Review of Smit et al., ***Intercomparison of IAGOS-CORE, IAGOS-CARIBIC and WMO/GAW-WCCOS Ozone Instruments at the Environmental Simulation Facility at Julich, Germany***

Reply to referee #1

We thank referee #1 for the complete and thoughtful review of our manuscript and providing thoughtful comments and suggestions that have helped us improve this manuscript. We also thank Editor Troy Thornberry for handling our paper and coordinating the reviews. Our responses to reviewer comments are provided below in red italic text.

Anonymous Referee #1, 18 February 2025

Summary:

This paper provides a summary of a number of experiments conducted at the Forschungszentrum Julich (FZJ) atmospheric profile simulation chamber designed to connect the ozone measurements profile measurements made as part of the In-service Aircraft for a Global Observation System (IAGOS) to those made on balloon sondes using the common, world-standard UV calibration instrument of Proffitt et al. (1982). As such this paper is an important contribution to the literature and will allow a harmonization of in situ ozone profiles across these measurement platforms.

In particular, the experiments conducted examined the performance of two versions of the aircraft O3 instruments (P1-O3 and CAR-O3) against the dual-beam UV-Ozone Photometer (OPM) of the World Calibration Center of Ozone Sondes (WCCOS) at FZJ. The instruments generally showed agreement to within 5-6% over the range of pressures studied. Interestingly, the P1-O3 instrument showed a consistent trend in offset from the OPM, starting at ~+2% at 1000 hPa and changing linearly to ~ -3% by 400 hPa. The paper was uncertain as to the cause, which does need to be identified and reconciled. It mentions that the performance of this instrument might be an artifact of the experimental set-up. That question should be resolved.

Recommendation:

Publish with relatively minor revisions – see my detailed comments below.

While it would be good to have the question of the drift in the offset of the P1-O3 instrument from the WPM resolved, it is worth getting these results into the literature sooner than later. If it is not resolved by the time of publication of this manuscript, a follow-up “note” should be submitted with an answer to the question.

>>> We share the concerns that this study needs as soon as possible more experimental efforts to obtain more statistical evidence concerning the observed drift of the P1-O3 instrument, but also to exclude any artifacts of the experimental set-up. Unfortunately, on the short term it is not possible to do any intercomparison experiments due to a shortage of operational P1-O3 instruments within IAGOS because nowadays all instruments are either “flying” or have been already scheduled to be flown in the upcoming year. However, we think the results of this study should be available to the scientific community the sooner the better. And we fully agree with your recommendation to do follow up intercomparison experiments and that they should be done as soon as possible. At present more intercomparisons are planned for 2026/2027. As soon as we have new results we will publish this of course as a “note”.

Detailed comments:

Line 28: How often do you recommend that these comparisons be performed? Is it possible that the offsets historically might have looked different if these comparisons had been done before? How stable are the instruments?

>>> At present it is too early to make a specific recommendation on how often this kind of intercomparison should be done. We first need more statistics on the variability of the observed differences to characterize these. However, it is not expected that historically the offsets would have been changing over time because the long-term stability of the tested ozone instruments have been regularly checked at laboratory pressure conditions over decades against NIST traceable ozone UV-photometers and no significant change in the offset or slope have been observed. For IAGOS-CORE a suite of ozone UV photometers have been flown since 1994 and all instruments consequently have been checked in the laboratory against a common (MOZAIC) ozone equipment (L147-L156). The long-term stability of the instruments is very good. This is confirmed in a comprehensive study by Blot et al. (AMT, 2021) investigating the internal consistency over more than 25 year of in-flight IAGOS-Core ozone measurements. It was shown that the stability among all the flown P1-O3 instruments is better than within a few percent.

Line 36: I might say, "anthropogenically influenced"

>>> Done.

Line 38: delete “and its impact on life on Earth.”

>>> Done.

Line 39: “Besides the traditional” (change first word and delete “of”)

>>> Done.

Line 45: “long-term”

>>> Done.

Line 47: “operation,”

>>> Done.

Line 47: “(9-12 km)” should match later reference of 10-12.5 km cruise altitude (line 78) – one or the other.

>>> Altitude ranges have been matched into 10-12.5 km.

Line 47-48: “and provides profiles of ozone from the surface to cruise altitude during take-off and landing. Since August 1994 more than 70,000…”

>>> Done.

Line 53: swap “instruments” in for “devices”

>>> Done.

Line 66: “chamber,”

>>> Done.

Line 68: “...that is approved as EASA…”

>>> Done.

Line 78: “(Z=10-12.5 km)” should match earlier reference of 9-12 km cruise altitude (line 47) - one or the other.

>>> Done.

Line 114: “considered, too, and that is also dependent…”

>>> Done.

Line 118: “...serves as the reference instrument.”

>>> Done.

Line 124: Delete the phrase, “It is to mentioned that”

>>> Done.

Line 137: What are the flow rates and cell volumes? I think this question is answered in the text below – just curious about the “flush” time for the cells when they are switched into zero air sampling mode.

>>> Based on cell volume (V_Cell) and volume flow rates (VFR_Cell)) the average residence time of an air sample in a cell: ART_Cell) = V_Cell / VFR_Cell)

OPM-O3: V_Cell = 50.6 cm3 & VFR_Cell = 4 l/min: ART_Cell = 0.75 s

P1-O3: V_Cell ≈ 30 cm3 & VFR_Cell = 1 l/min: ART_Cell = 1.70 s

CAR-O3: V_Cell = 9.5 cm3 & VFR_Cell = 1 l/min : ART_Cell = 0.57 s

Critical is that after switching the cells from measuring mode into zero mode or vice versa, the flushing times are long enough such that the air in the cells is refreshed by more than 99.5 %. Experiments in the past have shown that usually after flushing times of about two times the specific ART_Cell this 99.5 % refreshing criterion is fulfilled. This applies for all instruments in discussion, P1-O3, CAR-O3 and OPM-O3 (see alsoTable 1).

Line 148: swap “evaluate” for “prove”

>>> Done.

Line 149: “...is responding linearly to ozone to within…” instead of “...that its linearity is…”
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>>> Done.

Line 150: “...comparison with an instrument with measurements traceable to the National Institute…”

>>> Done.

Line 151: Confused about the word “above” at the end of this sentence.

>>> The sentence at L151 is corrected into: “The overall uncertainty is better than ± 2 ppbv for $O_3 < 100$ ppbv and ±2 % for $O_3 \geq 100$ ppbv. (Nédélec et al., 2015).” This has been also corrected in Table 1.

Line 152: “...IAGOS-CORE is compared…”

>>> Done

Line 209: swap “supply equivalent air samples to” in for “provide”

>>> Done.

Line 224: “CAR-O3 uses a 2 m tube (ID = 4 mm), while the P1-O3 inlet line goes…”

>>> Done.

Line 242-243: “...the manifold was monitored…”

>>> Done.

Line 246: “...when P1-O3 was directly connected…”

>>> Done.

Line 251-252: “...of the aircraft. On IAGOS-CARIBIC…”

>>> Done.

Line 253: “...about 12.5 km, the lowest…”

>>> Done.

Line 255: “...thus to a value of the lowest total…”

>>> Done.

Line 256: “Note, however, as P1-O3…”

>>> Done.

Line 258: “...both instruments span the relevant…”

>>> Done.

Line 262: “...usually falls in the range 800-850…” Question: By your argument in the text above this point, if you are determining the maximum difference, should you not be using 250 hPa here instead of 280 hPa? That would result in a 600 hPa difference instead of 570 hPa. Maybe I misunderstood the goal?

>>> You are right. Thanks for attending us to this mistake. We have corrected the numbers accordingly in the text of the revised manuscript.

Line 268: “...instrument does not use a pump…”

>>> Done.

Line 279: “...simulation experiments, numbered 3 to 7, which…”

>>> Done.

Line 295: For Figure 2, it might be helpful to include the 0% difference line across the top plot.

>>> Included. The figures have been revised, majorly on request of referee#2

Line 304: “...underlying cause. In a subsequent test (May 2024), KIT found an issue…” What is “KIT”?

>>> KIT = Karslruher Institut für Technologie. Has been included in the text and the List of Acronyms

Line 307: “...after the repair of the AD-converter…”

>>> Done.

Line 310-311: “...compared to the OPM. We only will present the pressure corrected…”

>>> Done.

Line 315: Figure 3 – the panels seem somewhat blurry. Do you have higher resolution versions for inclusion in the final publication?

>>> The figure has been exchanged by a higher resolution one.

Line 320: “...and the cruise altitude section at 400 hPa (Figure 4b).”

>>> Done.

Line 321: “...during ascent and descent, and no indication…”

>>> Done.

Line 354 and elsewhere: It would be good to formulaically define what you mean by relative difference.

>>> We add at L292 the exact definitions of the relative differences:

The relative differences in % of the μ_{O3} (VMR) readings of P1-O3 and CAR-O3, respectively, shown in this study are consequently defined with regard to the μ_{O3} readings of the OPM-O3 instrument acting as the reference as follows:

$$Rel.\,Difference of P1O3 = \frac{(\mu_{O3,P1O3} - \mu_{O3,OPMO3})}{\mu_{O3,OPMO3}} \qquad (3)$$

$$Rel.\,Difference of CARO3 = \frac{(\mu_{O3,CARO3} - \mu_{O3,OPMO3})}{\mu_{O3,OPMO3}} \qquad (4)$$

Line 363: Figure 6 – what are the spikes that appear in the red trace at the step changes in ozone concentration? Are those real or artifacts of the processing/measurement system?

>>> The O_3 spikes observed at the step changes are real and are caused by the "overshooting effect" of the fast response of the flow controllers of the OPS (Ozone Profile Simulator) on the sudden, abrupt change of the settings of the simulated μ_{O3} profile (see also section 2.2.2 on the OPS).

Line 380: "..to within +/- 3%."

>>> Done.

Line 392: "...at discrete values typically found at the corresponding…"

>>> Done.

Line 398: "...again (as in Exp #3 and #4) around -(1-2)% and is constant…"

>>> Done.

Line 399: "...400 - 1000 hPa with ozone volume mixing ratios…"

>>> Done.

Line 399-400: "...follow the changes in ozone levels below 100 ppbv, only relative…"

>>> Done.

Line 401-402: "...CAR-O3 in more detail. Figure 10 shows the three ozone VMR…"

>>> Done

Line 418-420: The lines-of-best-fit in Figure 10 are forced through the origin. Is that the right approach?

>>> We have changed the approach of Fig.10 and Table 3. As before the offsets of the three instruments have been determined during the periods of zero ozone exposure, while the slopes were obtained from linear fits of the scatter plots in Fig.10-a., b., c. respectively but not forced through the origin. In addition, similar graphs are shown for the lower ozone ranges for the corresponding three pressure levels (Fig.10-d., e., f.). For the 6 graphs in Fig.10 we also determined the slopes for the periods of upward and downward ozone step levels. The corresponding scatter plots and linear fits are displayed in Fig. S1 and S2 of the Supplement for the P1-O3/ OPM and CAR-O3/OPM, respectively. All results are summarized in Table 3 and discussed in the new manuscript in following paragraph:

"From Table 3 it is seen that the behaviour between the three instruments observed at ozone levels larger than about 100 ppbv is consistent with the results obtained from the Exp. #3 and Exp. #4. At lower ozone values below 100 ppbv, however, the slopes for P1-O3/OPM differ slightly by -(1-2) % compared to their corresponding slopes of P1-O3/OPM derived for higher ozone values, respectively. Breaking down the slopes into the upward and downward part of the ozone step levels, P1-O3/OPM reveals a small hysteresis effect of about a 2 % which is most pronounced in the lower range of ozone levels. CAR-O3 shows no hysteresis, neither at the higher nor at the lower ozone levels (Table 3 and Figs. S1 and S2 in the supplement). The observed differences are not really understood but are still within the experimental reproducibility of about ±1 % as mentioned in Section 3.2.2. "

Line 420: "...P1-O3 and CAR-O3" space added between "O3" and "and"

>>> Done.

Line 424: replace "for" with "of"

>>> Done.

Line 427-428: Should the formula be: "100% X (P1-O3 - OPM)/OPM? Same for the CAR-O3 calculation…

>>> We add at L292 the exact definitions of the relative differences where it explicitly mentioned that these definitions (Eq.3) and (Eq.4) throughout this entire study consequently will be used.

Line 443: "(i.e., the pressure under real flight conditions, see section 2.3.2)."

>>> Done.

Line 446: "...10 minutes, the difference declined to…"

>>> Done.

Line 448: "...the OPS and ESC; however, no indication of any malfunction of any…"

>>> Done.

Line 448-449: Delete "Although"..."The cause is still not understood; it is a subject for…"

>>> Done.

Line 455-456: "unrealistically high and most likely impacted by the high temperatures of the electronics of the instrument." Is there a way to check this hypothesis?

>>> From our long year JOSIE experiences we have observed that when the temperature of the lamp or the light detector electronics are exceeding 50 °C, the detector signal noise is getting larger and increasing with increasing temperatures. Lamp or light detector temperatures larger than 45-50 °C are observed only incidentally after long operation times and which most likely occurs when the laboratory temperature is above 25-30 °C. This was the case at the end of that day of doing the experiment. We changed the sentence accordingly:

“The OPM showed a small negative offset about - (0.05 – 0.10 mPa), but a rather noisy signal, unrealistic high and most likely due to the enhanced temperatures of the UV-light detector electronics exceeding the 50 °C threshold that occured during the experiment.”

Line 468: “P1-O3 showed a good performance…” Should the consistent slope and the 5% change from bottom to top worry users? Can this be corrected?

>>> Although the observed differences among the three different instruments are in general consistent within about a 5 % range, the P1-O3 instrument reveals a small but consistent pressure dependent change of about 5 % compared to the OPM. the results are significant to alert the community, but further investigations in the near future are needed to analyze P1-O3 versus OPM characteristics. At present, it is too early to draw solid conclusions to recommend any corrections of the P1-O3 data because this study deals only with the results of a first intercomparison of one single P1-O3 instrument against the OPM of the WCCOS. More intercomparisons of several different P1-O3 instruments versus OPM are needed.

Line 473-475: Comment – if you had swapped the positions of the instruments in the chamber set-up, could you have possibly seen different results?

>>> We did not really swapped the positions of the instruments, but at the beginning of the campaign we changed the connection of the P1-O3 to the manifold as written in section 2.3.1 (Experimental Setup at L244-L247 in the original manuscript) : “The P1-O3 sample flow we had to branch off from the ozone profile simulator flow before entering the manifold (Fig.1), because it was shown that the high sampling volume rate of P1-O3 pump box would otherwise cause leakage effects when P1-O3 was directly connected with a Teflon fitting at the inlet glas tube of the manifold.” The leakage effects were causing P1-O3 readings with a pressure dependent deviation of -5% at lab pressure up to -15% at lower pressure compared to the OPM. After we branched off the P1-O3 inlet tube from the ozone profile simulator flow before entering the manifold (See Fig.1) the effect seemed to be gone, however, a remaining pressure dependent artefact cannot be fully excluded (See also L471-L473 in the original manuscript).

>>> By simply swapping the positions of the instruments connected to the ozone manifold we didn’t expect to obtain different results because the air pressure P_M inside the manifold is strictly kept a few hPa higher than the air pressure inside the chamber, such that any leakage of chamber air into the manifold would be avoided (L242-L244 in the original manuscript).

Line 477-478: “...of the OPM as a standard, in combination…”

>>> Done.

Line 478-479: “...set up, to within about +/- 1%. A primary standard for O3-UV photometer measuring only exists at Earth surface conditions (at the Bureau…”

>>> Done.

Line 480: delete “respectively”

>>> Done.

Line 483: “...reference instrument.” delete “to refer to”

>>> Done.

Line 487: “...complementary, their records do not typically cover the same time period.”

>>> Done.

Line 497: “...has only a small, in any, impact of less…”

>>> Done.

Line 499: “...have been flown…”

>>> Done.

Line 502: “...stratosphere, be efficient enough that the impact…”

>>> Done.

Line 503: “...essential, and could be…”

>>> Done

Line 538: LIDAR = “Light Detection and Ranging”

>>> Done.

Line 548: I believe UTC = “Coordinated Universal Time”

>>> Done.