their own monthly
 835 climatologies, e.g. based on microwave radiometer-derived ozone profiles. Comparisons of the
 836 integrated ozonesonde ozone profile plus the partial column above the top of flight can then be
 837 made with ground-based and satellite measurements of total column ozone (e.g. Dobson
 838 spectrophotometer, Brewer spectrometer, OMI, GOME-2).
 839

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

844

845 The GRUAN ozonesonde data product shall adopt the following guidelines:

- 846 • The integrated ozone column amount (in DU) up to 10 hPa or balloon burst, whichever is
847 lower. Profiles above 10 hPa have high uncertainty due to the degradation of the pump
848 efficiency [Witte et al., 2017].
- 849 • Total column ozone from ozonesondes shall only be calculated where the balloon bursts
850 above the ozone peak.
- 851 • The ozone residual column amount (in DU) above burst pressure and ozone peak can use
852 the McPeters et al. [2012] climatology, an updated version, or a site-specific climatology
853 shall that has been peer-reviewed and shown to be as accurate, of not more so, than
854 commonly used ozone residual climatologies.
- 855 • It is recognized that there may be gaps in the profile measurements due to intermittent
856 telemetry. Profiles with large data gaps shall be identified and evaluated on a case-by-
857 case basis and the flight total column ozone value and, importantly, its uncertainty,
858 calculated according.
- 859 • If available, co-located ground-based or space-based measurements of total column
860 ozone shall be included.

861 **2.8. Dependence on the radiosonde**

862 Radiosonde pressure and temperature measurements are used to calculate the geopotential
863 heights. Thus, radiosonde measurement errors will cause the measured ozone to be assigned
864 incorrect altitudes and pressures. As with ozonesondes, there are a number of radiosonde
865 manufacturers whose instruments have changed in model, material, and algorithm since the
866 1970s. There are measurable differences between manufacturers, i.e. Vaisala vs iMET (Stauffer
867 et al., 2014), and between models, i.e. Vaisala RS-80 vs RS-92, that impact the ozonesonde
868 measurement, particularly at low pressures [Smit et al., 2014; and references therein]. GRUAN
869 shall document radiosonde manufacturer, model and type of interface so that appropriate
870 calibrations and corrections to the pressure and temperature, as well as RH, can be made in the
871 pre- and post-processing calculations of the geopotential height.

872

873 **GRUAN procedure protocol**

874

- 875 • Calibration of the radiosonde surface pressure, temperature, RH and determination of any
876 offset between geopotential and GPS height measurements, if and when available, shall
877 follow the processing guidelines dictated by the GRUAN Radiosonde Technical
878 Document.
- 879 • Handling biases in the geopotential height calculation in the absence of GPS
880 measurements shall be the responsibility of the Task Team Radiosondes, WG-GRUAN,
881 and Lead Centre.

- 882 • Radiosonde/Ozonesonde offsets in height and pressure, if any, shall be documented and
883 geopotential heights shall be recalculated by the Lead Centre GOASS (refer to Section
884 3.7).
- 885 • Quantifying the contribution of the radiosonde uncertainty to the ozone measurements, if
886 any, shall be the responsibility of the Task Team Radiosondes, WG-GRUAN, and Lead
887 Centre.

888 **2.9. Conversion efficiency**

889 One of the terms in the ozone uncertainty calculation is the contribution of the uncertainty in the
890 conversion efficiency. The conversion efficiency refers to 1:1 ratio assumed in the $I_2:O_3$
891 relationship. Interferences with this one-to-one relationship can arise from the buffering of the
892 solution [Johnson et al. 2002; Vömel and Diaz, 2010]. The cathode solution contains a buffer of
893 sodium-hydrogen phosphate to maintain the solution concentration and a neutral pH of 7.0
894 during flight. GRUAN shall follow a half buffered cathode solution for ENSCI sensors and a full
895 buffer for SPC, as recommended by WMO/ASOPOS [Smit et al., 2012; 2014]. Johnson et al.
896 [2002] performed stoichiometric sensitivity and pH tests and measured excess ozone at low
897 pressures due to the buffering effect. This would yield an $I_2:O_3$ relationship larger than unity.
898 This offset in the stoichiometry has been documented by others (Smit et al., 2014, section 3.2.2
899 and references therein; Johnson et al, 2002, section 2.1 and references therein). In the ozone
900 partial pressure equation, Equation 1, the conversion efficiency is assumed to be unity and is
901 therefore excluded from the equation. However, the uncertainty of this unity assumption can be a
902 significant contributor to the ozone uncertainty estimates and is addressed in Section 6.6.

903 **2.10. Transfer Functions**

904 There have been a number of studies that have used laboratory, dual-sonde, and multi-sonde
905 payloads to derive methods of calculating transfer functions that characterize differences in
906 instrument and solution concentration [Smit et al., 2007; Kivi et al., 2007; Deshler et al., 2008;
907 Stübi et al., 2008; Mercer et al., 2008; Deshler et al., 2017].

908
909 As part of the SPARC-IGACO-IOC-NDACC (SI2N) initiative, the Assessment of Standard
910 Operating Procedures for Ozone Sondes (ASOPOS) working group established empirical
911 transfer functions specifically for the SPC and ENSCI type ozonesondes using either the 1% full
912 buffer or 0.5% half buffer solutions [Smit et al., 2012]. These formulae are based on work done
913 by Deshler et al., [2017] which uses all data taken from the above campaigns. Their aim is to
914 homogenize long-term ozonesonde records that use these sensor/solution combinations for ozone
915 assessments of changes in the vertical distribution of ozone [[http://igaco-
916 o3.fmi.fi/VDO/documents.html](http://igaco-o3.fmi.fi/VDO/documents.html)].

917
918 These transfer functions represent the quantitative differences of the ozonesonde response based
919 on changes in instrumentation and stoichiometry of the conversion of O_3 to I_2 with a change in
920 solution concentration. They are not a reflection of changes in SOP. Smit et al. [2007] and
921 Thompson et al. [2007] showed that there are discontinuities in the time series of a single site
922 that have used a variety of instruments and solution strength, citing the need to homogenize the
923 long term records of individual ozonesonde sites. The conversion relationship is summarized in
924 Table 3 of Smit et al. [2012].

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GRUAN processing protocol

1. Where applicable, transfer functions derived by Deshler et al. [2017] shall be applied and be part of the ozonesonde Standard GRUAN Data Product (SGDP).
2. Data records where transfer functions should be applied but do not yet exist shall remain in the Level 2 stage and 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.

3. THE OZONE UNCERTAINTY BUDGET

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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 uncorrected and original ECC ozonesonde data to produce an ozonesonde 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. JOSIE (Jülich Ozonesonde Inter-comparison Experiment) has played a key role in describing/analyzing all sources of ECC 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.

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).

965 3.1. The ozone uncertainty equation

966 Since the 1990's tests conducted by JOSIE-led experiments, campaigns such as BESOS, and dual
967 flight experiments have clearly demonstrated the need to characterize singular features of the
968 ECC ozone sensors and standardize measurements. These activities have lead to the creation of
969 the ASOPOS panel whose goals are to (i) standardizing the ozonesonde conditioning and
970 preparation procedures, (ii) establishing guidelines for the reprocessing and homogenization of
971 ozonesonde data records, and (iii) determining the contributions of the individual uncertainties of
972 the different instrumental parameters to the ozone measurement. The treatment of uncertainty in
973 the GRUAN ozonesonde data processing will follow the recommendations and definitions of the
974 ASOPOS panel documented in Smit et al. [2012]. These uncertainty parameters are part of the
975 ozonesonde SGDP. We provide only a brief summary of uncertainty calculations derived for
976 each variable in the ozone partial pressure equation (Eqn. 1). GRUAN shall adopt the following
977 ozone uncertainty equation taken from Equation E-3-2 in Smit et al., [2012]:

978
979 Eqn. 3.1.1

$$980 \frac{\Delta P_{O_3}}{P_{O_3}} = \sqrt{\frac{(\Delta I_M)^2 + (\Delta I_B)^2}{(I_M + I_B)^2} + \left(\frac{\Delta \eta_C}{\eta_C}\right)^2 + \left(\frac{\Delta \Phi_{Ground}}{\Phi_{Ground}}\right)^2 + \left(\frac{\Delta T_P}{T_P}\right)^2 + \left(\frac{\Delta \Psi}{\Psi}\right)^2}$$

981
982

983 where the term, $\left[\frac{(\Delta I_M)^2 + (\Delta I_B)^2}{(I_M + I_B)^2}\right]$ is the contribution of the uncertainty in
984 background current, the $\left(\frac{\Delta \eta_C}{\eta_C}\right)^2$ term is the contribution of the conversion efficiency
985 uncertainty, the $\left(\frac{\Delta \Phi_{Ground}}{\Phi_{Ground}}\right)^2$ term is the pump flow rate uncertainty at the ground, the
986 $\left(\frac{\Delta T_P}{T_P}\right)^2$ term is the contribution of the pump temperature, and the $\left(\frac{\Delta \Psi}{\Psi}\right)^2$ term is the pump
987 flow correction factor uncertainties. Equation 3.1.1 is the sum of the squares of the uncertainty in
988 each term of the ozone partial pressure equation (Section 2.1, Eqn. 1). The uncertainties are
989 assumed to be random and gaussian and therefore follow the gaussian law of error propagation.
990 Each instrumental uncertainty term is discussed briefly in subsequent sections.

991 3.2. Contribution of the uncertainty in background current

992 The term $\left[\frac{(\Delta I_M)^2 + (\Delta I_B)^2}{(I_M + I_B)^2}\right]$ from equation 3.1.1 is the contribution of the uncertainty
993 in background current, where ΔI_M is the uncertainty in the measured current, I_M , and ΔI_B is the
994 uncertainty in the background current, I_B .

995

996 There is no standard or statistically robust method for estimating the uncertainty of the
997 background current. JOSIE experiments used small sample sizes, less than 14 ECC sensors, to
998 conduct the background current experiments published in Smit et al, [2007] and ultimately used
999 in the WMO/ASOPOS guidelines [Smit et al, 2012; 2014]. Results from Table 7 of Smit et al.
1000 [2007] record an average I_{B0} measurement ('background current before O₃-exposure') and 1-
1001 sigma uncertainty of $0.02 \pm 0.02 \mu\text{A}$ using ENSCI sensors with a 0.5% half buffer KI solution and
1002 $0.023 \pm 0.013 \mu\text{A}$ using Science Pump Corporation (SPC) sensors with a 1.0% full buffer KI
1003 solution.

1004

1005 Based on the JOSIE results above, for ozonesonde sites that use I_{B0} as their final background,
1006 GRUAN will adopt a $\pm 0.02 \mu\text{A}$ background current uncertainty, ΔI_B , for ENSCI 0.5% half buffer
1007 KI solution and a $\pm 0.013 \mu\text{A}$ uncertainty for Science Pump ECC 1.0% full buffer KI solution
1008 because there are no other uncertainty estimates for I_{B0} in the literature. Furthermore, there is the
1009 added complication that this is a single measurement per unique ECC sensor so uncertainties
1010 cannot be directly ascertained.

1011

1012 For sites that use I_{B2} as the final background current, GRUAN will adopt a $\pm 0.03 \mu\text{A}$ uncertainty
1013 for ENSCI/0.5% and $\pm 0.02 \mu\text{A}$ for SPC/1.0% based on results from Witte et al., [2017].

1014

1015 The uncertainty in the ozone current, ΔI_M , shall be set to $0.1 \mu\text{A}$ which is the resolution of the
1016 digital interface board (Terry Deshler/UWy and Herman Smit/Forchungszentrum, personal
1017 communication).

1018

1019 The uncertainty constants for the standard pairs are summarize in Table 3.1.1 below.

1020

1021 Table 3.1.1 Constants in the ozone current uncertainties for standard ECC/Solution pairs.

ECC/Solution	Final I_B	ΔI_B	ΔI_M
ENSCI/0.5%	I_{B0}	$\pm 0.02 \mu\text{A}$	$\pm 1\%$ of measured currents above $1 \mu\text{A}$, and $\pm 0.01 \mu\text{A}$ for currents below $1 \mu\text{A}$.
	I_{B2}	$\pm 0.03 \mu\text{A}$	
SPC/1.0%	I_{B0}	$\pm 0.013 \mu\text{A}$	
	I_{B2}	$\pm 0.02 \mu\text{A}$	

1022

1023 Background uncertainties outside the ENSCI/0.5% and SCP/1.0% pairs shall have to undergo
1024 similar rigorous testing to establish uncertainty estimates. In this case, profiles shall be archived
1025 until such time as background uncertainties can be establish and applied to create the ozonesonde
1026 SGDP. SGDP cannot be generated unless all uncertainty contributions to ozone in Equation 3.1
1027 are known.

1028 3.3. Contribution of the uncertainty in pump flow rate at the ground

1029 From Section 2.4 Equation 2.4.1 the final mean flow rate is corrected for the humidification
1030 effect, C_{PH} , and differences between the internal pump temperature and the ambient air, C_{PL} .

1031

1032 The full equation to calculate the pump flow rate uncertainty at the ground is expressed in the
1033 following equation

1034

1035 Equation 3.3.1
$$\frac{\Delta \Phi_{Ground}}{\Phi_{Ground}} = \sqrt{\left(\frac{\Delta \Phi_{Measured}}{\Phi_{Measured}}\right)^2 + (\Delta C_{PL})^2 + (\Delta C_{PH})^2}$$

1036

1037 The uncertainty in C_{PH} and C_{PL} are site specific. For existing sites that have established at least
1038 one year's worth of ozonesonde launches, i.e. a minimum of 24 total launches, relative
1039 uncertainties, ΔC_{PH} and ΔC_{PL} , can be calculated following Smit et al., [2012] recommendations
1040 (See section 8.4).

1041
 1042 For new GRUAN Ozonesonde Programmes with no launch history it is impossible to estimate
 1043 ΔC_{PH} and ΔC_{PL} . In this case, the term shall not be used in the ozone uncertainty equation until
 1044 after one years worth of ozonesonde launches have been processed by the GRUAN Lead Centre.
 1045 Until such time, profiles shall be archived until ΔC_{PH} and ΔC_{PL} can be calculated and then used to
 1046 create the ozonesonde SGDP. These terms will change as the data record expands, thus ΔC_{PH} and
 1047 ΔC_{PL} should be continually re-evaluated by the Ozonesonde Programmes annually to check for
 1048 large deviations from its constant value and assess whether and how fluctuations in the
 1049 uncertainty terms affect the ozone uncertainty significantly. It may be that re-processing of the
 1050 entire data record of a given site is required if ΔC_{PH} and ΔC_{PL} statistics changes significantly over
 1051 time.

1052 **3.4. Contribution of the uncertainty in pump correction factor (PCF)**

1053 The uncertainty in the pump correction factors (PCF), $\Delta\Psi$, shall be taken from Table 2.5.1.
 1054 Calculating $\Delta\Psi$ between data points shall be done on a log pressure scale with 2nd order
 1055 polynomial interpolation. The GRUAN GOASS shall use the following PCF uncertainties to the
 1056 following ECC sensors:

- 1057 (i) K86 $\Delta\Psi$ for SPC ECCs
- 1058 (ii) K95 $\Delta\Psi$ for ENSCI ECCs.

1059 New ECC sensors shall have to undergo similar JOSIE testing, laboratory and field tests to
 1060 establish and validate their PCF values and uncertainties. GRUAN protocols for managing a
 1061 change in sensor technology shall follow guidelines put forth in Section 7.1.

1062 **3.5. Contribution of the uncertainty in pump temperature**

1063 Calculating the adjusted pump temperature is discussed in detail in Section 2.6 and the
 1064 associated uncertainties are summarized in Table 3.5.1 below. Note that all units are in degrees
 1065 Kelvin.

1066
 1067 Table 3.5.1 Uncertainties based on the location of the pump temperature thermistor.

Case	Location	Sonde Type	ΔT_p	ΔT_{PCase}	$\Delta T_{Piston-internal}$
1	Bottom of circuit board	SPC 2A, 3A, 4A	$\pm 1.0K$	$\pm 1.0K$	$\pm 0.5K$
2	Suspended in the styrofoam box in the vicinity of the pump	SPC 5A	$\pm 0.5K$	3.9–1.13Log ₁₀ (P) for P > 70hPa 3.0–1.13Log ₁₀ (P) for P ≤ 70 hPa	$\pm 0.5K$
3	Taped thermistor at the pump base	SPC 5A	$\pm 0.5K$	Same as Case 2	$\pm 0.5K$
4	Epoxied at the pump base	SPC 5A	$\pm 0.5K$	$\pm 0.5K$	$\pm 0.5K$
5	Mounted inside the pump body, close to the piston	EnSci Z & 2Z, SPC 6A	$\pm 0.5K$	No uncertainty	$\pm 0.5K$

1068
 1069 The additional correction to account for differences between moving piston, T_{piston} , and the
 1070 internal pump, or pump based, temperatures is defined as $\Delta T_{\text{piston-internal}} = \pm 0.5\text{K}$ and is true for all
 1071 cases.

1072
 1073 The full contribution of the measured pump temperature to the ozone uncertainty is expressed as
 1074

1075 Equation 3.5.1
$$\frac{\Delta T_P}{T_P} = \sqrt{\left(\frac{\Delta T_P}{T_P}\right)^2 + \left(\frac{\Delta T_{\text{pase}_i}}{T_P}\right)^2 + \left(\frac{\Delta T_{\text{piston-internal}}}{T_P}\right)^2}$$

1076

1077 **3.6. Contribution of the uncertainty in the conversion efficiency**

1078 GRUAN shall adopt the WMO/GAW uncertainty calculation for the conversion efficiency [Smit
 1079 et al., 2014, Equation E-3-4], written as

1080

1081 Equation 3.6.1
$$\frac{\Delta \eta_C}{\eta_C} = \sqrt{\left(\frac{\Delta \alpha_{O_3}}{\alpha_{O_3}}\right)^2 + \left(\frac{\Delta S_{O_3:I_2}}{S_{O_3:I_2}}\right)^2} \text{ where,}$$

1082

1083 $\Delta \eta_C / \eta_C$ = conversion efficiency uncertainty term

1084 α_{O_3} = absorption efficiency from the gas into liquid phase of the sensing solution = 1.0

1085 $\Delta \alpha_{O_3} = \pm 0.01$

1086 $S_{O_3:I_2}$ = stoichiometry of the conversion of O_3 to $I_2 = 1.0$

1087 $\Delta S_{O_3:I_2} = \pm 0.02$ at $Z=0\text{km}$ with a linear increase to ± 0.05 at $Z=35\text{km}$. This translates to the linear
 1088 equation, $\Delta S_{O_3:I_2}(Z) = 0.000857143 * Z + 0.02$

1089

1090 Setting the absorption efficiency (α_{O_3}) equal to one applies to cases where the volume of the
 1091 cathode solution is 3.0 cm^3 . GRUAN will use the following WMO/GAW equations to calculate
 1092 α_{O_3} for a 2.5 cm^3 volume, as follows

1093

1094 Equation 3.6.2 $\alpha_{O_3}(P) = 1.0044 - 4.4 \times 10^{-5} * P$ $100 \text{ hPa} < P < 1050 \text{ hPa}$

1095 Equation 3.6.3 $\alpha_{O_3}(P) = 1.0$ $P \leq 100 \text{ hPa}$

1096

1097 $\Delta \alpha_{O_3}$ is ± 0.01 for both cathode volumes.

1098

1099 GRUAN shall require new candidate sites to use 3.0 cm^3 volume cathode sensing solution to
 1100 reduce added uncertainty in the ozone uncertainty equation and maintain a constant absorption
 1101 efficiency throughout the profile measurements.

1102 **3.7. Contribution of the uncertainty in the radiosonde pressure to ozone** 1103 **uncertainty**

1104 The designated GRUAN Ozonesonde Lead Centre shall adopt the GRUAN Radiosonde
 1105 Technical Report processing procedures for calculating the uncertainties associated with the
 1106 radiosonde measurements. Handling biases in the geopotential height calculation in the absence

1107 of GPS measurements shall be the responsibility of the Radiosonde WG-GRUAN, assigned task
1108 team, and responsible Lead Centre.

1109

1110 **4. GRUAN OZONESONDE PROGRAMMES**

1111 The GRUAN Guide (GCOS-171) states that the primary objective of GRUAN is to provide
1112 reference measurements for a range of upper-air climate variables. Reference quality
1113 observations are based on key concepts in metrology, in particular traceability. Metrological
1114 traceability is the process whereby a measurement and its uncertainty, can be related to a
1115 reference through a documented, unbroken chain of calibrations.

1116

1117 Confidence in the long-term stability of the ozonesonde data records across the network as a
1118 whole, the instrumentation, SOP, and data processing must be established in such a way that
1119 measurements from individual GRUAN Ozonesonde Programmes generate data sets that are
1120 homogeneous in both space (i.e. across the network) and time. For this reason, certification of
1121 GRUAN Ozonesonde Programmes (see Section 4.1) applies to the overall infrastructure
1122 underlying the ozonesonde measurement and the subsequent production of a final GRUAN
1123 ozonesonde reference data product. This infrastructure is defined here as a GRUAN Ozonesonde
1124 Programme, and includes the:

1125

- 1126 1. SOP that prescribe how ozonesonde flights shall be performed at a GRUAN site,
- 1127 2. Mandatory collection of metadata used to characterize the singular features of each
1128 ozonesonde and its inflight performance,
- 1129 3. Acquisition of the uncorrected original data and metadata by the RSLaunchClient utility
1130 (GRUAN-TD-3) for central processing,
- 1131 4. Steps involved for creating a final homogenized GRUAN ozonesonde data product,
- 1132 5. Storage and dissemination of the GRUAN ozonesonde data product.

1133

1134 To be GRUAN-certified each GRUAN Ozonesonde Programme must provide to the Lead Centre
1135 and to the GRUAN centralized ozonesonde data processing facility a GRUAN Ozonesonde
1136 Instrumentation and Measurement Report (GOIMR). This document describes the site's
1137 ozonesonde measurement programme and capabilities, as well as documenting the history of its
1138 ozonesonde data record, if any. The GOIMR shall include all aspects of the programme such as
1139 instrumentation inventory, SOP used, measurement schedules, and up-to-date data acquisition
1140 and archiving status. In addition, the site must provide proof of its ability to provide all essential
1141 metadata (defined in Section 4.6) and original data to the central processing facility using the
1142 RSLaunchClient utility (GRUAN-TD-3). All ozonesonde metadata uploaded by the
1143 RSLaunchClient shall be consistent with the latest version of a recommended check list
1144 (examples found in Appendix A-1 and in Appendix A-2 for refurbished sondes). Once certified,
1145 GRUAN Ozonesonde Programmes will be audited at least quadrennially, and reviewed annually
1146 to confirm compliance with the requirements and recommendations of GCOS-171 and this
1147 Technical Document.

1148 **4.1. GRUAN Ozonesonde Programme site assessment and certification**

1149 Sites seeking to have their ozonesonde measurements certified as a GRUAN Ozonesonde
1150 Programme will be assessed using criteria described in this section. In addition, each such site

1151 seeking certification must follow the requirements regarding site assessment and certification
1152 described in Section 5.1 of GCOS-171.

1153
1154 GRUAN recognizes that sites will vary in infrastructure and financial support. To comply with
1155 the mandatory operating protocols defined in Section 5.3 of GCOS-171, each GRUAN
1156 Ozonesonde Programme must:

- 1157
- 1158 1. Provide reference quality ozonesonde measurements, i.e., observations characterized by
1159 traceable calibrations, readily accessible documentation, and complete metadata
1160 availability.
- 1161 2. Assure long-term storage of these data either at the site, at another GRUAN facility, or at
1162 another internationally accessible archive in accordance with the GRUAN Data Policy
1163 document (referred to in Section 8.2 GCOS-171).
- 1164 3. Provide, to the extent possible, redundant reference observations of the vertical ozone
1165 profile or total column measurements from co-located ground-based instruments for
1166 independent evaluation and validation of the ozonesonde measurements and their
1167 uncertainties.
- 1168 4. Provide annual reports summarizing the ozonesonde operations at the site, including any
1169 changes in instrumentation, how those changes were managed, and any improvements
1170 made in the Programme.
- 1171 5. Manage change proactively as defined in Section 7 of this Document.
- 1172 6. Actively communicate with the GRUAN Lead Centre, WG-GRUAN and GRUAN TTR
1173 through attendance at meetings and emails.

1174
1175 Specifically, certification of a GRUAN ozonesonde programme shall be cognizant of:

- 1176
- 1177 1. The content and completeness of the GOIMR each ozonesonde candidate site is required
1178 to file.
- 1179 2. The level to which the candidate ozonesonde site conforms to the GRUAN prescribed
1180 SOP which is necessary to guarantee data product homogeneity across the network.
1181 Determining whether the operating procedures of an existing site meet the prescribed
1182 SOP will be done against the requirements outlined in Section 4.5. Metadata
1183 requirements are addressed in Section 4.4.3.
- 1184 3. Added value the candidate site brings to the GRUAN network of ozonesonde
1185 programmes, as a whole. This is outlined in detail in Section 4.2.1.

1186 **4.2. GRUAN Ozonesonde Programme assessment and certification process**

1187 Two scenarios are foreseen:

- 1188 1. The candidate site has no other GRUAN certified measurement programme.
- 1189 2. The candidate site has at least one other GRUAN certified measurement programme.

1190
1191 In the case of scenario (1) the certification of the site's ozonesonde programme also constitutes
1192 certification of the site as a GRUAN site. Refer to GCOS-171 for the additional requirements for
1193 site certification under scenario (1). Under either scenario, the following sequence of events
1194 defines the process specific to the certification of the GRUAN Ozonesonde Programme at the
1195 site:

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1. The GRUAN Lead Centre will provide the site with this Document, as well as any additional documentation related to data submission protocols and the procedures that must be followed when data are submitted to the GRUAN ozonesonde central data processing facility.
 2. The response from the candidate site shall be given in the form of the GOIMR submitted to the GRUAN Lead Centre and should include:
 - 2.1. A complete description of how the ozonesonde measurement programme will be conducted. Such information would include launch frequency and scheduling, detailed SOP, a copy of the check list and metadata inventory, and data storage policies. This information must be sufficient to establish the capability of the site to meet the mandatory operating protocols outlined in Sections 4.5 - 4.7.
 - 2.2. Include any cooperative agreements with other sites. This is desirable to ensure that expertise is disseminated to similar measurement programmes in operation at other sites.
 - 2.3. The management structure of the site and a general description of the manner in which the site is operated. This should include a description of current and expected future funding levels for ongoing operation of the site.
 - 2.4. A description of which data centres the ozonesonde measurements are, in addition to GRUAN, being submitted to and have been submitted to in the past.
 - 2.5. A description of how past ozonesonde measurements have been processed. This will be used to assess whether the time series to date meets the standards for a GRUAN reference measurement. Particularly important in this regard will be detailed documentation about how changes in SOP over the history of the measurement programmes have been managed to derive a homogeneous time series of measurements.
 - 2.6. 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.
 - 2.7. A list of the ozonesonde experts, if any, employed at the site who would likely participate in the analyses of the data collected at the candidate site and who could share their expertise with other GRUAN sites. 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 be submitted to the WG-GRUAN who will evaluate the proposal within 3 calendar months against the requirements listed in Sections 4.5 and 4.6. One or more visits to the site by members of the WG and/or Lead Centre within this 3-month period may be required to obtain specific additional information about the ozonesonde measurement programme. If accepted, the ozonesonde programme will then be included in the GRUAN certification for the site.

- 1241 5. Regardless of the outcome, the WG-GRUAN and Lead Centre will provide written
1242 constructive feedback to the candidate site outlining the strengths and weaknesses of their
1243 programme for GRUAN purposes and suggestions as to future improvements for GRUAN
1244 operational purposes. This feedback is non-binding and is rather intended to provide useful
1245 guidance and support.
1246
- 1247 6. Annual reports shall summarize the operation of the Ozonesonde Programme at the site,
1248 identifying any changes in the instrumentation used in the programme (e.g. ozonesonde type,
1249 radiosonde type, ground-check equipment), scheduling, procedures, and any improvements
1250 implemented. The intent of the annual report is to ensure that GRUAN ozonesonde SOP have
1251 been adhered to, and to identify changes that may require additional reprocessing that have
1252 not already been taken into account or require re-assessment of GRUAN certification. These
1253 reports will be presented at annual GRUAN meetings.

1254 **4.2.1 Criteria for assessing added value**

1255 The GRUAN Ozonesonde Programme assessment and certification process follows closely the
1256 more general GRUAN site certification process described in Section 5.5 of GCOS-171.

1257 Achieving all of the measurement programme requirements is not mandatory for the inclusion of
1258 a site in GRUAN. The extent to which a site can meet Section 4.1 requirements will determine,
1259 in part, the additional value that that site brings to the network. Once a site has committed to
1260 supporting the minimal set of measurement programmes under the protocols defined in Section
1261 5.2.2 of GCOS-171, the added value that a site flying ozonesondes brings to GRUAN will be
1262 assessed according to:

- 1263 • *Location.* For example, programmes located in a large region of the globe containing no
1264 other GRUAN Ozonesonde Programmes and fulfilling all other minimum requirements
1265 of a site will be assessed as adding more value to the network than a site located close to
1266 other GRUAN sites making ozonesonde measurements.
- 1267 • The extent to which the site provides profile measurements of ozone in regions of
1268 atmospheric phenomena which were not previously sampled by the network.
- 1269 • The extent to which the site contributes unique observational and/or analysis capabilities
1270 aligned with GRUAN's scientific objectives and the likelihood of being able to propagate
1271 those capabilities across other sites in the network.
- 1272 • The extent to which the site is prepared to forgo locally established ozonesonde operating
1273 procedures and adhere to the SOP detailed in this Document (see Appendix A.1).
- 1274 • The availability of historical measurements that conform to the GRUAN standard. All
1275 else being equal, a candidate site that extends an existing multi-decade time series of
1276 reference quality ozonesonde measurements will be assessed as adding more value to the
1277 network than a site that would initiate the same measurement programme starting at the
1278 present. Detailed documentation in the GOIMR would be required describing how
1279 changes in SOP, instruments, calibration procedures, data processing algorithms and
1280 operators over the history of the measurement programmes have been managed to ensure
1281 that the historical measurements are reference quality. Where historical reference quality
1282 measurements are available, consideration will be given by the Lead Centre to provide
1283 these as GRUAN data through the GRUAN data archives.

- 1284 • The extent to which the site can provide redundant observations of the vertical ozone
1285 profile or can conduct periodic inter-comparisons and laboratory studies.
- 1286 • The extent to which a site is capable of measuring other ECVs identified in GCOS-112 as
1287 being desired quantities.
- 1288 • The level of institutional support for the site and commitment to maintaining long-term
1289 reference quality measurement programmes. If, in addition, a site can demonstrate that it
1290 is actively pursuing resources to enhance its capability, such as the addition of new
1291 measurement programmes. It is also desirable that there is full host institution
1292 commitment to GRUAN-related activities and that this commitment is not dependent on a
1293 single individual.
- 1294 • The level of institutional support for the site (and any partner institutions) to undertake
1295 fundamental scientific research of the measurements from the site and other GRUAN
1296 sites. Because GRUAN includes aspects of both operational and research networks, a
1297 strong and ongoing science programme is required to ensure that GRUAN fulfills its role
1298 as a research network.
- 1299 • The degree of historical or planned cooperation with other sites both within and outside
1300 GRUAN including other GRUAN-relevant networks e.g. NDACC, SHADOZ, GAW, and
1301 WOUDC.

1302 Such assessments of added value shall rely on the expert judgement of the WG-GRUAN and
1303 Lead Centre.

1304 Determining optimal locations for GRUAN sites intending to fly ozonesondes shall consider:

- 1305 1. The representation of major climate regions.
- 1306 2. The ability of the ozonesonde network to diagnose dynamically driven changes in ozone
1307 e.g. stratosphere-troposphere exchange, the QBO, regional tropospheric ozone pollution,
1308 and regions where halogen-induced ozone depletion is expected.
- 1309 3. The ability of the network to provide measurements across a range of environments, e.g.
1310 tropics, mountainous, deserts, and islands.

1311 **4.3 GRUAN Ozonesonde Training Programme**

1312 A component of uncertainty in the GRUAN ozonesonde data product may be related to
1313 instrument set-up and operation. To minimize these sources of uncertainty, and to ensure
1314 network-wide homogeneity of ozonesonde instrument operation, the Lead Centre and WG-
1315 GRUAN shall identify Ozonesonde Programmes where instrument operators would benefit from
1316 training on GRUAN ozonesonde SOP, and shall organize cost-efficient training courses. A
1317 designated Ozonesonde Programme representative at each participating GRUAN site who is
1318 primarily responsible for the operation of that programme, should attend an initial training
1319 session in which the GRUAN-specific ozonesonde best measurement practices, and the use of
1320 RSLaunchClient are taught. Training of new or additional members of the ozonesonde team at a
1321 GRUAN site can either be done by the GRUAN Ozonesonde Programme site representative, and
1322 ozonesonde expert, or at a training session at a GRUAN site where SOP are kept up-to-date.

1323
1324 For those GRUAN Ozonesonde Programmes already partnered with an ozonesonde expert,
1325 training and maintaining up-to-date practices shall be coordinated between the two partners.

1326 Sites hosting GRUAN Ozonesonde Programmes where re-training is sought can make a formal
1327 written request for re-training to the Lead Centre. It is also possible that the WG-GRUAN may,
1328 on reviewing a site's annual report, request re-training to guarantee consistency of quality.
1329 Finally, an audit (see Section 4.10) may reveal deficiencies in the operating procedures that
1330 would trigger the need for re-training.

1331 **4.4. GRUAN Ozonesonde Programme data management**

1332 General considerations shall follow those detailed in Section 8 of GCOS-171.

1333 **4.4.1 Overview of the data flow**

1334 Refer to Figure 3 of GCOS-171 that shows a schematic representation of the flow of data in
1335 GRUAN to the user community.

1336
1337 GRUAN data levels relevant to ozonesondes are based on the GRUAN Data Management
1338 Manual:

- 1339 • Level 1 (L1): Converted raw data (CRD). This is telemetry data convert by the
1340 ozonesonde ground station to a common well-described file format intended for long-
1341 term storage. They are pre-processed ozone data that have not yet had the necessary
1342 corrections and transfer functions applied and might already represent parameters to be
1343 used in an end-user's application.
- 1344 • Level 2 (L2): SGDP resulting from all processing steps applied to the Level 1 data from a
1345 single flight.

1346
1347 Measurements and metadata are bound together in each of these data levels. CRD are ingested
1348 from all GRUAN sites hosting an Ozonesonde Programme into the internal GRUAN data
1349 archive for ozonesonde data.

1350

1351 **From CRD data submission to processing, storing and dissemination of SGDP**

1352

- 1353 1. Level 1 CRD and metadata shall be collected by the RSLaunchClient utility. Only
1354 original data that have not been processed apart from the ground station data acquisition
1355 system shall be submitted to the RSLaunchClient utility.
- 1356 2. Each GRUAN site is responsible for back-up storage of the CRD and associated metadata
1357 in its original format and in digital format.
- 1358 3. Processing of the ozonesonde CRD will be held in the designated GRUAN internal data
1359 archive at the Lead Centre.
- 1360 4. The Lead Centre GOASS will be responsible for taking the CRD and metadata to create
1361 the final standard ozone products (SGDP), as outlined in Section 4.7. This processing
1362 should include applying the necessary corrections, transfer functions, and uncertainty
1363 estimates in a consistent and traceable manner across identical instrument/solution
1364 pairings from other Ozonesonde Programmes.
- 1365 5. The SGDP, including their metadata, will be provided to the user community through the
1366 external GRUAN data archive hosted at NCEI.

1367

1368 A performance monitoring process (see Section 9 of GCOS-171), implemented at the Lead
1369 Centre, will provide feedback on performance to individual sites.

1370 **4.4.2 GRUAN data policy**

1371 Since GRUAN is co-sponsored by WMO, GRUAN ozonesonde data dissemination and use shall
1372 comply with WMO Resolution 40 (Cg-XII) which calls for free and unrestricted international
1373 exchange of data. Refer to Section 8.2 of GCOS-171 for further details on the data dissemination
1374 and exchange policy.

1375 **4.4.3 Collation of Metadata**

1376 To provide the best evaluation for the ozonesonde measurement uncertainty, a detailed
1377 understanding of the instrumentation is required for the conditions under which it is used. The
1378 ozonesonde metadata summarizes the unique characteristics of each ozonesonde instrument in
1379 response to standard operational procedures, and it makes all factors that contribute to the
1380 measurements traceable. Metadata shall be collected from a specified check list sheet that
1381 GRUAN ozonesonde site operators shall use. An example is the SHADOZ check list sheet found
1382 in Appendix A.1 that goes beyond the minimum metadata requirements recommended by
1383 WMO/GAW. The RSLaunchClient utility will be responsible for ingesting profile metadata to be
1384 saved and stored at a designated GRUAN archive. A candidate site should demonstrate that all
1385 essential metadata found in A.1 are recorded and shall be submitted to the RSLaunchClient
1386 utility. Ozonesonde Programmes are required to keep original copies of their metadata at their
1387 own storage facility, as secondary storage back-up.

1388
1389 Metadata documents related to historical operations at GRUAN sites and to historical data
1390 archives should be inventoried and properly conserved until such time as their information
1391 content can be transferred to a medium which supports multiple users' access and conforms to
1392 GRUAN reference measurement guidelines.

1393
1394 Metadata needs to have the same level of commitment as observed data. Incomplete, outdated, or
1395 inaccurate metadata can be as detrimental, indeed in some cases worse, than no metadata at all.
1396 Regular reviews of metadata content for confirmation and accuracy should be part of regular
1397 GRUAN operations.

1398 **4.4.4 Ozonesonde Standard GRUAN Data Product**

1399 The GOASS shall use the CRD, in conjunction with the metadata also collected from the
1400 RSLaunchClient, to generate the ozonesonde SGDP. Section 4.7 goes through the GOASS steps
1401 required to generate the ozonesonde SGDP from the CRD. The family of ozonesonde SGDP are
1402 listed in Table 4.1. Apart from the uncertainty estimates, it is not mandatory for all variables
1403 under the ozonesonde SGDP family to be measured. For example, heritage ozonesonde
1404 measurements used radiosondes that did not have the means or capability of acquiring GPS
1405 information.

1406
1407 **Table 4.1 Collection of Ozonesonde SGDP**

- 1408
1409 1. Time [s]
1410 2. Radiosonde Pressure [hPa]
1411 3. Radiosonde Pressure Offset [hPa]
1412 4. Geopotential height [gpm]

- 1413 5. Radiosonde Temperature [K]
- 1414 6. Radiosonde Temperature Offset [K]
- 1415 7. Radiosonde Relative Humidity [%]
- 1416 8. Radiosonde RH offset [%]
- 1417 9. Radiosonde Horizontal Wind Direction [decimal degrees] (range: 0:360)
- 1418 10. Radiosonde Horizontal Wind Speed [m/s]
- 1419 11. Radiosonde GPS Geometric Height [m]
- 1420 12. Radiosonde GPS Longitude [decimal degrees] (range: -180:+180)
- 1421 13. Radiosonde GPS Latitude [decimal degrees]
- 1422 14. Rise rate [m/s]
- 1423 15. Ozone Partial Pressure an uncertainty [mPa]
- 1424 16. Ozone Mixing Ratio per volume [ppm]
- 1425 17. Box or Pump Temperature and uncertainty [K]
- 1426 18. Ozone Current and uncertainty [μ A]
- 1427 19. Background Current and uncertainty [μ A]
- 1428 20. Pump Flow rate and uncertainty
- 1429 21. PCF and uncertainty
- 1430 22. Ozonesonde Conversion efficiency
- 1431 23. Integrated Column Ozone and uncertainty [DU]
- 1432 24. Pressure above which the TCO is calculated [hPa]
- 1433 25. Ozone residual above (23) and uncertainty [DU]

1434
 1435 Uncertainty estimates shall form part of the ozonesonde SGDP collective. GOASS shall be
 1436 responsible for calculating these estimates addressed in Section 4.7.

1437 **4.4.5 File naming convention**

1438 The filename convention described here is taken from Section 2.1 of the Manual for the Data
 1439 Management in GRUAN [GRUAN-TD-1 DRAFT v0.3 (2010-132010-07-13)] and will apply to
 1440 metadata, CRD, SGDP data files in the designated GRUAN Lead Centres file archive. The
 1441 obligatory parts of the file names should be:

- 1442
- 1443 • Unique Station Identifier → GAW ID and station location name, i.e.
- 1444 NRB_Nairobi_Kenya
- 1445 • Data level → L2 or L2
- 1446 • Date / Time of launch → in universal standard time (GMT)
- 1447 • Data product description → “Metadata”, “CRD” or “SGDP”
- 1448 • Version of data product → number
- 1449 • Date / Time of the creation of the file
- 1450 • Identification of the specific instrument → 'ECCSonde'
- 1451 • Identification of central tracer → 'Ozone'

1452
 1453 An example file is,
 1454 NRB_Nairobi_Kenya_20170301T23:50:12_L1_CRD_V1.0.0_20170323T09:01:48_ECCSonde_Ozone.csv

1455 **4.4.6 Data format**

1456 Metadata, CRD and SGDP will be stored in CSV ASCII format. ASCII format is an accepted
1457 standard output used by the leading ozonesonde archiving centers (WOUDC, NDACC, and
1458 SHADOZ) and is readily accessible to the global scientific community.

1459 **4.4.7 Data dissemination**

1460 Users of GRUAN data shall have access not only to the measurements and their uncertainties,
1461 but also to the metadata information that includes instrument specifications, operating
1462 procedures, data algorithms used, and when changes to any of these occurred through the
1463 complete time period of the data set.

1464 **4.4.8 Data archiving**

- 1465 • The ozonesonde metadata, CRD and SGDP will be stored at the nominated GRUAN
1466 central data processing facility Lead Centre.
- 1467 • A designated GRUAN storage facility shall be established. This would:
 - 1468 ◦ Allow the Lead Centre to maintain statistics on data usage. This would be useful
1469 when applying for funding to support GRUAN operations.
 - 1470 ◦ Allow end-users to be informed if and when newer versions of the data become
1471 available.
 - 1472 ◦ Facilitate reporting of potential errors, flags, and anomalies in the data by end-users.
- 1473 • The metadata and SGDP shall be made available at the NCEI.
- 1474 • Ozonesonde data dissemination shall comply with the data policy guidelines in Section
1475 8.2 of GCOS-171.
- 1476 • It is important that the GRUAN archive include all previous versions of any given data
1477 set such that analyses using previous versions of data can be repeated if required.

1478 **4.4.9 Handling data gaps**

1479 GRUAN recognizes that there may be gaps in the profile measurements due to telemetry
1480 interference, hardware, and software issues. Profiles shall not be excluded if data gaps occur.
1481 There is useful data extending from the surface up to the stratosphere that satisfies the four key
1482 user groups of GRUAN data products defined in Section 1.2. Depending on where data gaps
1483 occur and the extent of these data gaps, there remains useable quality reference data that can still
1484 satisfy one or more of these four communities. Profiles with very large and intermittent data gaps
1485 should be identified and evaluated in the annual reports and periodic audits. Ultimately, it is up
1486 to the end-user to determine the best use of the data.

1487 **4.5. The GRUAN Standard Operating Procedures**

1488 GRUAN seeks to ensure that all sites operate to the same reference quality standard to guarantee
1489 homogeneity of quality across the network. The WMO/GAW SOP is designed to reduce random
1490 errors by maintaining consistent and reproducible ozonesonde measurements. Standardization of
1491 the SOP has been shown to improve the precision and accuracy to less than $\pm 5\%$, while non
1492 uniformity in SOP will lead to inhomogeneities in the time series and between station data
1493 records [Smit et al, 2007, Deshler et al, 2008].
1494

1495 GRUAN recommends that Ozonesonde Programmes use, at the very minimum, the WMO/GAW
1496 ozonesonde conditioning and preparation procedures outlined in detail in Annex A of GAW
1497 Report No. 201. GRUAN recommends Programmes adopt of the SHADOZ check list (Appendix
1498 A-1) that is rigorous in metadata reporting requirements. It is strongly recommended that
1499 potential site candidates use this check list in place their own SOP, but it is not required as long
1500 as sites can demonstrate that all metadata found in Appendix A-1 are recorded.

1501 **4.5.1 Refurbished Sonde SOP**

1502 Refurbished sensors must follow more rigorous conditioning and testing. The ASOPOS panel
1503 concluded that at present it is not clear how often recovered ozonesondes can be re-used after
1504 reconditioning. Currently there are no quality assurance standards for refurbished sensors and a
1505 number of ozonesonde sites fly refurbished sondes using their own set of SOP. Sites risk
1506 potentially introducing artifacts in the data records if the re-conditioning procedures are not done
1507 properly. A basic set of SOP for refurbished sensors can be found in Appendix A-2, although
1508 manufacturer SOP should not be discounted. Further discussion on refurbished sensors can be
1509 found in Section 5.5. GRUAN strongly recommends and encourages that JOSIE studies,
1510 independent laboratory tests, and inter-comparison field measurements be conducted to establish
1511 SOP for refurbished sondes that GRUAN can draw on to incorporate across the Ozonesonde
1512 Programme network. Sites that launch refurbished ECC-sensors should follow the NOAA re-
1513 conditioning SOP in Appendix A-2 or manufacturer SOP.

1514 **4.6. The RSLaunchClient Utility**

1515 The RSLaunchClient utility will collect and manage uploaded metadata and ozonesonde CRD to
1516 the GRUAN Lead Centre. GRUAN defines essential data as input requirements to the
1517 RSLaunchClient. Regarding metadata, GRUAN Ozonesonde Programmes will be required to
1518 provide essential metadata, defined in Appendix A.1, to the RSLaunchClient. If one of the basic
1519 essential metadata variables is missing a flag will be given or, in some cases, the entire profile
1520 will be rejected (e.g. large gaps in metadata reporting or missing key variables in the
1521 measurement system that are a component of the SGDP).

1522

1523 Variables specific to the radiosonde data stream, such as P-T-U calibrations, offsets, and
1524 uncertainty calculations, shall use the Radiosonde Analysis Software in the GRUAN Radiosonde
1525 Technical Document.

1526 **4.7. The GRUAN Ozonesonde Analysis Software System (GOASS)**

1527 The GRUAN Ozonesonde Analysis Software System (GOASS) is the centralized data
1528 processing software that analyzes the CRD of all certified GRUAN Ozonesonde Programmes
1529 submitted through the RSLaunchClient utility. Before processing the CRD, the GOASS
1530 reconciles the metadata received from the RSLaunchClient with those contained in the GOIMR.
1531 Any inconsistency is immediately reported, thus providing a near-real-time check of the
1532 measurement traceability and stability, as well as a quick identification of change. The GOASS
1533 must be transparent, i.e., must be developed and optimized in consultation with all GRUAN
1534 Ozonesonde Programme representatives/investigators, as well as the GRUAN Lead Centre, WG-
1535 GRUAN, and TTR. These investigators shall meet regularly to discuss the implementation of
1536 updates to the GOASS, and whether processing changes pertain to one or all of the GRUAN

1537 Ozonesonde Programmes. The output of the GOASS consists of certified ozonesonde metadata,
1538 CRD, and SGDP.

1539

1540 GOASS must integrate correction methods and associated uncertainties that are accepted by
1541 GRUAN and user communities as being appropriate for the science application foreseen. It is
1542 therefore the GRUAN Lead Centre, TTR, and GRUAN Ozonesonde Programme
1543 Representative's joint responsibility to develop and maintain the operational GOASS. Failure of
1544 GRUAN Ozonesonde Programmes to use an operational version of the RSLaunchClient and
1545 GOASS will result in delivery delays of the ozonesonde SGDP, and therefore can result in the
1546 cancelation of the Programme's certification at the time of its audit.

1547

1548 The GOASS shall perform the following steps to transform the CRD to the final Level 2
1549 GRUAN standard ozonesonde product (SGDP):

1550

- 1551 1. Apply filtering criteria to test the performance of an individual ECC sensor, summarized
1552 in Table 4.7.1 below. Aspects of the conditioning process should fit within the following
1553 specific thresholds. GRUAN site operators shall use these threshold criteria to gauge the
1554 quality of the ECC sensor and perform repeat tests if necessary to bring the ECC sensor
1555 into compliance. Ideally, ozonesonde original data should not be uploaded to the
1556 RSLaunchClient if certain threshold criteria are violated.
- 1557 2. For the case where $IB_{final} > 0.05 \mu A$ GOASS shall recalculate ozone using the minimum
1558 of IB_0 , IB_1 , and IB_2 as IB_{final} . If that minimum background current still exceeds the 0.05
1559 μA threshold then a flag shall be recorded in the metadata. Programmes should specify
1560 which background current is used as IB_{final} .
- 1561 3. GOASS shall apply the RH correction, C_{PH} , and C_{PL} , explained in detail in Section 2.4 to
1562 calculated the final flow rate, Φ_{Ground} .
- 1563 4. Radiosonde/Ozonesonde offsets in height and pressure, if any, shall be documented in the
1564 metadata and geopotential heights shall be recalculated, in accordance with the GRUAN
1565 Radiosonde Technical Document.
- 1566 5. Adjusted pump temperatures using Equation 2.6.5 and sub-equations shall be calculated.
- 1567 6. After the above corrections are applied, the ozone partial pressure shall be recalculated
1568 using Section 2.1 Equation 1.
- 1569 7. Uncertainties, covered in Section 3, for each measured parameter in the ozone partial
1570 pressure equation shall be calculated as defined by Smit et al. [2012].
- 1571 8. A total column product shall then be calculated based on the processing protocol defined
1572 in Section 2.7.

1573 Table. 4.7.1 Threshold criteria for ECC ozonesondes by the RSLaunchClient to test the
 1574 performance quality of each sensor. These are specifically for SPC and ENSCI ECC types.
 1575

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

1576

1577 **Flagged Data**

1578 Data that are not within threshold levels itemized in Table 4.7.1 shall not be rejected but must be
 1579 flagged and documented in the final archived metadata. Flagged metadata shall be included as a
 1580 diagnostic tool in each GRUAN Ozonesonde Programmes annual report. Audits shall use the
 1581 statistics gathered on flagged metadata and the SGDP to help evaluate the continuity of GRUAN
 1582 Ozonesonde Programmes.

1583 **4.8. GRUAN ozonesonde calibration management**

1584 Ozonesonde ground stations generally do not require calibration at the manufacturing,
 1585 instrumentation, or operational levels. Calibration of the ECC sensor comes from adhering to the
 1586 SOP and completing the metadata check list requirements. At the time of this document, there is
 1587 no precedent or standard rules that require sites to test or calibrate aspects of the ground station
 1588 equipment, nor is there a mechanism to ensure equipment standards and quality. It would ideal
 1589 to establish guidelines by which a GRUAN Ozonesonde Programme can calibrate its ground
 1590 station equipment such that sources of error and uncertainty can be further identified, traced, and
 1591 included as part of the uncertainty budget for ozonesondes.
 1592

1593 **World Calibration Center for Ozonesondes (WCCOS)**

1594

1595 The World Calibration Center for Ozonesondes (WCCOS) at the Forschungszentrum, Jülich,
1596 Germany periodically conducts inter-comparison experiments (JOSIE) to establish and maintain
1597 quality assurance of the ozonesondes sensors. JOSIE performs routine testing of existing and
1598 newly manufactured ECC ozone sensors to (i) check the instrument performance in a controlled
1599 environment, (ii) maintain up-to-date SOP, (iii) test individual ECC sensor capabilities, and (iv)
1600 develop uncertainty estimates for the individual instrument parameters. The WG-GRUAN shall
1601 use findings from the JOSIE reports to evaluate current best practices and whether changes to the
1602 ozonesonde SOP or processing procedures are required. Members of the WG-GRUAN are
1603 encouraged to participate in JOSIE initiatives to keep abreast of new findings. It is highly
1604 desirable for GRUAN sites to endorse and participate in JOSIE-led activities.

1605

1606 **Calibration of the ozonizer test unit**

1607

1608 The ozonizer used to condition and prepare an ECC sensor does not generate a traceable amount
1609 of ozone. Comparisons against an independent calibrated reference, such as a TEI surface ozone
1610 monitor, to generate a known ozone amount would be very useful. It is desirable for sites to
1611 provide traceable ground/instrument checks, such as a surface ozone monitor (e.g. TEI) at the
1612 time of each profile measurement, prior to launch and independent of the manufacturer. In the
1613 case of refurbished ECC sensors it is strongly recommended that a calibrated source of ozone to
1614 test the instrument performance be used and included as part of their SOP. Ozonesonde
1615 programmes shall use digital test units capable of measuring background currents to at least three
1616 significant digits. Audits (Section 4.10) shall include the periodic testing of the ozonizers by
1617 using a calibrated source of ozone from a reliable instrument. Members of ASOPOS and the
1618 TTR+WG-GRUAN shall determine the calibration method and testing.

1619 **4.9. Ozonesonde Programme versioning system**

1620 A system of traceable version numbers and dates for all GRUAN Ozonesonde Programmes shall
1621 be developed to allow for a full identification and tracking of changes in SOP, and data
1622 processing since the initial certification. Every reprocessing of the metadata, CRD, and SGDP
1623 must be reflected in an increment in the data version and an update to the date of creation by the
1624 GOASS (see file naming convention in Section 4.4.5) as prescribed in the data versioning
1625 protocols developed by the GRUAN Lead Centre. Such data updates must also be communicated
1626 to users who have accessed earlier versions of the data and who have voluntarily registered to
1627 receive notifications of such data updates (see Section 8.6 of GCOS-171). For this reason it is
1628 also important that all older versions of any data set are always archived and made available
1629 through the GRUAN Lead Centre's archive.

1630 **4.10. GRUAN Ozonesonde Programme auditing**

1631 Certification of GRUAN measurement programmes are not a one-time-only event. GRUAN sites
1632 will be audited by members of the WG-GRUAN at 3-4 year intervals to ensure that programmes
1633 continues to meet GRUAN standards. The audit will involve:

1634

1635 1. A review of the site's annual reports.

- 1636 2. An ozonesonde launch in front of WG-GRUAN auditors that demonstrates that the SOP
1637 are being followed in accordance with Section 4.5. (Can be by video for very remote
1638 station?)
- 1639 3. Calibration/testing of the ozonizer.
- 1640 4. Check lists will be reviewed against the GRUAN Check lists if not used.
- 1641 5. Discussions with the site representatives responsible for the Ozonesonde Programme.
- 1642 6. In the eventuality of identified site problems the following protocols shall be followed
1643 (taken from Section 5.6 of the GCOS-171):
- 1644 1. Should a measurement programme at an existing GRUAN site show significantly
1645 reduced observational capability over more than a year, as evaluated by the criteria
1646 listed above, the WG-GRUAN and Lead Centre shall investigate the circumstances at
1647 that site, and, if needed, exclude that programme from the GRUAN certification for
1648 that site. The WG-GRUAN and Lead Centre shall work proactively with sites to
1649 resurrect such programmes, providing training, technical and in-kind support as
1650 practical and as needed.
- 1651 2. Should the overall contribution of a site be deemed sufficiently diminished to call into
1652 question its continued presence in the network, the site shall be informed immediately
1653 in writing. The site shall be given three months to form a capabilities recovery plan,
1654 in consultation with the Lead Centre and WG-GRUAN. Should this plan be accepted
1655 the sites should promptly implement agreed key aspects. In the eventuality that this is
1656 not achieved, the site shall be suspended with an invitation to submit anew at such a
1657 time as problems are remedied.
- 1658 3. An existing GRUAN site may also request the temporary suspension of some or all of
1659 the measurement programmes at that site from GRUAN certification. This could
1660 occur, for example, in cases of unforeseen budget limitations, non-availability of
1661 personnel, or some other unavoidable circumstance affecting the measurement
1662 programmes at the site. Such a request must be submitted in writing to the WG-
1663 GRUAN and the Lead Centre. At some later time, should the site request
1664 recertification of their measurement programmes previously suspended, the procedure
1665 for certification as outlined in Figure 2 of GCOS-171 shall be followed.

1666
1667 Along with the cooperation and goodwill of participating sites, nations, and individuals, the
1668 establishment of these GRUAN site assessment and certification guidelines provides one of the
1669 main foundations for ensuring that GRUAN meets its goals as a climate observing network.

1670 **5. GRUAN OZONESONDE INSTRUMENTATION**

1671 As described in Section 2 (and elsewhere) of the GCOS-171, one key requirement of GRUAN
1672 instruments is to provide reference measurements, i.e., using principles based on key concepts in
1673 metrology such as (but not limited to) traceability. Traceability must apply at all levels of the
1674 data acquisition and processing chain, including instrumentation. An entire ozonesonde system
1675 comprises the following components:

- 1676
- 1677 1. Electrochemical concentration cell (ECC) ozonesonde which is encased in a molded
1678 polystyrene weatherproof box for ascent into the lower stratosphere.
 - 1679 2. Radiosonde.

- 1680 3. Interface electronics, if applicable, to couple the ECC ozonesonde to the radiosonde.
- 1681 4. A ground station for receiving data provided by the radiosonde manufacturer. The ground
- 1682 station consists of an antenna, pre-amplifier, and coaxial cable connecting the antenna to
- 1683 a 400-405 MHz receiver.
- 1684 5. A computer with pre-installed data acquisition and processing software. This allows data
- 1685 to be received and processed during the balloon flight.
- 1686 6. Software or 1200 baud modem.
- 1687

1688 Refer to the GRUAN Radiosonde Technical Report for instrument details pertaining to
1689 radiosondes and their ground stations and data acquisition systems. Refer to the ECC manuals
1690 for information pertaining to the materials and electronics of the ECC sensor mainframe, and
1691 type interface circuitry which couples the sensor to the particular type of meteorological
1692 radiosonde [e.g. DMT, 2014; SPC, 1999].
1693

1694 The requirements and recommendations on ozonesonde instrumentation provided in this section
1695 apply only to the ozonesonde techniques recognized to be mature enough to be providing
1696 reference measurements of ECVs of highest-enough priority for GRUAN. As of this Document,
1697 these include the SPC and ENSCI instruments:
1698

- 1699 • Both manufacturer types are considered the leading industry standard for ECC
- 1700 ozonesondes and have a long heritage of launches.
- 1701 • The commercial demand for SPC and ENSCI is sufficient to support the production and
- 1702 use of the instrument for the expected multi-decade deployment within GRUAN.
- 1703 • There is no reason to expect that both instrument manufacturers will stop production in
- 1704 the foreseeable future, even if a newer (but not necessarily better) instrument is
- 1705 developed and marketed.
- 1706 • All ozonesonde stations with long-term ECC records use one or both types and are
- 1707 archived at WOUDC, NDACC or SHADOZ.
- 1708 • Finally, all WMO-supported ECC inter-comparison studies (JOSIE), campaigns
- 1709 (BESOS) and other laboratory and field studies have included these two manufacturing
- 1710 types. Thus, there is a substantial body of literature documenting their performance and
- 1711 measurement uncertainties.
- 1712 • Through JOSIE and independent dual-launch studies, the precision and accuracy claims
- 1713 for both instruments and its resultant data is sufficiently robust and meets the uncertainty
- 1714 and stability standards under Section 4.1 of GCOS-171.
- 1715

1716 Radiosonde and ground station data acquisition system packages shall be assessed through the
1717 TTR to ensure compliance with GRUAN measurement standards. It is important to note that
1718 GRUAN shall not prescribe any instrumentation system and setup in particular. Rather, GRUAN
1719 shall provide simple and practical recommendations that encourage sites to use the best practices
1720 in full compliance with the requirements and recommendations detailed in this Guide.
1721

1722 GRUAN recognizes that ECC sensor technology is constantly evolving and that not all sites
1723 within GRUAN will operate the same ECC sensor, e.g. a new site may decide to adopt a new
1724 ECC-sensor that has not been yet been included in JOSIE studies, or an existing site may
1725 continue to use an older manufacturing model or obsolete sensing solution (e.g. 2% unbuffered)

1726 to avoid potentially introducing a discontinuity in the measurement time series. That said, the
1727 fewer the number of different types of instruments and measurement techniques deployed within
1728 and among GRUAN Ozonesonde Programmes, the more likely network homogeneity will be
1729 achieved.

1730
1731 In the event that a new ECC ozone sensor is commercially developed, GRUAN expects the
1732 manufacturer to (i) actively participate in JOSIE and other instrument inter-comparisons, (ii) be
1733 willing to disclose the necessary information required to form a fully traceable chain of sources
1734 of measurement uncertainty in accordance with the GCOS-171 mandatory operating
1735 requirements, and (iii) make available the algorithms used for corrections within the data
1736 processing software to conduct uncertainty analysis. In accordance with GCOS-171 guidelines, it
1737 is a 'fundamental requirement that the information required to reprocess the data at any time in
1738 the future must be made available (though not necessarily publicly available)'.
1739

1740 **5.1. The SCIENCE PUMP CORPORATION ozonesonde**

1741 The earliest Science Pump Corporation (SPC) ECC ozonesonde measurements occurred in the
1742 late 1960's [Komhyr, 1969]. Table 1 from Johnson et al. [2002] summarizes the model
1743 production dates and design changes from the earliest SPC design (SPC-1A). The first known
1744 operating guidelines for preparing ozonesondes for flight was created for the now retired SPC-
1745 4A model in the NOAA technical memorandum [Komhyr, 1986]. The current manual has been
1746 optimized for the SPC-6A model design [SPC Manual, 1999].

1747

1748 **GRUAN protocol procedure**

1749

1750 As of this document, the GOASS shall process CRD from SPC-4A models and higher to produce
1751 the ozonesonde SGDP using procedure protocols established in this document. All other historic
1752 SPC profiles from older SPC models should be inventoried and properly conserved until such
1753 time as their information content can be evaluated, assessed, and assigned uncertainty estimates
1754 that conform to GRUAN reference standards and guidelines.
1755

1756

1757 While the SPC modifications over time improved ECC performance, error characterization in
1758 models older than SPC-4A are not as well known. The first SOP manual was conceived with the
1759 SPC-4A model design in mind and changed with model design as they were altered to optimize
1760 performance. Given that these older SPC models no longer exist and are no longer flown, JOSIE-
1761 type studies or campaigns are necessary to determine error estimates or empirical corrections to
all historic instrumental parameters.

1762 **5.2. The ENSCI ozonesonde**

1763 ENSCI Corporation started in the mid 1990's with similar ECC sensor instrument configuration
1764 to that of the SPC-5A model (refer to Table 1 of Johnson et al., [2002]). Komhyr [1997]
1765 published the first ENSCI operations handbook for the 2Z model. There is no significant
1766 instrumental differences between the Z and 2Z models [Bryan Johnson/NOAA, personal
1767 communication]. The Z model is configured to be compatible with interface boards of other
1768 ground station systems (e.g. Vaisala) while the 2Z has a built-in V7 interface board compatible

1769 with the iMET ground station. Since the late 2000's Droplet Measurement Technologies (DMT)
1770 took over the manufacturing of ENSCI ECCs. The model design has remained unaltered at the
1771 helm of DMT, thus GRUAN does not make a distinction between the two companies. As of this
1772 document, the most up to date ENSCI manual has been published by DMT [2014] and includes
1773 much of the WMO/GAW SOP recommendations and protocols. In 2015 ENSCI has separated
1774 from DMT and is once again it's own manufacturing entity.

1775

1776 **GRUAN protocol procedure**

1777

1778 The GRUAN archive shall accept ENSCI Z, 2Z ozonesonde instrument profiles to produce the
1779 ozonesonde SGDP.

1780 **5.3. Measurement Redundancy**

1781 “Having different instruments at GRUAN sites measuring the same atmospheric parameters will
1782 be invaluable for identifying, understanding and reducing systematic effects in measurements”
1783 - GCOS-171
1784

1785 Examples of redundant instruments that measure profile ozone are the ozone Lidar and
1786 Microwave Radiometer. Other ozone monitoring instruments to consider that can complement
1787 ozonesonde profile measurements are the TEI surface ozone monitor and UV Vis
1788 instrumentation. All these instruments can provide uninterrupted hours of measurements at one
1789 given location. Unlike these fixed located instruments, balloon-borne ozonesondes provide in-
1790 situ measurements at varying locations and altitudes with time. The challenge therefore is to
1791 match the ozonesonde altitude and time with those other instruments with careful considerations
1792 about the geographic displacement from the ground-based instrument site. Section 6.4.2 in
1793 GCOS-171 provides an overview of the characteristics of Lidar and microwave instrumentation.
1794 Methods on resolving the time/altitude differences from these instruments shall draw on
1795 information found in the GRUAN technical documents for Lidar and Microwave Radiometers.
1796 GRUAN shall draw on methods developed by Calisesi et al. [2005], Bodeker et al. [2013],
1797 Hassler et al., [2008] and references therein, that create site atmospheric state best estimates
1798 (SASBE) of ozone profiles from combining ozone instrumentation of varying temporal and
1799 spatial resolutions to provide objective evaluation of ozonesonde performance. Ozonesonde
1800 measurements themselves may be part of SASBE.

1801 **5.4. A typical GRUAN ozonesonde data acquisition system**

1802 The ozonesonde is interfaced with a radiosonde and uses its data acquisition system to transmit
1803 and record the ozone cell current and other parameters used to calculate the ozone partial
1804 pressure (see Equation 1 in Section 2.1). The ozonesonde/radiosonde equipment and data
1805 acquisition system shall also be referred to as the 'ozonesonde ground station'. From to Section
1806 6.1 of GCOS-171

1807 “GRUAN will not prescribe the use of specific instruments in the network since the
1808 emphasis is not on prescribing an instrument, but rather on prescribing the capabilities required
1809 of an instrument and allowing individual sites to select an instrument that achieves those
1810 capabilities.”
1811

1812 As of this Document, there are a number of ozonesonde/radiosonde ground station systems
1813 operating with varying degree of publicly available documentation. These include Vaisala
1814 (Finland), iMET (USA), Lockheed-Martin-Sippican (LMS, USA), Meisei (Japan), Modem
1815 (France), GRAW (Germany), and ChangFeng (China). The Vaisala type ground station system is
1816 the most commonly used, having a heritage of long-term records of ozonesonde and radiosonde
1817 measurements. Specific to radiosondes there is a large body of literature that have characterized
1818 the uncertainties and biases among the Vaisala models (Dirksen et al., [2014] and references
1819 therein; Hurst et al. [2011]; Nash et al. [2006; 2011]; Steinbrecht et al., [2008] and references
1820 therein; and Vömel et al. [2007]). Hurst et al. [2011] and Stauffer et al [2014] were among the
1821 first inter-comparison studies of iMET and Vaisala models. Both iMET and Vaisala adhere to the
1822 instrument selection requirements addressed in Section 6.1 in GCOS-171. This includes, but is
1823 not limited to, information content, instrument heritage (e.g., maturity), sustainability (e.g.
1824 sufficient commercial demand), robustness of measurement uncertainty, and manufacturer
1825 support. Both ozonesonde ground station systems are known to provide all the essential raw data
1826 and metadata.

1827

1828 As of this Document, there is varying degree of documentation that is publicly available on the
1829 other ozonesonde/radiosonde ground station systems mentioned above. However, meeting the
1830 GCOS-171 instrument selection criteria and GRUAN data quality assurance and measurement
1831 standard policies can be assured provided that the manufacturer is:

1832

- 1833 • Willing to provide essential CRD and metadata to generate the SGDP.
- 1834 • Prepared to actively participate in instrument inter-comparisons (e.g. JOSIE) and field
1835 campaigns (e.g. BESOS).
- 1836 • Willing to disclose the necessary information required to form a fully traceable chain of
1837 sources of measurement uncertainty (e.g. releasing SOP and algorithms used for any
1838 corrections within its data processing software).

1839

1840 **GRUAN procedure protocol**

1841

- 1842 1. GRUAN requires that candidate sites use ground stations that provide the essential
1843 metadata (see Appendix A.1) and CRD necessary to generate SGDP (see Table 4.1).
- 1844 2. GRUAN shall encourage all ozonesonde/radiosonde ground station manufacturers to
1845 participate in JOSIE-led and other WMO-sponsored intercomparison activities.
- 1846 3. GRUAN shall encourage ozonesonde/radiosonde ground station manufacturers to provide
1847 documentation on laboratory and/or dual sonde launches to demonstrate that the precision
1848 and accuracy fits within $\pm(3-4)\%$ and $\pm(4-5)\%$ of the JOSIE results, respectively. These
1849 results have been determined by Smit et al. [2000] using the leading SPC and ENSCI
1850 ECC sensors in chamber experiments.

1851 **5.5. Refurbished Ozonesondes**

1852 The ASOPOS panel concluded that at present it is not clear how often recovered ozonesondes
1853 can be re-used after reconditioning. The general recommendation by the ASOPOS panel is not to
1854 fly re-used ECC-sondes. However, for a number of ozonesonde sites it is the most cost-effective
1855 way to ensure financial stability of their programme and maintain their ozonesonde launch
1856 schedule. GRUAN shall (i) encourage sites at unique locations (refer to Section 4.2.1 on added-

1857 value criteria) that regularly launch re-used sondes to apply to become a GRUAN site and (ii) not
1858 prohibit existing Ozonesonde Programmes from including data from refurbished ozonesondes,
1859 provided that all operating conditions set forth by this Document are met.

1860
1861 Refurbished sensors falls under one of the “9 items” under managing changes in Section 7 of this
1862 report. Thus, established GRUAN Ozonesonde Programmes that wish to include refurbished
1863 sensors falls under the guidelines of a “change event” and programmes shall follow steps in
1864 Section 7.1 to include refurbished ozonesondes into their programme. For new candidate sites
1865 seeking to become a GRUAN site this information should be included as part of their GOIMR.

1866
1867 For individual GRUAN Ozonesonde Programmes re-using ECC-sensors, the re-conditioning
1868 SOP of recovered sondes should be done by trained personnel in such a way that the resulting
1869 metadata is always within the threshold criteria defined in Table 4.5. For refurbished
1870 ozonesondes it is recommended that Ozonesonde Programmes following the modified NOAA
1871 prescribed re-conditioning instructions found in Appendix A-2 or re-conditioning procedures as
1872 given by the sensor-specific manufacturer.

1873
1874 In recognition of the heterogeneity of the GRUAN ozonesonde network, the WG-GRUAN and
1875 GRUAN Lead Centre shall evaluate individual candidate sites ability to launch refurbished
1876 sondes based on the following:

1877 • GRUAN Ozonesonde Programme applicants will first be assessed according to their
1878 ability to meet the mandatory operating protocols defined in Section 5.3 of GCOS-171
1879 and specifically 4.1 of this report, and then according to the added value they bring to the
1880 network, as defined in Section 4.2.1 of this Document. This will enable candidate sites to
1881 operate their ozonesonde programme to GRUAN standards.

1882 • Consideration shall be given to, but not be limited to, the following:

- 1883 ◦ Historical data – sites with long term homogenous data records is a desirable factor.
- 1884 ◦ Operation set-up.
- 1885 ◦ The ability and skill of site operators to re-condition sensors following re-
1886 conditioning operating protocols (Appendix A-2 or manufacturer specific).
- 1887 ◦ Funding constraints.
- 1888 ◦ The launch schedule, which is a defining factor in assessing the extent to which the
1889 candidate site can become a fully operational GRUAN Ozonesonde Programme.

1890
1891 Candidate sites must clearly demonstrate that each refurbished ozonesonde is measuring ozone
1892 with an accuracy and uncertainty similar to that of a new ozonesonde. This can be done using
1893 calibrated ozone instrumentation, e.g. a TEI ozone photometer, that tests the sensor performance
1894 against known quantities of ozone, and through dual sonde inter-comparisons.

1895

1896 **6. OZONESONDE MEASUREMENT SCHEDULING**

1897 As detailed in Section 5.2.1 of GCOS-171, a fully equipped GRUAN site is required to make
1898 weekly ozone profile measurements. While it is not stipulated whether such measurements
1899 should be made using ozonesondes, lidar or microwave radiometer, the expectation is that an

1900 ozonesonde measurement programme would be a fundamental part of a GRUAN vertical ozone
1901 profile measurement programme.

1902 Scientifically, measurement scheduling for GRUAN ozonesonde programmes is likely to be
1903 driven by:

- 1904 • The needs of the stratospheric ozone change detection community. Ozonesonde flights need
1905 to be made sufficiently frequently to provide ozone time series suitable for detecting trends
1906 in the vertical distribution of ozone.
- 1907 • The needs of the air quality assessment community. Because ozone is a component of urban
1908 air quality, ozonesonde measurements need to be made sufficiently frequently to support air
1909 quality process studies.
- 1910 • The needs of the satellite validation community. To the extent possible ozonesonde launches
1911 should be timed to coincide with overpasses of satellite which are also making
1912 measurements of the vertical profile of ozone.

1913
1914 Ozonesonde protocols will continue to develop over time and, in the case of conflict between
1915 GCOS-171 guidelines and this Ozonesonde Technical Document, the schedule outlined in this
1916 Document shall take precedence (see Section 7.5 of GCOS-171).

1917
1918 Measurement scheduling for GRUAN ozonesondes is driven by one main factor: financial
1919 support for expendables which include the ozonesonde sensor, solutions, interface electronics,
1920 and the balloon payload. Once an ozonesonde is launched it is typically irretrievable. It is not
1921 common for sites to retrieve, re-condition, and re-launch the same sensor. Geography, land
1922 restrictions, weather, and additional resources can prohibit such rescue attempts. Schedules will
1923 depend upon available expendables and so there cannot be a proscriptive solution. GRUAN shall
1924 adopt the following schedule guidelines:

- 1925
1926 • In seeking a practical balance between sites with funding constraints and GRUAN
1927 scientific goals, GRUAN shall accept a minimum requirement of two times per month
1928 launches to be spaced every other week. Candidate GRUAN ozonesonde programme
1929 sites shall first be assessed according to their ability to meet the mandatory operating
1930 protocols defined in Section 5.3 of GCOS-171 and then according to the added value they
1931 bring to the network, as defined in Section 4.2.1.
- 1932 • A fully equipped GRUAN ozonesonde programme shall make weekly launches. If and
1933 when possible, GRUAN shall encourage candidate or newly certified sites to become a
1934 fully equipped GRUAN site.
- 1935 • Sites shall be expected to, in good faith, upload metadata and CRD to the
1936 RSLaunchClient utility as soon as the launch is complete and that site has successfully
1937 archived their metadata and CRD.
- 1938 • Sites shall commit to launching at around the same time of day. This is to maintain the
1939 representativeness and homogeneity of the data record. Variable launch times may affect
1940 the accuracy of trend assessments [Thompson et al., 2014].
- 1941 • To the extent possible, launches should be timed to coincide with satellite overpass times
1942 that measure total column ozone and/or vertical profiles of ozone.

1943 • Weather permitting; GRUAN advises launching the same day for bi-monthly to weekly
1944 sounding schedules. Altering a planned launch date due to inclement weather such as a
1945 natural disaster, strong winds, heavy rains, and storms that would impede a successful
1946 launch is expected. Altered scheduled launches shall be included as part of the annual
1947 report summaries.

1948 • Where possible, measurement schedules for redundant systems should be synchronized
1949 so as to avoid sampling biases when combining the measurements into a single data
1950 product.

1951 • Measurement scheduling shall remain stable unless there is a clear requirement for
1952 change, which would then have to be agreed with the relevant GRUAN sites.
1953 Amendments to the GRUAN measurement scheduling protocol shall follow guidelines
1954 outlined in Section 7.1 of this report.
1955

1956 When laboratory studies and dual ozonesonde launches are proposed, the regular launch
1957 schedule must not be interrupted.

1958 **6.1. General considerations from Section 7 of the GRUAN Guide**

1959 The candidate site shall work with the WG-GRUAN and TTR to define a measurement schedule
1960 that allow the resultant ozone data products to best capture all important scales of temporal
1961 variability, both for trend analysis and for process understanding.
1962

1963 In designing the Ozonesonde Programmes measurement schedule it will be necessary for the
1964 TTR and WG-GRUAN to work closely with individual sites since scheduling will be site
1965 specific. For example, some sites are more likely to (i) experience specific or unique atmospheric
1966 conditions related to the understanding of associated processes compared to other sites, (ii) be
1967 more financially constrained compared to other sites, and (iii) experience limit operating
1968 capabilities compared to other sites.
1969

1970 Given that task teams have a finite operating life, should the TTR no longer exist, this scheduling
1971 guidance responsibility shall fall to selected members of the WG-GRUAN who may include
1972 participants from the wider GRUAN community to assist with revising measurement scheduling
1973 protocols.
1974

1975 **7. MANAGING CHANGES**

1976 Changes in instrumentation, operating procedures, and data processing algorithms are likely to
1977 introduce sources of operational uncertainty into the ozone profiles measured within GRUAN
1978 Ozonesonde Programmes. The primary goals are to (i) avoid unnecessary changes, i.e. those
1979 changes that have no scientific, financial or operational benefit, and (ii) where changes are
1980 beneficial and/or necessary, to manage those changes in a way that the homogeneity of the
1981 ozonesonde data record is maintained across the transition and that the change does not
1982 compromise the integrity of the long-term record.
1983

1984 Ozonesondes have gone through several modifications since they were first introduced in the
1985 1960s and there is no reason to believe that those modifications will cease. Without such
1986 modifications there would be no opportunity to improve the performance of the instruments.
1987 Therefore, while GRUAN encourages ozonesonde manufacturers to improve the performance of
1988 the instruments, GRUAN also recognizes that managing such changes in instrument design or
1989 function is essential for maintaining long-term stability of the ozonesonde data products.

1990
1991 Factors influencing trends in an ozonesonde dataset to consider include the following changes
1992 (termed as “9 items” hereinafter):

- 1993
1994 1. SOP
1995 2. GOASS data processing algorithms
1996 3. ECC-sensor
1997 4. Solution concentration
1998 5. Location of launch site
1999 6. Operating environment of the ozonesonde
2000 7. Ground station system
2001 8. Radiosonde manufacturer
2002 9. Inclusion of refurbished ECC-sensors

2003
2004 These are all likely to introduce inhomogeneities into ozonesonde SGDP time series. This
2005 section describes the protocols for managing changes for a GRUAN Ozonesonde Programme.
2006 This section is developed based on the section “Managing change” of the GCOS-171 GRUAN
2007 Guideline.

2008 **7.1. Change Event Notification**

2009 A change event begins with the start of change of any one of the above “9 items”. The impact of
2010 new ozonesonde systems or changes to existing systems should be assessed by GRUAN prior to
2011 archiving with a suitable period of overlap between new and old items. This will be dictated by
2012 the GCOS-171 guidelines and is addressed further in Section 7.7. GRUAN recognizes that
2013 regular operations will continue regardless of GRUAN’s official acceptance.

- 2014 • The GRUAN site, in writing, shall first issue a change event notification to the
2015 GRUAN Lead Centre.
- 2016 • The Lead Centre, a GRUAN Ozonesonde Programme, an ozonesonde instrument
2017 manufacturer, or another member of the GRUAN community may also initiate a
2018 proposal for changes.
- 2019 • The Lead Centre must act as a clearinghouse for all proposed changes to (a) assure
2020 high stability and (b) decide when an improvement merits a change to the GRUAN
2021 ozonesonde procedures.
- 2022 ◦ The Lead Centre, in consultation with ozonesonde experts, makes an initial
2023 evaluation of the proposed change.
- 2024 ◦ If considered to be worth pursuing, the Lead Centre assesses the advantages,
2025 disadvantages, and potential impacts of the proposed change.

- 2026
- 2027
- 2028
- 2029
- 2030
- 2031
- *Justification of change:* Any change to the “9 items” 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, if relevant, should be included in the assessment report. Any relevant results in the peer-reviewed literature should be included in any change assessment.
- 2032
- 2033
- 2034
- 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.
- 2035
- 2036
- 2037
- *Preparing for change:* the Lead Centre must undertake a quantitative assessment of the impacts of any planned change before the GRUAN GOASS implements the change.
- 2038
- The assessment must cover a sufficient period of time, not just the change period.
- 2039
- 2040
- 2041
- 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)).
- 2042
- 2043
- 2044
- If additional laboratory studies or dual ozonesonde launches are required, such studies must be undertaken by with participation by the GRUAN site representatives and identified ozonesonde experts.
- 2045
- 2046
- A change event ends with the official acceptance of the change that has been made after a careful and rigorous assessment.

2047 **7.2. Guiding Principles?**

2048 The impact on the ozonesonde SGDP product and its uncertainty needs to be assessed in such a
2049 way that

- 2050
- 2051
- 2052
- 2053
- 2054
- 2055
- 2056
- 2057
- 2058
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 in terms of continuity, accuracy or integrity. 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.

2059 If the GRUAN Ozonesonde Programme decides to proceed and implement the change, any data
2060 and metadata collected as part of the change process must be recorded in the metadata submitted
2061 to the RSLaunchClient utility. This information will then be archived as part of that
2062 programme’s metadata record in the designated GRUAN archive.

2063

2064 *Validating impacts:* No discontinuities in the measurement series or schedule should occur if a
2065 change has been properly managed. This is done through the *justification* and *preparing for*
2066 *change* items in Section 7.1. Validation of the process can be achieved by subjecting the entire

2067 measurement series to homogenization tests, or may require a reprocessing of historical data.
2068 Impacts of changes must be assessed in light of the different intended uses of the SGDP.

2069
2070 *Change and uncertainty:* Knowledge of an ozonesonde measurement system can never be
2071 complete or perfect. Transitioning from an old to a new measurement system always introduces
2072 an additional source of uncertainty that must be captured in the uncertainty estimate on the
2073 measurements.

2074
2075 *Supporting reprocessing:* As new and more in-depth knowledge of ozonesonde instrumentation
2076 and processing is gained, reprocessing of historical data may be necessary. Such reprocessing
2077 may require revision of the homogenization procedures. It is essential, therefore, that original
2078 CRD data, as well as detailed metadata collected during change events, are archived so that
2079 such reprocessing can be done with minimal impact to the measurement accuracy.

2080
2081 *Single change requirement:* Whenever a measurement system is changed, as many similarities as
2082 possible between the old and new systems should be maintained e.g. both the ozonesonde and
2083 ground-station should not be simultaneously changed. Multiple simultaneous changes must be
2084 avoided so that the quantitative assessment of the impact of the change on the measurement and
2085 its uncertainty is not confounded with other simultaneous changes.

2086
2087 *Monitoring changes:* Most changes are planned and therefore can be managed. However, some
2088 changes may be unplanned (e.g. natural disaster, changes in funding). Under these
2089 circumstances, a GRUAN Ozonesonde Programme shall be placed on hold until the site can be
2090 re-established. It may be that re-certification is required. This shall be determined by a site visit
2091 from members of the Lead Centre (see Section 4.2).

2092
2093 *Use of independent, redundant measurements:* Redundancy in ozone measurement systems
2094 provides a powerful tool for validating the management of changes to the ozonesonde system. To
2095 take advantage of measurement system redundancy, it is essential that these independent systems
2096 are not changed simultaneously.

2097
2098 *Manufacturer involvement:* Efforts must be undertaken to avoid unknown changes e.g. the
2099 instrument manufacturer making unannounced changes. GRUAN needs to establish close
2100 working relationships with instrument manufacturers so that any changes implemented in the
2101 manufacturing of an instrument are made known to the GRUAN ozonesonde community.

2102 **7.3. Managing changes in instrumentation**

2103 Efforts must be undertaken to avoid unknown instrument changes e.g. the instrument
2104 manufacturer making unannounced changes to the material or configuration of the ECC sensor,
2105 or a ground station software update. Late response to changes or upgrade announcements may
2106 result in discrepancies in the measurement time series. One way to ensure that instrument
2107 changes are identified, characterized, and recorded such that there is no discontinuity in the
2108 network, as a whole, is for mandatory GRUAN representation at future JOSIE and other
2109 collaborative intercomparison studies. This will not only safeguard the homogeneity of datasets
2110 due to instrumentation changes but will also ensure that GRUAN (1) follows retractions or
2111 addenda to the original GAW Report No. 201 recommendations and SOP protocols, (2) be

2112 informed of changes in manufacturer design and materials, and how these affect ozonesonde
2113 performance, (3) be aware of changes in the processing software, and (4) be advised of
2114 additional concerns in the SOP.

2115
2116 GRUAN Lead Centre needs to establish close working relationships with ozonesonde instrument
2117 manufacturers (e.g. SPC and ENSCI) and ozonesonde/radiosonde ground station manufacturers
2118 (e.g. Vaisala, Modem, Chang Feng, etc) so that any changes to be implemented or having been
2119 implemented are known to them. Preferably the changes can be known substantially in advance
2120 of deployment, allowing sufficient time to investigate, understand, prepare for and document the
2121 change and its likely impacts.

2122 **7.4. Managing changes in SOP and operating environment**

2123 Currently, there are multiple variations in ozonesonde preparation procedures since the first
2124 manual was written [Komhyr, 1986]. Besides modifications in the manufacturer's instructions in
2125 past the decades, scientific institutions have established their own modified operating
2126 procedures. There are also a number of ozonesonde processing software systems that apply their
2127 own treatment of the variables that go into Equation 1. Smit et al., [2007] reports that
2128 maintaining SOP improves the precision of the overall measurements better than $\pm 3-5\%$.
2129 GRUAN recommends that each station maintain the GRUAN Lead Centre certified set SOP for
2130 pre-flight and day of flight conditioning established by WMO/GAW to ensure consistency and
2131 homogeneity in operating practices. The goal here is not to disrupt the continuity of the long-
2132 term practices.

2133
2134 As described in Section 4.5, while implementing these SOP is not mandatory, sites are required
2135 to document where they have deviated from the GRUAN certified SOP and, when audited, are
2136 assessed for their ability and willingness to adhere to the SOP within GRUAN.

2137
2138 Some changes in the operating environment may be unplanned, such as in the event of a natural
2139 disaster, erosion of the field site or land-use changes that necessitates moving the operating
2140 environment. Under these circumstances, a GRUAN Ozonesonde Programme shall be placed on
2141 hold until the physical site can be re-established. It may be that the new location is far enough
2142 away from the original location that a new GRUAN site needs to be established in place of the
2143 old site. The task team assigned by the Lead Centre shall determine this. In this case, re-
2144 certification will be required because the new location and operating conditions will need to be
2145 re-assessed. The process of re-certification shall follow the guidelines addressed in Section 4.2.
2146 In their annual report, each site shall document any changes to their current certified SOP and
2147 operating environment and include (1) why those changes occurred, (2) how those changes were
2148 managed, and (3) the impact, if any, on the homogeneity, accuracy, and integrity of their
2149 measurements.

2150
2151 GRUAN sites shall follow the change protocol outlined in Section 7.1 if changes to items (1) and
2152 (6) of the "9 items" occur.

2153 **7.5. Managing changes in data processing algorithms**

2154 As in any data processing situation, there will be occasional re-processing of the ozonesonde
2155 CRD after updates/upgrades of the GRUAN GOASS, addressed in Section 4.7. The GOASS
2156 must be transparent, i.e., developed and optimized in consultation with WG-GRUAN members.
2157 WG-GRUAN shall meet regularly to discuss the implementation of updates to the GOASS,
2158 whether they pertain to one site or the entire ozonesonde network. Planned changes in data
2159 processing algorithms should be dealt with in a fashion similar to planned changes in SOP.

2160

2161 Changes in the GOASS may be due to:

- 2162 1. New or modified transfer functions
- 2163 2. Updated uncertainty calculations
- 2164 3. Changes in the pump efficiency factors
- 2165 4. Changes in the partial ozone column calculation above balloon burst
- 2166 5. Changes in the metadata reporting

2167

2168 These changes will likely result in the complete reprocessing of entire data sets across the
2169 network. Since there is a time and administrative cost associated with the reprocessing of a
2170 record, such reprocessing should only be undertaken when justified.

2171

2172 Traceability is a leading component of GRUAN. Every single GOASS update must be associated
2173 with an increment of the data processing version. A system of traceable version numbers for all
2174 ozonesonde level products shall be developed to allow for a full identification and tracking of the
2175 data processing changes made since the initial product delivery. The Lead Centre task team shall
2176 determine this product versioning system (see Section 4.9).

2177

2178 Data processing updates must be communicated to users who have accessed earlier versions of
2179 the data and who have voluntarily registered to receive notifications of such data updates (see
2180 Section 8.6 of the GRUAN Guide). Therefore, all older product versions must be made available
2181 through the GRUAN archives.

2182 **7.6. Managing changes in calibration**

2183 When ozonesondes are calibrated to fundamental calibration standards (e.g. SOP) as part of the
2184 pre-flight ground-check, changes in sonde performance can be more easily managed. If possible,
2185 the impacts of a change in calibration should be quantified through traceability of the calibration
2186 standard. For example, the WCCOS in JOSIE studies satisfies the protocols for maintaining
2187 ozonesonde continuity, accuracy and integrity through periodic quality checks of instrumental
2188 performance of ozonesonde from different manufacturers, and establishing up-to-date SOP.

2189 It would ideal to establish guidelines by which a GRUAN Ozonesonde Programme can calibrate
2190 its ground station equipment such that sources of error and uncertainty can be further identified,
2191 traced, and included as part of the uncertainty budget for ozonesondes. Metadata also provides a
2192 traceable source from which a change in the essential characteristics of each unique ozonesonde
2193 sensor can be identified, measured, and recorded.

2194 **7.7. Validating changes using parallel observations**

2195 Cases where parallel observations are applicable to the ozonesonde programme are the following
2196 (hereafter called “4 cases”):

- 2197
- 2198 1. A new ECC sensor is developed
- 2199 2. A new sensing solution recipe is developed
- 2200 3. Change in SOP
- 2201 4. Change in radiosonde manufacturer and/or model
- 2202

2203 If any of the above changes occur, a combination of JOSIE studies, other laboratory inter-
2204 comparisons, and dual sonde launches must be made to establish (1) new precision and accuracy
2205 estimates, if any, (2) changes in uncertainties, and (3) new transfer functions to maintain
2206 homogeneity within a time series of a single site and within the network. While these studies are
2207 proposed and conducted, the regular observations schedule must not be interrupted. In the case
2208 when laboratory studies cannot be reconciled, this must be noted as part of the metadata. In this
2209 case, a proposal of how to resolve the discrepancy should be developed by the Lead Centre or a
2210 task force commissioned by the Lead Centre.

2211
2212 *Measurement redundancy*: Measurement redundancy (see Section 6.2 of GCOS-171) highlights
2213 the benefits for managing instrumentation change. If parallel observations of the above four
2214 changes are not feasible, the availability of additional redundant measurements with similar
2215 sampling attributes (vertical resolution, temporal sampling frequency etc.) is essential for
2216 validating a managed change.

2217
2218 *Inter-comparisons*: Formal measurement inter-comparisons, in the form of dual or multi-payload
2219 ozonesonde launches are essential for developing the in depth understanding required to manage
2220 changes in the “4 cases”. For this reason, participation in inter-comparison campaigns is
2221 expected. Outcomes from such inter-comparisons must form an important component of the
2222 metadata archived at the GRUAN Lead Centre. GRUAN Ozonesonde Programme should
2223 participate in, or leverage from WMO and partner networks (e.g. SHADOZ and NDACC)
2224 instrument inter-comparison campaigns.

2225 **7.8. Implementation of Network-wide changes**

2226 Considering the critical importance of change management and that GRUAN sites should not act
2227 unilaterally in implementing changes without informing the GRUAN Lead Centre, a procedure
2228 for implementing network-wide changes has been described in Section 2.3.11 of the GRUAN
2229 Guide to Operations.

2230
2231 The Lead Centre should consult with ozonesonde experts (e.g. members of the ASOPOS panel),
2232 science experts from the four key user communities, and other ozonesonde archive centres such
2233 as SHADOZ and NDACC to thoroughly evaluate the potential implications of network wide
2234 implementation of the proposed change. If the proposed change is approved, the Lead Centre, in
2235 consultation with the nominated central processing facility, will develop a formal change plan for
2236 implementation across the network. The formal change plan is then communicated to all
2237 GRUAN Ozonesonde Programmes within the network.

2238 **7.9. Data and metadata traceability**

2239 It is essential that metadata capture information regarding any change events (see Section 7.1).
2240 Metadata must tie the new SGDP via a comparable traceability chain, back to the same
2241 recognized standard as the old SGDP. Detailed archiving of instrument metadata will be vital to
2242 managing changes in instrumentation.

2243
2244 *Storage:* It is essential that digital storage of metadata and CRD be maintained at each GRUAN
2245 site. Each Ozonesonde Programme's data storage policy shall be evaluated by the WG-GRUAN
2246 as part of the site assessment and certification process (Section 4.2), and re-evaluated in audits
2247 and annual reports.

2248
2249 *Metadata changes from the GRUAN check list:* As described in Section 4.6, while using the
2250 GRUAN check list is not mandatory, sites are required to document where they have deviated
2251 from the prescribed check list and, when audited, are assessed for their ability and willingness to
2252 adhere to them within GRUAN.

2253

2254 **8. Quality Management**

2255 This section defines the principles and framework for GRUAN operations, and details how
2256 activities will be coordinated to manage and control data quality within GRUAN. This section
2257 draws heavily from Section 10 of GCOS-171 and reiterates much of the data management
2258 policies central to all GRUAN measurement programmes.

2259

2260 Quality management is required at all points in the measurement process from network planning
2261 and training, through installation and site operations, to data transmission and archiving. Quality
2262 management within GRUAN consists of quality assurance and quality control:

2263

2264 *Quality assurance (QA):* The purpose of quality assurance is to provide confidence that the
2265 requirements for achieving quality are fulfilled. QA includes all the planned and systematic
2266 activities that will be implemented such that quality requirements for a product or service are
2267 fulfilled.

2268

2269 *Quality control (QC):* The purpose of quality control is to ensure that the expectations created by
2270 QA are fulfilled. QC is associated with those operational methods, techniques and activities used
2271 to ensure that the quality requirements (as defined by QA) are fulfilled.

2272

2273 The GRUAN quality management policy is to achieve a level of data quality that allows the
2274 primary goals of GRUAN to be met for all potential users of GRUAN data products. QA and QC
2275 are both required at all stages of the GRUAN ozonesonde data production. Because SGDP are
2276 intended to be used for long-term trend detection, quality assurance and control are further
2277 extended to data re-processing (addressed in Section 7 of this Document).

2278

2279 Methods by which QA for Ozonesonde Programmes can be achieved is through the following:

2280

- 2281 1. The use of redundant measurements, as described in Section 5.3, serves to assure the
2282 quality of the GRUAN data products. Agreement of two independent measurements (e.g.

2283 Lidar and Microwave Radiometer), preferably based on different measurement
2284 principles, provides a high degree of confidence that no significant systematic effect was
2285 disregarded and uncertainties were not under-estimated.

- 2286
- 2287 2. Laboratory tests are fundamental methods for establishing and confirming uncertainty
2288 estimates and transfer functions for GRUAN data products. Laboratory tests provide an
2289 opportunity to investigate, in detail, the performance of instruments under controlled
2290 conditions and to measure differences against certified references or other standards (e.g.
2291 JOSIE). Data from these experiments can be used to detect biases that may be corrected
2292 for and to determine calibration uncertainties.
 - 2293 3. Field inter-comparisons (dual or multi sonde launches on a single payload) allow multiple
2294 in-situ sensors to be directly compared under the actual atmospheric conditions of the
2295 required measurement, including the complex environmental conditions (temperature,
2296 humidity, pressure, wind/flow rate, radiation, and chemical composition) that cannot be
2297 fully reproduced in the laboratory. These complementary activities increase confidence
2298 that measurements are subject to neither unanticipated effects nor undiscovered
2299 systematic uncertainties. Therefore field experiments are particularly useful for assuring
2300 the quality of GRUAN data products.

2301

2302

2303 QC will be achieved through the application of the various measurement protocols defined in this
2304 Document and in related measurement system documents (e.g. Lidar, Radiosonde technical
2305 documents). To the extent possible, visual inspection of all data by science/instrument experts
2306 will be required for ozonesondes to minimize anomalies that slip through automated routines.
2307 The Lead Centre shall coordinate this effort, which shall be distributed across different GRUAN
2308 sites and other interested parties as deemed appropriate including task teams and members of
2309 WG-GRUAN. Uncertainty estimates covered in Section 3 of this Document will be used as a
2310 metric to compare the site-to-site quality of the observations.

2311

2312 A key aspect of quality management within GRUAN will be fulfilling customer requirements.
2313 To this end, systems shall be developed to:

- 2314
- 2315 1. Inform users of GRUAN products of site-specific or network-wide changes in
2316 measurements systems.
 - 2317 2. Provide an incident reporting system that can flag data anomalies to users.
 - 2318 3. Inform users of updates to previously accessed data products.
 - 2319 4. Provide “help desk” support to users of GRUAN data products.

2320 **8.1. Assuring the quality of GRUAN Ozonesonde Programmes**

2321 Ozonesonde sites vary in levels of maturity (length of operation), resource (launch frequency),
2322 and possess varying levels of infrastructure (air-conditioned versus ambient laboratory
2323 conditions) and financial support (piecemeal, intermittent, or stable funding). The purpose of
2324 quality management is to ensure that GRUAN data meet the requirements in terms of
2325 uncertainty, resolution, continuity, homogeneity, representativeness, and timeliness for their
2326 intended use.

2327

2328 Five critical components are required to assure the long-term quality of GRUAN Ozonesonde
2329 Programmes:

2330

- 2331 1. Maintaining consistent, up-to-date SOP to minimize systematic errors and lend
2332 confidence in the observed trends.
- 2333 2. GRUAN-specific training of the representative and ozonesonde technicians of candidate
2334 ozonesonde sites, the purpose of which is to ensure that the latest GRUAN-recommended
2335 best practices for ozonesonde operations are observed.
- 2336 3. The RSLaunchClient utility, the purpose of which is to upload, the raw measurement data
2337 and metadata to the GRUAN central ozonesonde data processing facility.
- 2338 4. The GOASS, the purpose of which is to analyze, in a consistent manner, the CRD and to
2339 generate the ozonesonde SGDP.
- 2340 5. Maintaining documentation and statistics on flagged metadata and data and significant
2341 data gaps are to be used as a diagnostic tool as part of the quality control assessment and
2342 to ensure the continuity of individual GRUAN Ozonesonde Programmes.

2343

2344 Routine testing through intercomparison peer-reviewed studies of new ECC models, changes in
2345 instrument design, or solution recipes will help to ensure confidence in observed trends in the
2346 future. Therefore, as part of the QA for ozonesondes that are in routine use, GRUAN shall follow
2347 protocols established by the Forschungszentrum Jülich that houses the World Calibration Center
2348 for Ozone Sondes (WCCOS). The simulation facility enables control of pressure, temperature
2349 and ozone concentration and can simulate flight conditions of ozone soundings up to an altitude
2350 of 35 km, whereby a UV photometer serves as a reference [Smit et al., 1998]. The long-term
2351 objective of WCCOS is to ensure three major QA-tasks:

- 2352 1. QA-Procedures: Establishment and up-date of SOP of different sonde types.
- 2353 2. QA-Manufacturers: Performance check of ozonesondes from different manufacturers.
- 2354 3. QA-Operation: Evaluation of ozonesonde operating practice of difference sounding
2355 laboratories.

2356 **8.2. Ozonesonde data product validation**

2357 Quality control at the CRD level is performed in two steps, first through uploads of the original
2358 data and associated metadata through the RSLaunchClient utility, then through the threshold
2359 quality checks at the early processing stage of the GOASS (selection criteria are addressed in
2360 Table 4.7.1 in Section 4.7). The suitability check of the CRD and metadata to be accepted as part
2361 of the GOASS processed stream serves as a means to verify the completeness of the information
2362 required by the RSLaunchClient.

2363

2364 Ozone profiles from GRUAN Ozonesonde Programmes will, in the first instance, be validated
2365 against available redundant ozone profile measurements made at GRUAN sites. Multiple
2366 measurements of ozone will be invaluable for identifying, understanding and reducing systematic
2367 effects in ozonesonde measurements. The cross-checking of redundant measurements for
2368 consistency should be an essential part of the GRUAN quality assurance procedures. Since all
2369 data are to be reported with uncertainties, a consistency check should, in principle, be a
2370 straightforward task.

2371

2372 Satellite-based measurements of total column ozone (e.g. OMI, GOME-2, TROPOMI) and
2373 profiles of ozone in the lower stratosphere (e.g. Aura/MLS, SAGE III) are common reference
2374 measurements that can be used to assess the quality of ozonesonde observations. GRUAN shall,
2375 where practical, schedule ozonesonde launches in near real-time (i.e. within 2 hours of a satellite
2376 overpass) to fulfill the requirement of providing a reference to satellite measurements.
2377

2378 In addition, GRUAN Ozonesonde Programmes are encouraged to participate in field campaigns
2379 that include measurements from an independent instrument, i.e. UV photometer. If two
2380 measurements are known to be dependent, the degree of this dependence as well as its
2381 consequences must be specifically described and taken into account in the product assessment.
2382 As stated in Section 10 of the GCOS-171, “Agreement of two independent measurements,
2383 preferably based on different measurement principles, provides a high degree of confidence that
2384 no significant systematic effect was disregarded and uncertainties were not underestimated”.

2385 **8.3. Performance monitoring system**

2386 Applying the principles described in Section 10 of the GCOS-171 to GRUAN Ozonesonde
2387 Programmes, performance monitoring is a non-real-time activity in which the performance of an
2388 individual GRUAN Ozonesonde Programme, or of an ensemble of GRUAN Ozonesonde
2389 Programmes, is examined for trends and systematic deficiencies. Performance monitoring within
2390 GRUAN Ozonesonde Programmes is primarily the responsibility of the Lead Centre and the
2391 TTR.
2392

2393 Certification and re-certification of GRUAN Ozonesonde Programmes is an essential component
2394 of performance monitoring. Examples of quantitative performance indicators are:
2395

- 2396 1. Ozonesonde SGDP downloads.
- 2397 2. Number of candidate sites wishing to become a GRUAN Ozonesonde Programme.
- 2398 3. Number of GRUAN sites participating in JOSIE and inter-comparison field campaigns,
2399 and conducting laboratory studies whose results appear in peer reviewed journals.
- 2400 4. The number of peer reviewed publications in which GRUAN ozonesonde data products
2401 have been used.
- 2402 5. The number of GRUAN Ozonesonde Programmes funded through national or
2403 international funding agencies.
2404

2405 All above indicators serve to provide a year-to-year traceability of GRUAN ozonesonde
2406 programmes' impact within the climate community.
2407

2408 **ACRONYMS**

- 2409 *ASOPOS*: Assessment of Standard Operating Procedures for Ozone Sondes
2410 *BESOS*: Balloon Experiment on Standards for Ozone Sondes
2411 *CRD*: Converted Raw Data
2412 *DMT*: Droplet Measurement Technologies
2413 *ECC*: Electrochemical concentration cell
2414 *ECV*: Essential Climate Variable
2415 *GATNDOR*: GRUAN Analysis Team for Network Design and Operations Research
2416 *GAW*: Global Atmosphere Watch
2417 *GCOS*: Global Climate Observing System
2418 *GOASS*: Ozone sonde Analysis Software System
2419 *GOME-2*: Global Ozone Monitoring Experiment-2
2420 *GPS*: Global Positioning System
2421 *GRUAN*: GCOS reference upper-air network
2422 *IGACO*: Integrated Global Atmospheric Chemistry Observations
2423 *IGPD*: Integrated GRUAN Product Data
2424 *IMet*: Internet (radiosonde)
2425 *IOC*: Intergovernmental Oceanographic Commission
2426 *JOSIE*: Jülich Ozone Sonde Inter-comparison Experiment
2427 *LMS*: Lockheed Martin Sippican
2428 *NDACC*: Network for the Detection of Atmospheric Composition Change
2429 *NCAR*: National Center for Atmospheric Research
2430 *NCEI*: National Centers for Environmental Information
2431 *NMI*: National Metrological Institute
2432 *NOAA*: National Oceanic and Atmospheric Administration
2433 *OMI*: Ozone Monitoring Instrument
2434 *PCF*: Pump correction factors
2435 *CRD*: Primary Raw Data
2436 *SAG*: Science Advisory Group
2437 *SASBE*: site atmospheric state best estimates
2438 *SGDP*: Standard GRUAN Product Data
2439 *SHADOZ*: Southern Hemisphere ADditional OZonesondes
2440 *SPARC*: Stratosphere-troposphere Processes And their Role in Climate
2441 *SPC*: Science Pump Corporation
2442 *Suomi-NPP*: Suomi National Polar-orbiting Partnership
2443 *TEI*: Thermo Environmental Instruments
2444 *TTR*: Task Team on Sondes
2445 *UTLS*: Upper Troposphere Lower Stratosphere
2446 *WCCOS*: World Calibration Center for Ozone Sondes
2447 *WG-GRUAN*: Working Group on GRUAN
2448 *WIGOS*: WMO Integrated Global Observing Systems
2449 *WMO*: World Meteorological Organization
2450 *WOUDC*: World Ozone and Ultraviolet Data Centre

2451 **Appendix A.1: SHADOZ SOP CHECK LIST**

2452 **Version: Mar 01, 2017 SHADOZ DIGITAL OZONESONDE CHECKLIST**

2453

2454 **INITIAL PREPARATION - NO LESS THAN 3 DAYS BEFORE FLIGHT.**

2455

2456 OPERATOR INITIALS: _____

2457 *FLT* # _____

2458 DATE (YYYYMMDD): _____ Station: _____

2459 O₃ SONDE SERIAL #: _____

2460 SOLUTION STRENGTH (1%, 0.5%, other) _____

2461 1. Run 10 minutes on *no* O₃ air: _____ (✓)

2462 2. PUMP CURRENT: _____ (μA)

2463 3. PUMP PRESSURE: _____ (psi)

2464 4. PUMP VACUUM: _____ (in Hg)

2465 5. Bypass Cathode chamber: Yes _____ No _____

2466 6. Add 5-6cc Cathode solution: _____ (✓)

2467 7. Run 30 minutes on *HIGH* O₃: _____ (✓)

2468 8. Run 5 minutes on *no* O₃: _____ (✓)

2469 9. Dump Cathode solution: _____ (✓)

2470 10. ADD _____ (✓) 2.5CC or _____ (✓) 3.0 CC FRESH CATHODE (Wait 2 min): _____ (✓)

2471 11. ADD 1.5 CC ANODE SOLUTION: _____ (✓)

2472 12. Run 10 minutes on *no* O₃: _____ (✓)

2473 13. RECORD O₃ CURRENT: _____ μA

2474 14. Run 10 minutes at 5μA O₃ _____ (✓) - then switch to *no* O₃ air.

2475 15. RECORD TIME TO DROP FROM 4.0 TO 1.5 μA: _____ sec.

2476 16. Run 10 minutes on *no* O₃: _____ (✓)

2477 17. RECORD O₃ CURRENT: _____ μA

2478 18. Add additional _____ (✓) 2.5CC or _____ (✓) 3.0 CC of CATHODE : _____ (✓)

2479 19. Short the cell leads and store in Styrofoam box: _____ (✓)

2480

2481 **IF DORMANT AFTER 1 WEEK REPLACE SOLUTIONS.**

2482 **DATE (YYYYMMDD) :** _____

2483

2484 1. CHANGE CATHODE SOLUTION: _____ 3cc or _____ 2.5cc (✓)

2485 2. CHANGE ANODE SOLUTION (1.5cc): _____ (✓)

2486 3. Run 5 minutes on *no* O₃ _____ (✓)

2487 4. RECORD O₃ CURRENT: _____ μA

2488 5. Run 5 minutes on 5μA O₃ _____ (✓)

2489 6. Switch to *no* O₃: _____ (✓)

2490 7. RECORD TIME TO DROP FROM 4.0 TO 1.5 μA: _____ sec

2491 8. Run 10 minutes on *no* O₃ – RECORD CURRENT: _____ uA

2492 9. Short cell leads and Store in Styrofoam box: _____ (✓)

2493

2494 **DAY OF FLIGHT PREPARATION IN LAB.**

2495

2496 OPERATOR INITIALS: _____

2497 DATE (YYYYMMDD): _____

2498

2499 1. Cathode solution # and date of bottle (*if applicable*): _____
 2500 2. CHANGE CATHODE SOLUTION: ____3cc or ____2.5cc (√)
 2501 3. CHANGE ANODE SOLUTION (1.5cc): ____ (√)
 2502 4. Run 10 minutes on *no* O₃: ____ (√)
 2503 5. RECORD O₃ CURRENT: BG#0 = _____ μA
 2504 6. Run 10 minutes at 5μA O₃: ____ (√)
 2505 7. Switch to *no* O₃: ____ (√)
 2506 8. RECORD TIME TO DROP FROM 4 TO 1.5 μA: _____ sec.
 2507 9. RUN 10 MINUTES ON *no* O₃ and RECORD O₃ CURRENT: BG#1 = _____ μA
 2508 10. ROOM TEMP (C): _____, ROOM RH (%): _____, ROOM Pressure (hPa) _____
 2509 11. Flow rate Correction (*if calculated*): _____ %
 2510 12. RECORD T100 FLOWRATE TIMES:
 2511 FLOWRATE #1: _____ sec
 2512 FLOWRATE #2: _____ sec
 2513 FLOWRATE #3: _____ sec
 2514 FLOWRATE #4: _____ sec
 2515 FLOWRATE #5: _____ sec
 2516 AVERAGE T100: _____ sec

DAY OF FLIGHT AT THE LAUNCH SITE.

2518
 2519 OPERATOR INITIALS: _____
 2520 RADIOSONDE TYPE/Model (Vaisala RS92, Modem M10, etc): _____
 2521 RADIOSONDE SERIAL #: _____
 2522 INTERFACE #: _____
 2523 O₃ BACKGROUND CURRENT BEFORE FLIGHT BG#2: _____ μA
 2524
 2525 GMT Date (YYYYMMDD): _____
 2526 LOCAL date (YYYYMMDD): _____
 2527 GMT Launch Time (HH:MM:SS): _____
 2528 LOCAL Launch time (HH:MM:SS): _____
 2529
 2530 BALLOON SIZE: _____ Grams: _____
 2531 BALLOON TYPE: TOTEX ____ Hwoyee ____ PAWAN ____ (√ one)
 2532 NOAA FPH Serial # (*if applicable*): _____
 2533 Other instruments: _____
 2534
 2535 SURFACE PRESS: _____ (hPa) SURFACE WIND SPEED: _____ (m/s)
 2536 SURFACE TEMP: _____ (C) SURFACE WIND DIR: _____ (deg)
 2537 SURFACE RH: _____ (%)
 2538
 2539 Dobson (*if available*): _____ (DU)
 2540 Brewer (*if available*): _____ (DU)
 2541 Other (*if available*): _____ (DU)
 2542
 2543
 2544 Sky Conditions and Remarks:

2545 **Appendix A.2: RECOVERED OZONESONDE CHECK LIST**

2546 *Follows the NOAA/ESRL/GMD Check list*

2547

2548 DATE (YYYYMMDD): _____

2549 OPERATOR INITIALS: _____

2550

2551 Was this a ozonesonde recovered on day of flight? ____ Yes/No

2552 If No, how many days between launch and recovery? ____ days

2553

2554 **HISTORY:**

2555 O₃ PUMP SERIAL #: _____

2556 FORMER FLIGHT #: _____

2557 DATE FLOWN (YYYYMMDD): _____

2558 DATE FOUND (YYYYMMDD): _____

2559 DATE RETURNED (YYYYMMDD): _____

2560

2561 **COMMENTS: OVERALL SONDE/PUMP CONDITION:** (looks new, dirt or coloring around
2562 pump present, signs of corrosion anywhere, 0-ring condition, pump noisy?, etc.)

2563

2564

2565

2566

2567

2568

2569

2570

2571 **INITIAL RINSE/RECONDITIONING – SOON AFTER DELIVERY:**

2572

2573 Check that the cam that drives the piston is not turning off-center, loose or rubbing too close to
2574 the metal frame. If it is too close or has come loose then the sonde will be noisy and run with a
2575 high current. Sonde should not be flown in this case.

2576

2577 Rinse off outside of cells with warm tap water. ____ (√)

2578 Squirt De-ionized water (DIW) through running pump inlet (2 or 3 times for about 5 seconds).

2579 ____ (√)

2580 Rinse cells and tubing with DIW. ____ (√)

2581 Fill cells about ¾ full of DIW. ____ (√)

2582 Store sheet and ozonesonde until ready for the 3-7 day pre-condition. ____ (√)

2583 Date stored on shelf until ready for the 3-7 day pre-condition (YYYYMMDD):

2584 _____

2585

2586 **During normal pre-conditioning preparations**, an ozone calibrator, e.g. TEI, is strongly
2587 recommended to test the performance of the refurbished sonde. Re-conditioned sondes should
2588 not be flown if the sonde values are $\pm 5\%$ of calibrated source.
2589

2590 **PRE-CONDITIONING CALIBRATION PROCEDURES:**

2591 **DATE (YYYYMMDD):** _____

2592 Operator Initials: _____

2593 Calibration Instrument/Model: _____

2594 Calibration Serial Number: _____

2595 1. Run 50 ppbv O₃ for 10 minutes: ____ (√)

2596 2. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ____

2600 3. Run 100 ppbv O₃ for 10 minutes: ____ (√)

2601 4. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ____

2602 5. Run 150 ppbv O₃ for 10 minutes: ____ (√)

2603 6. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference:

2604 _____

2605 7. Run 200 ppbv O₃ for 10 minutes: ____ (√)

2606 8. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ____

2607 9. Run 50 ppbv O₃ for 10 minutes: ____ (√)

2608 10. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference:

2609 _____

2610 11. Run *no* ozone air for 10 minutes: ____ (√)

2611 12. Record: CALIBRATOR: _____ ppbv OZONESONDE: _____ ppbv % Difference: ____

2612 If the percentage differences for the 100 ppbv and ozone-free air exceeds $\pm 5\%$ do not fly re-used
2613 sonde.
2614

2615

2616

2617 FINAL COMMENTS:

2618

2619

2620

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