1 2 3 4 5	Ozonesonde Quality Assurance: The JOSIE-SHADOZ (2017) Experience
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52 Abstract. The ozonesonde is a small balloon-borne instrument that is attached to a standard 53 radiosonde to measure profiles of ozone from the surface to 35 km with ~100-m vertical 54 resolution. Ozonesonde data constitute a mainstay of satellite calibration and are used for 55 climatologies and analysis of trends, especially in the lower stratosphere where satellites are 56 most uncertain. The electrochemical-concentration cell (ECC) ozonesonde has been deployed at 57 ~100 stations worldwide since the 1960s, with changes over time in manufacture and procedures, 58 including details of the cell chemical solution and data processing. As a consequence, there are 59 biases among different stations and discontinuities in profile time-series from individual site 60 records. For 22 years the Jülich [Germany] Ozone Sonde Intercomparison Experiment (JOSIE) 61 has periodically tested ozonesondes in a simulation chamber designated the World Calibration 62 Centre for Ozonesondes (WCCOS) by WMO. In October-November 2017 a JOSIE campaign 63 evaluated the sondes and procedures used in SHADOZ (Southern Hemisphere Additional 64 Ozonesondes), a 14-station sonde network operating in the tropics and subtropics. A distinctive feature of the 2017 JOSIE was that the tests were conducted by operators from eight SHADOZ 65 66 stations. Experimental protocols for the SHADOZ sonde configurations, which represent most 67 of those in use today, are described, along with preliminary results. SHADOZ stations that 68 follow WMO-recommended protocols record total ozone within 3% of the JOSIE reference 69 instrument. These results and prior JOSIEs demonstrate that regular testing is essential to 70 maintain best practices in ozonesonde operations and to ensure high-quality data for the satellite 71 and ozone assessment communities. 72 **Capsule:** Data from ozonesondes form a backbone of satellite algorithms and monitoring 73 stratospheric ozone recovery. The ozonesonde community regularly evaluates sonde procedures

and instrumentation, as in this experiment featuring operators from the tropical SHADOZ

- 75 network.
- 76

#### 77 JOSIE History and Background

78 The periodic ozone assessments sponsored by WMO/UNEP (1991; 1995; 2011; 2015) and 79 related studies have long recognized the role of ozonesondes in the suite of global observations 80 because sondes are the only technique practical for in-situ monitoring of profiles. The sonde 81 instrument is easy to deploy in remote locations and is relatively inexpensive. Sondes operate in 82 both troposphere and stratosphere (Sidebar 1) and in clouds, precipitation and periods of 83 darkness. Most important, as they ascend, ozonesondes measure ozone with an effective 84 resolution of 100-150 m, far better than satellites. Indeed, sondes, like the ground-based 85 networks of lidar, Dobson and other spectrometers, constitute an essential component of satellite 86 calibration and cross-calibration (Fishman et al., 2008; Hubert et al., 2016; Steinbrecht et al., 87 2017; Tarasick et al., 2018). The vertical structure of ozone as measured at a typical tropical 88 station appears in Sidebar 1, along with background on ozone in the atmosphere. Although 89 dozens of stations began launching ozonesondes in the 1970s and 1980s, the concepts of 90 standardizing and testing instruments in a coordinated network, did not evolve until the 1990s 91 (Mohnen, 1996; Melamed et al., 2015). This was the period when both the Jülich Ozone Sonde 92 Intercomparison Experiment (JOSIE) and Southern Hemisphere Additional Ozonesondes 93 (SHADOZ) project began.

94 [Insert Sidebar 1 Here]

Over 50 years of ozonesonde data-taking, there have been several instrument designs.
Furthermore, as instruments have changed and preparation and data-processing techniques have
evolved over time, time series of data from individual stations often display discontinuities and
gaps that lead to inhomogeneous data records. Thus, the reliability of ozonesonde trends was

99 questioned in some of the earlier ozone assessments (WMO/UNEP 1991; 1995;

100 SPARC/IOC/GAW, 1998) (See Acronym List).

101 Two approaches have been used to address these deficiencies. First, evaluations of 102 ozonesonde types in a controlled laboratory environment were undertaken in the 1990s, a process 103 that continues periodically to this day. Second, in a similar manner, by testing different sonde 104 preparation methods and protocols for data recording and processing, a set of standard operating 105 procedures (SOP; Smit et al., 2014) was developed through consensus with the ozonesonde 106 research community. Finally, there are recommended methods for reprocessing long-term 107 records compromised by inhomogeneities (Smit et al., 2012, Deshler et al., 2017). 108 The need to have recommended instruments and procedures for emerging WMO/GAW 109 stations in the 1990s provided a framework for the first intercalibration and intercomparisons of 110 existing ozonesonde types. In order to assess the performance of the various ozonesonde 111 instrument types used within GAW, the environmental simulation chamber (ESC) at the 112 Forschungszentrum Jülich (FZJ, Germany) was established as the World Calibration Centre for 113 Ozone Sondes (WCCOS) in 1996. The chamber enables control of pressure, temperature, and 114 ozone concentration as it simulates flight conditions of ozone soundings up to an altitude of 35 115 km (Smit et al., 2000). This controlled environment and comparison of the ozonesonde profiles 116 with an accurate UV-photometer as a reference (Proffitt and McLaughlin, 1983) are essential 117 requirements for addressing instrument issues that arise from field and laboratory operations. 118 The initial JOSIE, performed in 1996 (Smit and Kley, 1998), was the first GAW activity 119 directed toward implementing a global quality assurance plan for ozonesondes in routine use. 120 By now, JOSIE experiments have provided over twenty years of ozonesonde data quality 121 assurance to the larger atmospheric research and remote sensing communities. JOSIE-1996 was 122 attended by eight laboratories from seven countries representing the major types of ozonesondes:

123 Electrochemical Concentration Cell (ECC) sondes of two manufacturers, the Brewer/Mast sonde 124 (BM-original), the Indian sonde (a modified BM-type), and the Japanese Meisei sonde (KC79). 125 JOSIE-1996 revealed important information not only about ozonesonde performance but also the 126 influence of operating procedures for sonde preparation and data correction that often varied 127 among the participating laboratories. The succession of JOSIE campaigns (Table 1) has shown 128 that there is an on-going need to evaluate ozonesondes because the instruments, preparation 129 procedures, and/or the sensing solutions are modified, often inadvertently, over time. Routine 130 testing of newly manufactured ozonesondes on a regular basis coupled with better 131 standardization of operating procedures help ensure more confidence in the data itself as well as 132 trends calculated from the data.

The overall objective of WCCOS and the JOSIE series of experiments has been the establishment of a facility for ozonesonde quality assurance (QA) that can be used by sonde manufacturers and the research community. Instrumental performance of sondes from different manufacturers is tested through comparison of profiling capabilities with a standard ozone profile that simulates a typical ascent in polar, mid-latitude or tropical conditions. Regular evaluation of procedures and methods at long-term ozone sounding stations with a single ozone reference instrument ensures the traceability and consistency of the records.

Over time, the SOP have been established and updated as needed. The first major SOP documentation appeared as a WMO/GAW Report (#201; See Smit and ASOPOS, 2014) with major contributions from prior reports and Smit et al. (2007). GAW 201 was also based on field tests of the major sonde types used in the JOSIEs up through 2009. A gondola of 18 instruments was flown along with same UV-photometer used in JOSIE-2000 as reported in Deshler et al. (2008).

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## SHADOZ and Unresolved Sonde Issues

148 The SHADOZ network began in 1998 as an international partnership to enhance the 149 number of tropical ozone soundings from operational stations (Thompson et al., 2003a,b; 2004; 150 2007; 2011). SHADOZ uses ECC ozonesondes that, over time, have been coupled with a variety 151 of radiosondes (Table 2). A history of ozonesonde-radiosonde pairings used at SHADOZ sites 152 appear in archival papers (Thompson et al., 2003a,b; Thompson et al., 2007; Witte et al., 2017). 153 At the time SHADOZ began, all known operational stations were in the southern hemisphere, but 154 gradually northern hemisphere stations joined: Kuala Lumpur, Paramaribo, Costa Rica; Hanoi, 155 and Hilo. The 14 long-term stations, defined as operating at least a decade during SHADOZ, 156 appear in Fig. 1. More than 7000 sets of ozone and pressure-temperature-humidity profiles from 157 SHADOZ are available at the website: https://tropo.gsfc.nasa.gov/shadoz. 158 Periodic evaluations of SHADOZ data have examined three parameters. First, total 159 column ozone (TCO) from the sonde, with an appropriate extrapolation above balloon burst, e.g., 160 McPeters and Labow, (2012), is compared to TCO from co-located ground-based instruments 161 (Brewer, Dobson, SAOZ) and satellite overpasses. Second, stratospheric profiles are compared 162 to satellite overpass ozone profiles from instruments like SAGE II (to 2005), SBUV (entire 163 record, 1998-2016) or Aura's MLS (2005-). Third, for the tropical stations (generally within 18° 164 latitude of the equator), stratospheric column ozone and profiles are compared. The tropical 165 TCO is typically constant to within 3-5 DU (Dobson Units), so measurement biases from station 166 to station can be identified (Thompson et al., 2017). 167 The first three years of SHADOZ TCO compared to the EP/TOMS satellite TCO disagreed 168 by  $\sim 8\%$  on average, with a number of stations displaying a discrepancy of greater than 10%; the 169 sonde TCO was usually lower than the satellite (or ground-based instrument). After the JOSIE-170 2000 campaign (Smit et al., 2007), in which the instruments and techniques used at all the

171 SHADOZ stations were tested, several stations changed their sensing solution type (SST), 172 resulting in reduced offsets (Thompson et al., 2007). Further changes in sonde preparation 173 procedures and subsequent reprocessing of the data, both in accordance with WMO/SPARC/ 174 IOC/NDACC guidelines (Smit and O3S-DQA, 2012; Smit and ASOPOS, 2014), brought TCO 175 for 12 of 14 stations to within 2% of TCO from three BUV-type satellites (EP/TOMS, OMI and 176 OMPS) operating over the 1998-2016 period (Thompson et al., 2017); the remaining two stations 177 show TCO data averaging within 5% of the satellite TCO. These improvements derive from the 178 application of "transfer functions" that relate a profile from each instrument–SST combination to 179 data from the standard reference. Each profile in a time-series is examined for possible

180 correction (Witte et al., 2017; 2018).

181 Although the reprocessing of prior SHADOZ data has greatly reduced systematic variations 182 in the record, JOSIE-SHADOZ was designed to address several outstanding issues. First, transfer 183 functions determined by Deshler et al. (2017) are used to homogenize SHADOZ readings that 184 are taken with different SST and/or instruments. This includes the 1%, KI, 0.1% buffer SST 185 used at stations supported by NOAA since the mid-2000s (Sterling et al., 2018). Second, a few 186 stations in SHADOZ changed SST unintentionally and introduced discontinuities in station time-187 series (Thompson et al., 2017; Witte et al., 2017; 2018). Finally, several stations employing a 188 given sonde type show sharp discontinuities after 2014 that appear to originate with changes in 189 manufacture (Sterling et al., 2018; Thompson et al., 2017).

190 [Insert Sidebar 2 here]

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## 192 JOSIE-SHADOZ-2017 Goals

193 Similar to prior JOSIE campaigns, the major objectives of JOSIE-SHADOZ are:

194 1. Evaluate ozonesonde instrument performance, specifically the pump and sensor as delivered

195		by the ECC-sonde manufacturer. Most of the SHADOZ stations operate with WMO-
196		recommended solutions and preparation and calibration procedures that allow the
197		experimenters to update typical performance of the instruments relative to the Ozone
198		Photometer (OPM) reference instrument (Proffitt and McLaughlin, 1983).
199	2.	Evaluate current preparation and operating procedures of each SHADOZ station. Unlike
200		prior JOSIE experiments, in 2017 personnel representing the practices of all currently
201		operating SHADOZ stations participated (Tables 2 and 3; see Sidebar 2). In most cases the
202		operators supplied solutions as prepared at their home institution. In the first part of the
203		JOSIE-2017, the operators followed their standard practice for pre-conditioning sondes and
204		for "day of flight" prior to simulation in the ESC. The goal was to understand the existing
205		ozone profiles archived in SHADOZ by reproducing current practices, techniques, and
206		solutions at each participating station as closely as possible.
207	3.	Evaluate the current WMO recommended SOP. Specific instrumental aspects examined in
208		these tests were details of pre-conditioning, background current, response time, pump flow
209		efficiency, and SST. In addition to two WMO-recommended SST, two alternatives, one of
210		which is employed at several SHADOZ stations, were included in the tests.

# 212 **The Ozonesonde Design**

The electrochemical concentration cell (ECC) ozonesonde uses a chemical reaction measured inside a pair of cells that is displayed schematically in **Fig. 3a.** As the sonde rises in the atmosphere (and during the laboratory calibration phase), air is pulled through the intake tube (left in **Fig. 3a**) and pushed into the cathode cell by means of a small pump. The pump maintains positive pressure as the air is sampled; the flow rate is measured during pre-flight calibration. The second cell (anode) is filled with a saturated version of the cathode solution and is located adjacent to the cathode, with an ion bridge separating the two cells. The reacting
chemical, oxidized by the ozone molecule, is dissolved potassium iodide (KI). The sensing
solution is maintained at a neutral pH with the addition of the paired phosphates (NaH<sub>2</sub>PO<sub>4</sub>•H<sub>2</sub>O/
Na<sub>2</sub>HPO<sub>4</sub>•12H<sub>2</sub>O). The ozone partial pressure is calculated by the following equation (taken
from Witte et al. 2018),

224 
$$R_{O3} = 4.307 \ 10^{-2} \frac{(I_{M} - I_{B})T_{R}}{Y_{R}F_{R}h_{C}}$$

225 where

- 226  $P_{O3} = Ozone partial pressure, mPa$
- 227  $I_M$  = Cell current,  $\mu A$
- 228  $I_B$  = Cell background current,  $\mu A$
- 229  $T_P = Ozonesonde pump temperature, K$
- 230  $\Phi_{\rm P}$  = Pump flow-rate, ml/s
- 231  $\Psi_P$  = Pump flow efficiency, unitless
- 232  $\eta_C$  = Conversion efficiency which is generally assumed to be 1.
- 233



- solution recipe, and mechanical degradation of the pump at low pressures (< 100 hPa). The
- volume mixing ratio is computed from the ratio of the ozone partial pressure  $(P_{O3})$  to the ambient
- 237 pressure determined from the radiosonde attached to the ozonesonde container as the two
- instruments ascend into the stratosphere (Fig. 3b). The typical ascent rate is 5 m/s.
- From the large body of SHADOZ data as well as instruments in the field and prior lab
- 240 intercomparisons it is known that the two major sources of systematic error are the manufacture
- of the instrument and the composition of the KI and/or buffers in the SST (Smit et al., 2007).

242 Random sources of error include operator handling and changing conditions in the station 243 calibration unit. Calibration practices and the method of data-processing can also lead to 244 systematic differences among station profiles (Johnson et al., 2002; Deshler et al., 2008; 2017). 245 In JOSIE-SHADOZ two types of protocols investigated these issues. The first five of ten tests in each session were carried out with the operators using their own solutions and preparation 246 247 technique. We refer to this as SHADOZ SOP (Standard Operating Procedure). In the second set 248 of tests, uniform calibration and preparation procedures were followed using JOSIE-prepared 249 solutions, hereafter referred to as the JOSIE SOP. Unified data collection by the Data 250 Acquisition System (DAS) eliminates variations due to operator data-processing. 251 252 General Operations during JOSIE-SHADOZ (2017). The JOSIE-SHADOZ 2017 campaign took place at the World Calibration Centre for Ozone Sondes (WCCOS) at the Research Center 253 254 Jülich (FZJ) in the Institute of Energy and Climate Research: Troposphere (IEK-8), Jülich, 255 Germany. Ozonesonde pre-conditioning test units and the ECC instruments were provided by 256 FZJ from a pool of loaned supplies. Participants were split into two groups (Table 3), each of 257 four teams operating ozonesondes of the type used in SHADOZ (**Table 2**). Each group 258 participated in a 12-day intercomparison campaign. Session No. 1 took place from 9 to 20 259 October 2017; Session No. 2 took place from 23 October through 3 November 2017. Each 260 session consisted of ten simulation experiments with all four participant sondes being "flown" 261 simultaneously in the chamber (see Sidebar 3) to an effective altitude of ~35 km. The overall 262 protocol for each campaign was similar but the second session tested two "JOSIE SSTs" (Table 263 4). During the SHADOZ SOP (first five simulations) participants used their own zero-air filter, 264 solutions, and preparation procedures. During the JOSIE SOPs the lab provided a single source

of high-quality zero-air, a common SST, and common operating procedures that all teams

followed. Data were collected by the DAS of the WCCOS test chamber.

267 [Insert Sidebar 3 here]

268 Because JOSIE-SHADOZ 2017 was focused on questions about SHADOZ operations, all

the chamber runs simulated tropical sounding conditions (**Fig. 4**). The test profiles described in

Fig. 4 and Table 4 represent three typical tropical profiles, one that is unpolluted throughout the

troposphere with very low ozone near the tropopause and two with higher levels of ozone in the

free troposphere and near the tropopause.

Four SST recipes were tested. All sonde data were processed by using a constant background current correction. Total ozone column normalization was not applied. The

- solutions, with references, follow:
- 1. <u>SHADOZ 1.0.</u> The WMO-recommended SOP (Smit et al., 2012) for use with the
- 277 Science Pump (SPC) instrument and is referred to as SST 1.0%-Full Buffer:
- 278 Cathode: 1% KI + Full-Buffer & KBr as described by Komhyr (1986)
- 279 Anode: Cathode solution with saturated KI
- 280 Pump flow efficiency factors (PEF): Komhyr (1986)
- 281 2. <u>SHADOZ 0.5.</u> The WMO-recommended SOP (Smit et al., 2012) for use with the ENSCI
   282 instrument is referred to as SST 0.5%-Half Buffer:
- 283 Cathode: 0.5% KI + Half of the Buffer & KBr as described by Komhyr et al. (1995)
- 284 Anode: Cathode solution with saturated KI
- 285 PEF: Komhyr et al. (1995)
- 3. JOSIE 1.0.1. Solution developed by NOAA for use with ENSCI sondes that has been
- 287 employed at Fiji, Samoa, Costa Rica, and Hilo stations since the late 2000's. The
- 288 formulation is SST 1.0%-1/10<sup>th</sup> Buffer:

289	Cathode:	1% KI+ 1/10 <sup>th</sup> Buffer, KBr as described by Komhyr (1986)
290	Anode:	Cathode solution with saturated KI
291	PEF:	New constants derived from recent pumpflow measurements made by
292	Nakano (2017	, private communication).
293 4.	JOSIE 2.0.1.	This variation on JOSIE 1.0.1 was used to test if ozone response in the
294	tropopause an	d stratosphere regions is improved by doubling the KI concentration:
295	Cathode:	2% KI + 1/10 <sup>th</sup> Buffer, KBr as described by Komhyr (1986)
296	Anode:	Cathode solution with saturated KI
297	PEF:	New constants derived from recent pumpflow measurements made by
298	Nakano (2017	, private communication).
200		

#### **300 Preliminary Results**

301 Preliminary data are used to answer three questions. (1) What is the accuracy of ozone 302 readings throughout the profile for each sonde-SST combination tested in the ESC? This is 303 answered by comparing both the ozone partial pressure profiles measured by the sonde with the 304 OPM and column-integrated ozone from the sondes with the OPM. For the latter, TCO and 305 segments for troposphere, stratosphere and the tropopause transition layer (TTL) in between the 306 stratosphere and troposphere are computed. (2) How do profiles and column segments from 307 sondes prepared with the SHADOZ SOP compare to those prepared with the JOSIE SOP? (3) 308 What differences are observed when the same instrument type is prepared with different SST or 309 when different instruments use the same SST? Differences are expected based on prior JOSIE 310 results and field tests.

311 SHADOZ SOP. Fig. 5 displays raw data from eight SHADOZ participants. The OPM

312 measurements are represented by the black dashed lines: Fig. 5a shows the data for a simulation 313 in Session 1 (No. 171) and Fig. 5b for a simulation in Session 2 (No. 182). The fundamental unit 314 in the tests is lapsed time; quoted "altitudes" are approximate. There is some arbitrariness in 315 designating the TTL, with lower-mid-troposphere below and mid to upper stratosphere above. 316 We adopt a TTL at 2200-3800 s (~12-18 km) when analyzing the test results. In this region the 317 signal-to-noise ratio is low, and therefore the uncertainty, is highest (Witte et al., 2017). 318 In **Fig. 5a** the ozone partial pressures are very small throughout the "troposphere" and up 319 to ~3500 s or ~17.5 km. This profile simulates a near-zero-ozone tropopause, mimicking 320 western Pacific profiles (Kley et al., 1996; Thompson et al., 2012; Rex et al., 2014; Newton et 321 al., 2016), where SNR in ozone readings is often low. In **Fig. 5b** ozone partial pressure 322 throughout the tropospheric profile is higher, representing stations influenced by biomass 323 burning pollution in the lower-mid troposphere (Thompson et al., 1996; Jensen et al., 2012). The 324 ozone transition near the tropopause and in the lower stratosphere in Simulation No. 182 (Fig. 325 **5b**) lacks the sharp gradient intentionally generated in **Fig. 5a**. The pattern in **Fig. 5b** resembles 326 that of SHADOZ stations that exhibit gradual ozone transitions in the TTL, e.g., Ascension, 327 Natal and Nairobi. Their upper tropospheric and TTL cross-sections and their contributions to 328 the zonal wave-one in tropical ozone are summarized in Thompson et al. (2003b; 2011; 2017). 329 The OPM TCO in Fig. 5a is 282 DU. The TCO from the four participants in Session 1 330 are all higher than the OPM by 3-26 DU (up to 9%). The OPM TCO in Fig. 5b is 334 DU. The 331 TCO from the four participants in Session 2 are all equal to or higher than the OPM, with the 332 largest offset 23 DU (7%) higher. Columns 2 and 3 in **Table 5** list the corresponding TCO 333 fractions for all 8 participants relative to the OPM.

The means of five simulations for all eight participants, expressed as absolute and percentage differences from the OPM and based on their SHADOZ SOP are displayed in **Fig. 6**. 336 The shapes of the mean profiles are broadly similar with the sonde partial pressures (relative to 337 the OPM, Fig. 6a) overlapping throughout the troposphere and TTL (to 3500s). In the 338 stratosphere (above 4000 s, ~20 km) differences are much larger. The fractional differences are 339 smaller in the stratosphere (Fig. 6b), however, because the ozone partial pressure peaks at over 340 20 mPa (Fig. 5). The relative differences with the OPM are largely within + 10% of the OPM 341 (zero-line in **Fig. 6b**) throughout the lower to mid-troposphere (0-2000 s, up to 10-12 km). 342 Around 2000 s, there is an inflection, with the offsets all turning more negative. The largest 343 relative differences occur within the upper troposphere (UT) and TTL (equivalent to 2500-3500 344 s, 13-18 km), exceeding 5% on average for all the stations. For participant nos. 4 and 5 the mean 345 relative differences exceed -20%. Witte et al. (2018) noted that SHADOZ ozone values are most 346 uncertain in the narrow region between 15 and 17 km (~3000-4300 s). However, the large 347 offsets recorded in Fig. 6b originate from four JOSIE tests conducted with TTL ozone equivalent 348 to 2 DU (e.g. Simulation 171, Fig. 5a); a value that applies to only ~ 5% of tropical SHADOZ 349 readings. Realistically, Fig. 8b in Thompson et al. (2017), based on > 6000 profiles, shows that 350 the actual TTL ozone for 12 of 14 SHADOZ stations is 8.0+1.5 DU. By 3000 s (~15 km) the 351 relative differences of all SHADOZ profiles with respect to the OPM start to increase. All 352 SHADOZ profiles show excellent agreement with OPM to within + 5% at 20-25 km (critical 353 ozone maximum). By 5000 s (~ 25 km) most SHADOZ profiles exceed OPM ozone and are 354 well-aligned with one another. The range of mean deviations in the region corresponding to 20-355 28 km is within 10%. This tighter clustering implies good measurement precision. By  $\sim$ 5500 s 356 (27.5 km) all the SHADOZ readings are higher than the OPM. Above 30 km the agreement 357 breaks down and there is a downturn in ozone readings relative to the OPM for most stations. 358 Exceptions are participant No. 1 and 7 that display +10% and 4% deviations, respectively (Fig. 359 **6b**). The negative relative differences are not surprising. Witte et al. (2017) showed that even

360 reprocessed SHADOZ ozonesonde data above ~30 km are highly variable and not as reliable. 361 How do column amounts for the SHADOZ participants compare on average to OPM 362 ozone? Answers appear in **Table 5.** For the five SHADOZ simulations all of the participants 363 record, on average, slightly more ozone than the OPM, with ratios from 1.017-1.040 (1.7% to 364 4.0% more O<sub>3</sub>). This result seems to validate the quality assurance practices of the SHADOZ 365 stations, with 7 of 8 participants following the WMO-recommended instrument SST 366 combinations and SOP (Smit et al., 2007; 2012). The segment column comparisons (columns 0-367 15 km, 12-18 km, 15 km-end in **Table 5**) demonstrate that the good agreement between sondes 368 and the OPM is dominated by the ozone column from 15 km-end, i.e., the stratospheric portion 369 of the profile. Because the WMO recommendations are largely based on JOSIE-2000, several 370 follow-on lab tests and the BESOS conducted in 2004, it can be inferred that the WMO 371 recommendations (Smit et al., 2012) are still valid. Agreement in the TTL (12-18 km column) 372 averages < 0.95 for half of the groups (**Table 5**). Because the OPM recorded only 5 DU on 373 average in this region, the larger offsets do not detract from the good agreement overall. 374 JOSIE SOP. The sonde partial pressure offsets from the OPM and relative differences 375 for the eight participants using the JOSIE 1.0.1 SST and preparation protocols appear in Fig. 7a 376 and **Fig. 7b**, respectively. When these results are compared to those with the SHADOZ SOP 377 (Fig. 6) two differences are observed. First, the divergence among stations is less with the more 378 uniform specifications of the JOSIE SOP, especially in the mid-troposphere through the TTL. 379 This is not surprising because the use of a single SST and SOP is expected to minimize 380 variations due to SST. The JOSIE SOP uses solutions with less buffer by a factor of 2 or 10. 381 Thus, due to the lower buffer the sonde responses show less hysteresis effect in the region with 382 relatively fast ozone changes, resulting in increased SNR. This is particularly true in the TTL at 383 the tropopause and just above, corresponding to the 2500 to 3500 s region in Fig. 6b and Fig. 7b. The second difference is that ozone readings throughout the profile are lower relative to the OPM with the JOSIE SOP than the SHADOZ SOP, particularly in the troposphere (**Fig. 7a** below 4000 s) and even more so in the stratosphere, where the offsets are -1 to -2 mPa ozone. The result is a mean sonde TCO offset with the JOSIE SOP relative to the OPM of 0.97 (first two entries in column three of **Table 6**) compared to a mean 1.03 TCO offset with the SHADOZ SOP. Background cell currents and response times improved significantly during the JOSIE SOP in both sessions when a shared zero-air system was used.

391 SHADOZ-JOSIE Comparisons. Fig. 8a displays the average differences between the 392 SHADOZ and JOSIE SOP profiles for Session 1. For each participant in Session 1, five 393 simulations were made totaling 20 profiles of each SOP, both using the same SST. Up to 10 km 394 the SHADOZ SOP resulted in relatively higher ozone readings; toward the TTL the JOSIE SOP 395 resulted in higher ozone readings. The stratospheric differences, however, show the JOSIE SOP 396 averages 3% lower TCO than the OPM while the SHADOZ SOP averages 3% higher TCO than 397 the OPM (and stratospheric segment, Table 6). Note that the near-zero simulated ozone 398 represents a small fraction of what is observed in SHADOZ records; thus, the large uncertainties 399 seen in Fig. 8a represent the extrema of the data set.

In Session 2, to compensate for the reduced sensitivity of the 1.0%, 1/10<sup>th</sup> Buffer SST 400 401 (JOSIE 1.0.1), solutions with the JOSIE SOP were prepared with twice as much KI but the same low buffer, the so-called JOSIE 2.0.1. JOSIE 1.0.1 comparisons were all made with ENSCI, 402 403 whereas the JOSIE 2.0.1 referred to a combination of SPC and ENSCI. Mean profile 404 comparisons with the different SSTs are summarized in Fig. 8b. The differences are not 405 statistically significant throughout the troposphere or TTL but the JOSIE 2.0.1 profile mean is closer to the OPM in the upper stratosphere (above 5000 s). In Session 2, the ratio of sonde to 406 407 OPM partial column ozone above 20 km for JOSIE 1.0.1 was 0.95, while for JOSIE 2.0.1 it was

408	0.97. Sondes filled with both SST show sondes measure less ozone than the OPM in the
409	stratosphere and are highly variable above 30 km, consistent with Fig. 7 and Witte et al. (2018)
410	findings.
411	Previous JOSIE campaigns and various field tests (especially the BESOS in 2004) noted that
412	throughout the ozone profile when the same SST is used, the ENSCI instrument tends to measure
413	more ozone than the SPC instrument. Of the 14 SHADOZ stations, 11 use the ENSCI
414	instrument and three use the SPC type (Thompson et al., 2017; Witte et al., 2017; 2018). Fig. 8c,
415	based on the combined session simulations (JOSIE 1.0.1), shows that, also for the less buffered
416	solutions, the ENSCI instrument measures slightly higher ozone than the SPC with the greatest
417	discrepancies in the troposphere, consistent with previous JOSIE studies.
418	
419	Conclusions
420	1. All 8 stations participating in JOSIE-SHADOZ-2017 measured ozone that agreed well
421	with the OPM.
422	2. The slight ENSCI – SPC ozone bias (ENSCI reads higher) previously observed (Smit et
423	al., 2007; 2012) remained in JOSIE-SHADOZ 2017.
424	3. JOSIE-2017 affirms the very high quality of the SHADOZ methods that use SOP and
425	SST-instrument combinations based on earlier JOSIE campaigns and field tests as
426	summarized in Smit et al. (2007; 2012). This is independent confirmation of the
427	accuracy of the large SHADOZ dataset that up to now has only been compared to data
428	from satellite and ground-based instruments (Thompson et al., 2017; Witte et al., 2017).
429	The ozonesonde community goals of "5% accuracy and precision in TCO" has been met
430	by SHADOZ operators engaging in collaborative ozonesonde "expert" activities since
431	2000. Except for the TTL, most instrument-SST combinations tested in JOSIE with

432	SHADOZ SOP agreed within 3% of OPM in total column amount (sonde higher) and 5-
433	10% throughout the ozone profile. The often large TTL ozone underestimate (>30%
434	relative to OPM in some tests) contributes only 2-3% of the total ozone column.
435	4. JOSIE tested solutions with a reduced buffer SST, of the type used at four SHADOZ
436	stations. As expected, agreement of sonde ozone data with the OPM in the TTL regions
437	was improved. However, sensitivity to stratospheric ozone is reduced, so TCO from
438	these tests averaged 3% lower than the OPM. The low-bias is reduced when the KI is
439	doubled (JOSIE2.0.1). However, the divergence of profiles with the different SST is so
440	small (~5%) that further analysis, such as taking into account individual sonde responses,
441	is required.
442	5. JOSIE SOP:
443	• Lower, uniform, and better reproducible background cell currents are achieved
444	using a high quality no-ozone filter source or purified air.
445	• The hysteresis effect ('memory' effect due to the buffering of the solution) is
446	minimized which may improve the response of the sonde, particularly in the TTL
447	where sharp ozone gradients are measured.
448	
449	Because SHADOZ represents virtually all current ECC sonde practices used by the
450	global ozone community, these findings and any SOP recommendations that ozonesonde
451	"experts" consider in light of JOSIE-2017 should be universally valid for ECC instruments.
452	Establishing SOP guidelines and standardization of ground equipment is essential to achieving
453	an uncertainty less than 5% between surface and 30 km altitude. The JOSIE-SHADOZ 2017
454	experience highlights the necessity of having a continuous reference calibration facility
455	(WCCOS) operating over the past 25 years. The capacity building exercise has empowered

456	participants to continue working towards ensuring high quality standard in sonde data-taking.
457	With well-trained and motivated operators, SOPs based on best practices, and experiments such
458	as JOSIE-SHADOZ, our aim of an uncertainty less than 5% can be achieved.
459	
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467	SHADOZ host nations and from Japan, Switzerland, France and the Netherlands.
468	
469	ACRONYMS
470	ASOPOS = Assessment of SOP for Ozone Sondes
471	DAS = Data Acquisition System
472	ECC = Electrochemical Concentration Cell

- 473 ENSCI = Environmental Science Corp.
- 474 ESC = Environmental Simulation Chamber
- 475 FZJ = Forschungscentrum Jülich
- 476 GAW = Global Atmospheric Watch
- 477 GSFC = Goddard Space Flight Center
- 478 IOC = International Ozonesonde Commission
- 479 JAMSTEC = Japan Agency for Marine-Earth Science and Technology
- 480 JOSIE = Jülich Ozonesonde Intercomparison Experiment

- 481 KNMI = Koninklijk Nederlands Meteorologisch Instituut
- 482 MLS = Microwave Limb Sounder
- 483 NDACC = Network for the Detection of Atmospheric Composition Change
- 484 OPM = Ozone Photometer
- 485 OPS = Ozone Profile Simulator
- 486 PEF = Pump Efficiency Factor
- 487 QA = Quality Assurance
- 488 SBUV = Solar Backscatter Ultraviolet
- 489 SHADOZ = Southern Hemisphere Additional Ozonesondes
- 490 SNR = Signal Noise Ratio
- 491 SOP = Standard Operating Procedures
- 492 SPARC = Stratospheric Processes And their Role in Climate
- 493 SPC = Science Pump Corporation
- 494 SST = Sensing Solution Type
- 495 TCO = Total Column Ozone
- 496 TTL= Tropical Tropopause Layer (or Tropopause Transition Layer)
- 497 UNEP = United Nations Environmental Programme
- 498 WMO = World Meteorological Organization
- 499 WCCOS = World Calibration Centre for Ozonesondes
- 500

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- 636
- 637 Sidebar 1: Ozone in the Earth's Atmosphere

638	The ozone molecule (O <sub>3</sub> ) plays several important roles in the earth's atmosphere. Its
639	absorption of radiation warms the stratosphere, leading to the temperature inversion between
640	troposphere and stratosphere (Fig. SB1). The inversion is typically referred to as the tropopause
641	but we use the term "tropopause transition layer" to signify that the tropopause is a region (~130-
642	70 hPa) in which a number of physical properties gradually change. Eighty-ninety percent of the
643	ozone molecules reside in the stratosphere so harmful uv radiation is blocked from reaching the
644	earth's surface. In the free troposphere, ozone acts as a greenhouse gas and is estimated to be
645	responsible for $\frac{1}{4}$ to $\frac{1}{3}$ of earth's warming over the past 200 years. Tropospheric ozone is also
646	a source of the OH free radical, the primary oxidant in the atmosphere, responsible for reacting
647	with hundreds of species (Thompson, 1992). Ozone at the surface is considered a pollutant,
648	harmful to human and plant health when it exceeds 3 mPa (Fig. SB1).

650 Sidebar 2: Capacity building during JOSIE-SHADOZ 651 652 653 A unique feature of JOSIE-SHADOZ was that the ozonesondes were prepared by 654 operators from organizations representing eight SHADOZ sites (see Fig. 2 showing group 655 photos taken during both sessions in front of the WCCOS chamber). Capacity-building 656 activities during both sessions included lectures on sonde quality-assurance, the importance 657 of metadata reporting, troubleshooting, and training with coaches from sponsoring 658 organizations: NASA/GSFC; NOAA/GMD; KNMI (Netherlands); KMI (Belgium); 659 Meteoswiss, Environment – Climate Change Canada; the Finnish Meteorological Institute. 660 Financial support for the tropical operators came from the UNEP-sponsored Vienna 661 Convention Trust Fund, administered by WMO. Operators are essential contributors to 662 ozonesonde quality assurance by providing detailed metadata information on each sonde 663 launch and maintaining uniformity in their preparation and launch procedures. Bringing

together SHADOZ operators for training and knowledge sharing helps to ensure that best
 practices are applied to operations in a consistent manner across the SHADOZ network.

666

# 667 Sidebar 3: Design of the ESC, Reference Instrument, Data System.

668		The WCCOS, the only one of its kind, was established in the mid-1990s at FZ-Jülich to
669	tes	st, calibrate and compare different types of balloon borne ozonesondes that are used to measure
670	the	e distribution of ozone in the troposphere and lower/middle stratosphere. The facility is
671	de	scribed in more detail in Smit et al. (2000): http://www.fz-juelich.de/iek/iek-
672	8/1	EN/Expertise/Infrastructure/ESF/ESF_node.html.
673		The setup of the simulation facility (Fig. SB2a), consists of four major components:
674	1.	Environmental Simulation Chamber. The ESC chamber is a temperature-controlled vacuum
675		chamber with a test room volume of about 500 liter (80 x 80 x 80 cm). Within the ESC the
676		pressure and temperature can be dynamically regulated, with pressures between 5 and 1000
677		hPa and temperatures between 200 and 300 K, with a maximum rate of $\pm 2$ K/min. Iso-
678		thermically operated, the temperature variations of the air as well as the wall inside the test
679		room can be maintained within $\pm$ 0.2 K. For more details see Smit et al. (2000).
680	2.	Ozone Photometer (OPM), Ozone reference. The OPM is a fast response dual-beam UV-
681		absorption photometer, originally developed by Proffitt and McLaughlin (1983) for use on
682		stratospheric balloons. The instrument was flown during Balloon Ozone Intercomparison
683		(BOIC) missions in 1983/1984 (Hilsenrath et al., 1986); it was used in the Balloon
684		Experiment on Standards for Ozone Sondes (BESOS) field campaign in Wyoming, in 2004
685		(Deshler et al., 2008). The OPM is an absolute measuring device with a 1-s response time at
686		a sampling volume flow rate of about 8 l/min. The overall accuracy of ozone measurements

687 made by the OPM is better than  $\pm 2\%$  for simulated altitudes up to 25 km (pressures down to 688 25 hPa) and  $\pm 3.5$  % at 30-35 km altitude (12-5 hPa). The instrument resides in a separate 689 vacuum vessel which is connected to the ESC such that the UV-photometer has the same 690 pressure conditions as inside the test chamber. 691 3. Ozone profile simulator (OPS). A gas-flow system that controls the ozone concentrations 692 sampled by the instruments in the ESC, with a gas flow rate of 12-15 l/min. The OPS can 693 simulate vertical ozone profiles between the surface and 35 km. The OPS can accommodate 694 up to four ozonesondes, including the OPM (Fig. SB2b). The OPS has an option to specify 695 ozone step functions or zero ozone to investigate the response time and background 696 characteristics of ozonesondes. 697 4. Data Acquisition System (DAS). The entire simulation process is automated by computer 698 control in order to have reproducible conditions with respect to the simulated pressure, 699 temperature and ozone versus time, and for recording and storing the large variety of

parameters measured during the simulation process. A special electronic interface (JOSIE/

701 ECC-interface) couples the ECC sonde to the DAS, transmitting cathode cell current, pump

temperature, pump motor current and pump motor voltage (12V). A small variable electrical

heater (0-10W) adjusts pump temperatures to values similar to actual flight temperatures.

±

1 Table List:

# 2 Table 1: JOSIE activities on ozonesonde procedures and related reports.

Campaign	Objective
JOSIE-1996 GAW Report #130	<ul> <li>Operating Procedures</li> <li>Profiling Capabilities</li> <li>Intercomparison sonde types (ECC, Brewer Mast, Meisei)</li> </ul>
GAW Report #57	Manufacturing ECC sondes (SPC, ENSCI)
JOSIE-2000 GAW Report #158 (Smit et al., 2007)	<ul> <li>Operating Procedures</li> <li>Focus on ECC sonde         <ul> <li>Different sensing solution types</li> <li>Different manufacturers (SPC, ENSCI)</li> </ul> </li> </ul>
BESOS-2004 (Deshler et al., 2008)	<ul> <li>Operating Procedures under flight conditions</li> <li>Focus on ECC sonde         <ul> <li>Different sensing solution types</li> <li>Different manufacturers (SPC, ENSCI)</li> </ul> </li> </ul>
ASOPOS 2002-2012 GAW Report #201	Define and establish Standard Operating Procedures for ECC sondes
JOSIE-2009	Manufacturers (SPC, ENSCI)
JOSIE-2010	Refurbished sondes
O3S-DQA Guidelines Report-2012	Homogenization and Uncertainties
JOSIE-SHADOZ-2017	<ul> <li>Operating procedures</li> <li>Tropical simulations</li> <li>Different sensing solution types</li> <li>Different manufacturers (SPC, ENSCI)</li> </ul>

3

# 4 Table 2: SHADOZ stations operating at least 10 years between 1998 and 2017

Station	Latitude, Longitude	Current ECC	Current Radiosonde
		Sensor	
Pago Pago, Am. Samoa	14.23S, 170.56W	ENSCI	iMet-1
Hilo, Hawaii	19.40N, 155.00W	ENSCI	iMet-1
San Cristobal, Galapagos,	0.92S, 89.60W	ENSCI	Vaisala RS92
Ecuador			
San Pedro, Costa Rica	9.94N, 84.04W	ENSCI	iMet-1
Paramaribo, Surinam	5.81N, 55.21W	SPC	Vaisala RS92
Ascension Is., U.K	7.98S, 14.42W	ENSCI	iMet-1
Natal, Brazil	5.42S, 35.38W	SPC	Lockheed-Martin-
			Sippican LMS6
Irene, S. Africa	25.90S, 28.22E	SPC	Vaisala RS92
Nairobi, Kenya	1.27S, 36.80E	ENSCI	Vaisala RS92
La Réunion, France	21.10S, 55.48E	ENSCI	Modem M10
Kuala Lumpur, Malaysia	2.73N, 101.70E	ENSCI	GRAW DFM-09
Hanoi, Vietnam	21.02N, 105.80E	ENSCI	Vaisala RS92
Watukosek-Java, Indonesia	7.57S, 112.65E	ENSCI	*
Suva, Fiji	18.10S, 178.40E	ENSCI	iMet-1

5 \*Operated Meisei RS II-KC79D radiosonde-ozonesonde system 1992-1999; Vaisala RS80 1998-2013.

# 7 Table 3: SHADOZ station operators and instruments tested in JOSIE. Stations 1-4

8 participated in Session 1 (9-20 October 2017); stations 5-8 participated in Session 2 (23

9	October -	- 3	November	2017).
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Participant	SST	Operator	Affiliation	Station
Number				
		Sessi	on 1	
1	1.0% Full Buffer	Tshidi Machinini	South African Weather Service	Irene, South Africa
2	1.0% Full Buffer	Francisco R. da Silva	Brazilian Space Agency	Natal, Brazil
3	0.5% Half Buffer	Kennedy Thiong'o	Kenyan Meteorological	Nairobi, Kenya
			Department	
4	0.5% Half Buffer	Ernesto Corrales	University of Costa Rica	San Pedro, Costa Rica
		Sessi	on 2	
5	1.0% Full Buffer	George Paiman	Meteorological Service of	Paramaribo, Surinam
			Suriname	
6	0.5% Half Buffer	Zamuna Zainal	Malaysian Meteorological	Kuala Lumpur,
			Department	Malaysia
7	0.5% Half Buffer	Françoise Posny	Université La Réunion, Météo-	La Réunion Is., France
			France, CNRS	
8	0.5% Half Buffer	Nguyen Thi Hoang Anh	Vietnam Meteorological and	Hanoi, Vietnam
			Hydrological Administration	

10

### 11 Table 4: Characteristics of JOSIE-SHADOZ-2017 simulations in the WCCOS chamber

12 with Simulation Numbers listed for the two Sessions. LT=lower troposphere, MT=mid-

13 troposphere, UT=upper troposphere and LS=lower-stratosphere. All profiles simulated

- 14 with nominal 5 m/s ascent velocity. The tropopause was located at Z=18-20 km with
- 15 minimum temperature ~-(70-80)°C. The stratospheric profile was specified to be the same
- 16 for all simulations.

	Session 1			
Simulation Number	Troposphere Profile Type	Profile Type Index**	Specifications	ECC Procedure
171	Recent deep convection	1	Extremely low O <sub>3</sub> values nearly uniformly up to tropopause with very steep gradient into LS	Station-supplied SST & procedures
172	Maritime background	2	Low $O_3$ in LT, moderate $O_3$ in MT, extremely low $O_3$ in UT	Station-supplied SST & procedures

173, 174, 175, 176*	Biomass burning	3	Enhanced $O_3$ in LT, high $O_3$ in MT, low $O_3$ in UT	Station-supplied SST & procedures
177, 178, 179, 181	Biomass burning	3	Enhanced $O_3$ in LT, high $O_3$ in MT, low $O_3$ in UT	JOSIE-supplied SST & WMO procedures
180	Maritime background	2	Low $O_3$ in LT, moderate $O_3$ in MT, extremely low $O_3$ in UT	JOSIE-supplied SST & WMO procedures
			Session 2	
Simulation Number	Troposphere Profile Type	Profile Type Index**	Specifications	ECC Procedure
182, 183, 184,186	Biomass burning	3	Enhanced $O_3$ in LT, high $O_3$ in MT, low $O_3$ in UT	Station-supplied SST & procedures
185	Maritime background	2	Low $O_3$ in LT, moderate $O_3$ in MT, extremely low $O_3$ in UT	Station-supplied SST & procedures
187, 188, 190, 191	Biomass burning	3	Enhanced $O_3$ in LT, high $O_3$ in MT, low $O_3$ in UT	JOSIE-supplied SST & WMO procedures
189	Maritime background	2	Low ozone in LT, enhanced ozone in MT and extreme low ozone in UT	JOSIE-supplied SST & WMO procedures

7 \* Due to a problem with the ESC, Simulation 176 only recorded profiles to 15 km.

18 \*\* In Figure 4, 1 = blue, 2= green, 3= red

19

# 20 Table 5: Total and partial column statistics from two SHADOZ simulations and means for

# 21 all 10 simulations (five each in Sessions 1 and 2). All simulations use SHADOZ SOPs.

Instrument	Sim 171	Sim 182	Mean	Mean	Mean	Mean
	(DU)	(DU)	OPM/Sonde	OPM/Sonde	OPM/Sonde	OPM/Sonde
			Ratio: TCO	Ratio: Trop	Ratio: TTL	Ratio: Strat O <sub>3</sub>
				O <sub>3</sub> (0-15 km)	O <sub>3</sub> (12-18	(15 km-end)
					km)	
OPM	282		337 DU	47.0 DU	4.93 DU	298 DU
Participant 1	1.07		1.03	1.09	1.02	1.04
Participant 2	1.09		1.04	1.09	1.03	1.04
Participant 3	1.03		1.03	1.02	0.95	1.03
Participant 4	1.01		1.02	1.06	1.01	1.02
OPM		334	313 DU	41.0 DU	5.30 DU	271 DU
Participant 5		1.00	1.03	0.85	0.77	1.03
Participant 6		1.04	1.04	0.89	0.87	1.05
Participant 7		1.07	1.04	0.93	0.93	1.05
Participant 8		1.00	1.02	0.88	0.87	1.02

#### Table 6: Total and partial column statistics from profile simulations, relative to OPM,

Methodology	No.	Mean	Mean	Mean	Mean
		Sonde/OPM	Sonde/OPM Trop	Sonde/OPM TTL	Sonde/OPM Strat
		TCO	O <sub>3</sub> (0-15 km)	O <sub>3</sub> (12-18 km)	O <sub>3</sub> (20 km-end)
SHADOZ SOP	40	1.03	1.01	0.94	1.04
JOSIE SOP	40	0.97	0.99	0.94	0.97
ENSCI 1.0%, 0.1B*	25	0.98	1.00	0.97	0.98
SPC 1.0%, 0.1B	10	0.97	0.96	0.90	0.98
ENSCI 0.5%, 0.5B	20	1.03	1.00	0.91	1.04
SPC 1.0%, 1.0B	15	1.03	1.01	0.95	1.04
ENSCI 2.0%, 0.1B	5	0.97	1.01	0.97	0.97
SPC 2.0%, 0.1B	5	0.97	0.94	0.90	0.96
* B=Buffer					

#### categorized by SOP and sonde/solution types.

26	Figure	Caption	List:
20	I is an c	Cupiton	LUDU.

28	Figure 1:	Map	of SHADOZ	stations.
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29

30	Figure 2(a): Session 1 participants: (1) George Brothers (NASA/WFF); (2) Kennedy
31	Thiong'o (Kenya Met Dept.); (3) Francisco Raimundo da Silva (INPE Natal); (4) Ernesto
32	Corrales (Univ. Costa Rica); (5) Peter von der Gathen (Alfred Wegener Institute); (6)
33	Herman Smit (FZ Jülich); (7) Ryan Stauffer (NASA/GSFC); (8) Gary Morris (St.
34	Edward's Univ.); (9) Gabi Nork (FZ Jülich); (10) Anne Thompson (NASA/GSFC); (11)
35	Bryan Johnson (NOAA ESRL); (12) Tshidi Machinini (South African Weather Service);
36	(13) Tatsumi Nakano (Japan Met Agency); (14) Rhonie Wolff (NASA/WFF).
37	
38	Figure 2(b): Session 2 participants: (1) Gonzague Romanens (MeteoSwiss); (2) Torben
39	Blomel (FZ Jülich); (3) Jennifer Gläser (FZ Jülich); (4) Nguyen Thi Hoang Anh (Vietnam
40	Meteorological and Hydrological Administration); (5) Anne Thompson (NASA/GSFC); (6)
41	Jonathan Davies (Env. Climate Change Canada); (7) Zamuna Zainal (Met Malaysia); (8)
42	Patrick Neis (FZ Jülich); (9) Gabi Nork (FZ Jülich); (10) Rigel Kivi (FMI); (11) Rene Stübi
43	(MeteoSwiss); (12) Patrick Cullis (NOAA ESRL); (13) Herman Smit (FZ Jülich); (14) Marc
44	Allaart (KNMI); (15) Roeland Van Malderen (Royal Meteorological Institute of Belgium);
45	(16) Jacquelyn Witte (NASA/GSFC); (17) George Paiman (Met Dept. of Suriname); (18)
46	Andreas Petzold (FZ Jülich); (19) Gilbert Levrat (MeteoSwiss); (20) Françoise Posny
47	(Univ. of La Réunion).

49	Figure 3: (a) Schematic of an electrochemical concentration cell (ECC) in operational
50	mode. (b) ECC instrument in Styrofoam box in which it is housed during JOSIE tests or in
51	deployment (when launched the sensor is sealed with a Styrofoam lid). Instrument and
52	solution type for each JOSIE-SHADOZ station appear in Tables 2 and 3, respectively.
53	
54	Figure 4: Simulated ozone profiles (in partial pressure) as a function of simulation time for
55	the troposphere and stratosphere until 33 km altitude (a) and up to 20 km in (b). Three
56	different tropospheric ozone profiles with extreme low ozone concentrations up to the
57	tropopause (Altitude $\approx 18$ km) in blue and two profiles with moderate to enhanced middle
58	tropospheric ozone values in green and red, respectively.
59	
60	Figure 5: Ozone "raw" profiles of typical simulations in Sessions 1 (a) and 2 (b).
61	Participants are listed in Table 3, simulation specifications are listed in Table 4.
62	
63	Figure 6: (a) Participant mean profiles relative to OPM in partial pressure (mPa), and (b)
64	% deviation (Sonde – OPM / OPM). Based on 5 simulations per participant.
65	
66	Figure 7: Same as Fig. 6, except for JOSIE SOP as described in Table 4.
67	
68	Figure 8: (a) Session 1 SHADOZ SOP (blue) and JOSIE SOP (red) mean profiles
69	subtracted from the OPM profile mean; (b) Session 2 JOSIE 2.0.1 (black) and JOSIE 1.0.1
70	(red) SST profile means subtracted from the OPM; and (c) Session 1 and 2 mean profiles of

71 ENSCI-OPM (red) and SPC-OPM (blue) for which JOSIE 1.0.1 SST and SOP was used. 1-

72 sigma standard deviations for all panels are included.

- 73
- 74 Figure SB1. Ozone and temperature profiles from a typical SHADOZ sounding at Natal,
- 75 Brazil, taken from the archive, <u>https://tropo.gsfc.nasa.gov/shadoz</u>.
- 76
- 77 Figure SB2: (a) Set up for the simulation of vertical ozone soundings with a schematic of
- 78 the Environmental Simulation Chamber, showing Ozone Photometer (OPM) standard
- 79 reference, control systems, placement of four ozonesondes ("TEO") in the chamber and
- 80 data acquisition system (DAS). (b) Photo of the chamber and DAS computer.





**Fig. 2. (a)** Session 1 participants: (1) George Brothers (NASA/WFF); (2) Kennedy Thiong'o (Kenya Met Dept.); (3) Francisco Raimundo da Silva (INPE Natal); (4) Ernesto Corrales (Univ. Costa Rica); (5) Peter von der Gathen (Alfred Wegener Institute); (6) Herman Smit (FZ Jülich); (7) Ryan Stauffer (NASA/GSFC); (8) Gary Morris (St. Edward's Univ.); (9) Gabi Nork (FZ Jülich); (10) Anne Thompson (NASA/GSFC); (11) Bryan Johnson (NOAA ESRL); (12) Tshidi Machinini (South African Weather Service); (13) Tatsumi Nakano (Japan Met Agency); (14) Rhonie Wolff (NASA/WFF).



**Fig. 2. (b) Session 2 participants**: (1) Gonzague Romanens (MeteoSwiss); (2) Torben Blomel (FZ Jülich); (3) Jennifer Gläser (FZ Jülich); (4) Nguyen Thi Hoang Ahn (National Hydro-Meteorological Service of Vietnam); (5) Anne Thompson (NASA/GSFC); (6) Jonathan Davies (Env. Climate Change Canada); (7) Zamuna Zainal (Met Malaysia); (8) Patrick Neis (FZ Jülich); (9) Gabi Nork (FZ Jülich); (10) Rigel Kivi (FMI); (11) Rene Stübi (MeteoSwiss); (12) Patrick Cullis (NOAA ESRL); (13) Herman Smit (FZ Jülich); (14) Marc Allaart (KNMI); (15) Roeland Van Malderen (Royal Meteorological Institute of Belgium); (16) Jacquelyn Witte (NASA/GSFC); (17) George Paiman (Met Dept. of Suriname); (18) Andreas Petzold (FZ Jülich); (19) Gilbert Levrat (MeteoSwiss); (20) Françoise Posny (Univ. of La Réunion).





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**Fig. 4.** Simulated ozone profiles (in partial pressure) as a function of simulation time for the troposphere and stratosphere until 33 km altitude (a) and up to 20 km in (b). Three different tropospheric ozone profiles with extreme low ozone concentrations up to the tropopause (Altitude  $\approx$  18 km) in blue and two profiles with moderate to enhanced middle tropospheric ozone values in green and red, respectively.



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Fig. 7. Same as Fig. 6, except for JOSIE SOP as described in Table 4.



**Fig. 8.** (a) Session 1 SHADOZ SOP (blue) and JOSIE SOP (red) mean profiles subtracted from the OPM profile mean; (b) Session 2 JOSIE 2.0.1 (black) and JOSIE 1.0.1 (red) SST profile means subtracted from the OPM; and (c) Session 1 and 2 mean profiles of ENSCI-OPM (red) and SPC-OPM (blue) for which JOSIE 1.0.1 SST and SOP was used. 1-sigma standard deviations for all panels are included.



Fig. SB1. Ozone and temperature profiles from a typical SHADOZ sounding at Natal, Brazil, taken from the archive, <u>https://tropo.gsfc.nasa.gov/shadoz</u>.



**SB2.** (a) Set up for the simulation of vertical ozone soundings with a schematic of the Environmental Simulation Chamber, showing Ozone Photometer (OPM) standard reference, control systems, placement of four ozonesondes in the chamber ("TEO") and data acquisition system (DAS). (b) Photo of the chamber and DAS computer.