Author comment on "Evaluation and optimization of ICOS atmospheric station data as part of the labeling process" by Camille Yver-Kwok et al.

Anonymous Referee #1
Received and published: 21 August 2020

We thank the reviewer for their positive review and their constructive and helpful comments. We answer them below, highlighted in bold and italic.

This paper represents a substantial contribution to scientific progress in atmospheric measurement techniques of greenhouse gases. It describes in detail the labelling process that atmospheric greenhouse gas measurements sites have to go through to receive approval to join ICOS, as well as the quality controls used to assure high quality and precise scientific data. To date, there are few papers outlining the steps taken to harmonise trace gas measurements from large networks with multiple stakeholders.
This paper bridges this gap, gives good lessons learnt during the process and provides great clarity on the ICOS atmospheric station labelling procedure that can sometimes be a little opaque to those outside of ICOS.

The paper is well written, with very good English and the scientific methods used are appropriate. The figures and tables are on the whole well-presented and add to the understanding of the manuscript. I thoroughly enjoyed reading and reviewing the manuscript.

Specific comments: There are a few inconsistencies within the manuscript that need to be addressed, including the mixing of units (e.g. ppm and μmol.mol-1) and whether species are written with subscripts or not (i.e. CO2 or CO2) within both the manuscript, tables and figures. Furthermore, there are a number of times where the authors have used atmospheric or atmosphere interchangeably to describe ICOS stations where atmospheric GHGs are measured (c.f. P3 L23 and P15 L20).
In addition, the use of abbreviations and their introduction into the manuscript aren't always consistent. For example, the abbreviation of greenhouse gas to GHG is used within the abstract whilst no abbreviation is used within the remaining sections of the manuscript. In contrast, station acronyms based on GAWSIS IDs for stations have been used within the manuscript but no full name has been given the first time that the station has been introduced in the text. For clarity, please include the full name, followed by an acronym, the first time it is used in the manuscript.
We will pay attention to this and correct accordingly.

Furthermore, there are some formatting issues with some of the tables and figures that need attending to, such as the inconsistencies of table presentation and the boarders of column titles. Some figure captions are lacking in basic information (e.g. what abbreviations mean within the figure, keys for schematics, etc.) and mean that if a reader were to come and look at the figure only, it is difficult to comprehend (see technical corrections for specific figure comments). Additionally, some colour combinations are hard for people with colour-blindness to decipher. Please consider altering some combinations, e.g. not having red and green together.
We will work on the captions to help the tables and figures be understandable as standalone. When possible, we will change the colors to address color-blindness. However the figures in the first part were made for the Step2 reports and are not easily reproduced. Thanks to your remark, we are working to improve the color code for the figures that are produced daily and are visible on the ATC website.

For the technical corrections, we will apply them. Specific answers can be find below.
Technical corrections:

P1 L8: text does not read well, try – ". . . calibration gases are
measured twice a month".
P1 L8: change "controlled" to "verified".
P2 L3: text does not read well, try – ". . . in a calibration sequence is possible, saving gas and extending the calibration gas lifespan".
P2 L10: text does not flow well, try – " Continuous, precise, greenhouse gas monitoring began in 1957 at the South Pole and in . . .".
P2 L21: remove "i.e." before "harmonized and high precision. . .".
P3 L1: seeing as the location of the ATC is stated in P3 L6, this should also be done for the Flask and Calibration Laboratory and the Central Radiocarbon Laboratory.
P3 L6-8: the location of the ATC is ambiguous, would be better to state outright that it is in France, i.e. "The Atmospheric Thematic Center (ATC, https://icos-atc.lsce.ipsl/fr/) is divided into three components; the metrology laboratory (MLab) responsible for instrument evaluation, protocol definition and PI support (located in France), the data centre (located in France) responsible for data processing, code development and graphical tools for PIs, . . .".
It is in fact located in France for the Mlab and data center and in Finland for the MobileLab. We will reformulate for accuracy.

P3 L10: add "the" before ATC.
P3 L15: it might be good to give an example of what elaborated products are available as those reading the manuscript who are not familiar with ICOS may not know what is offered.
P3 L28-29: text does not read well, try - ". . . adhering to the WMO guidelines (WMO, 2018) for greenhouse gas observations but are elaborated on more in ATC and Laurent (2017) and presented in section 2.4.
P4 L15: What is the frequency of routine data evaluation sessions?
We usually go for once a month.

P4 L26-27: It is not clear here what it meant by the list of Class 1 parameters that aren't necessary for a station to be labelled. Is it that out of the three parameters (boundary layer height, GHGs and 14C values from flasks), two do not need to yet be in place for a site to be labelled; or should the sentence read three parameters? Additionally, could more clarity be given on what is meant by GHGs, seeing as in situ CO2 and CH4 measurements are mandatory and are GHGs.
We will clarify. There are only two parameters: BLH and flask measurements. For the flask we measure GHG (the one we sample quasi-continuously and some we don't such as SF_6 and H_2) and radiocarbon. For the flasks, there were delay with the development of the automatic flask sampler.

P5 L1: Please provide a reference for the specification document if publicly available. In addition, is the list of accepted analysers publicly available?
The list is in the specification document which is publicly available (ICOS RI (2020): ICOS Atmosphere Station Specifications V2.0 (editor: O. Laurent). ICOS ERIC. https://doi.org/10.18160/GK28-2188)

P5 L15-18: the relative pronoun "whose" on L16, in the parentheses, should be replaced with "for which".
P5 L25: Try to avoid double parentheses.
P6 L6: What mixing ratios do you suggest for the long-term target to ensure that it is representative for more than 10 years?
In the specifications, the recommended long-term target mixing ratio is 450ppm for CO_2 for background stations, 470 ppm for peri-urban sites. You can find the values for the other species in the specification document. Of course this value will pass from a relatively high to a low value over time compared to most of the ambient air measurements. However, since this tank is really

intended to check the long term consistency of the measurements we could not find a better option to cope with the trend.

P6 L7-8: For clarity, change to "It is recommended to send the long-term target, as well as the calibration set, for recalibration approximately every 3 years to the CAL-FCL to investigate and take into account any possible composition changes in the gases, especially for CO.
P6 L10: To make the manuscript more accessible for colour-blind readers, change the end of the line to "The instrument calibration dates are included at the bottom of the plot by the open orange circles.".
P6 L15: replace "depending" with "dependant".
P6 L19: Include definite articles (the) in front of long-term and short-term target.
P6 L22: replace "are going" with "go".
P6 L23: To remove potential misunderstandings with the meaning of the word "control" in relation to station PI's reviewing data, replace "control" with "verify" or "review".
P6 L28: Please state which server you are referring to at the beginning of the line.
P6 L28: Where are the ATC data products located that station PIs check? Are they the plots shown on the ATC website (e.g. https://icos-atc.lsce.ipsl.fr/SAC)? If so, please state that these are publicly available for stations that have been labelled and give the link to the website.
Yes, indeed, they are located on the website. We will add the link there.

P6 L30: Please outline what is used as the flagging scheme. Is this already published in Hazan et al. (2016)?
In Hazan et al. (2016), the automatic flagging scheme is described but not the user part of it. Raw data are controlled day by day. For valid data, we can choose additional information such as "Maintenance", Quality assurance operation" or " Non-background conditions" but this is not mandatory. Data have to be invalidated only for a objective reason which has to be chosen in a list to carry on the QC. The reasons can be (non exhaustive list): "Calibration Issue", "Flushing period", "Maintenance with contamination", "Inlet leakage"... We will add this short description.

P6 L31: As for P6 L23, change "controlled" to "verified" or "reviewed" to remove misunderstandings.
P7 L22-25: Establishing if your sample intake line has a leak or not is an important consideration. What is done at sites to establish if there are leaks if the mast cannot be climbed easily due to reasons outside of the control of the PIs and there is no infrastructure installed to alter intake configurations remotely?
Up to now, all Pis of the labeled stations have managed to perform the intake line at least once. Also, to minimize leaks, the specifications recommends to have sampling lines in one part, without connections.
One more point we are promoting is a check of the consistency of the vertical profiles of CO_2, CH_4 and CO during mid-afternoon periods in well mixed conditions (see Matthias Lindauer presentation during the 2020 ICOS conference, "Vertical gradients of greenhouse gases at 8 German atmospheric ICOS Stations").

P8 L1-2: More information is needed for this test to be replicated by someone reading this paper and is not part of ICOS. It is not clear to me if a humidification loop is used, as in Stavert et al. (2019; https://doi.org/10.5194/amt-12-4495-2019) to conduct this test or is another method used within ICOS? In addition, what mixing ratios within the cylinder are suggested by ICOS for the test?
We will rephrase for clarity. No humidification loop is used. We inject from a syringe directly in the inlet of the instrument in the case of the CRDS (they have an internal filter) and through a filter for the OA-ICOS. The cylinder used is with ambient air mixing ratios.

P8 L9: Please provide a hyperlink for the automatically generated plots on the ATC website.
P8 L14: Please alter “bi-monthly” to “twice-monthly” or “every 15 days” to remove ambiguity.
P8 L30: Please include three letter identifier after Lindenberg to aid the reader in finding the example in Figure 4.
P9L8-9: Please include a space between numbers and units.
P9 L18: Calibration drift is misleading as a title, as it suggests the drift of mole fractions within the calibration cylinders. This may be the case for some species and over longer periods of time than 2 weeks; however, the authors are discussing the assessment of instrumental drift in this section. I would suggest changing the sub-heading to “Instrumental drift and calibration optimization”.
Thanks for this comment, we will do so.

P9 L20: Is instrumental drift ever estimated over shorter timescales than 2 weeks? In my personal experience with optical instruments, some can drift quite significantly over periods of time less than 1 day. This is especially the case in environments where there is poor thermal stability (e.g. no air conditioning or too large thermal switches on air conditioning units).
For some instruments, such as the ones measuring CO and N_2O, we definitively observe short-term drifts, in the scale of hours to days. In this case, we use a “short-term working standard” to correct for such drift. This standard is calibrated by the twice-monthly calibrations.

P9 L30: Are there specific types of analysers that are worse than others for temperature dependence, e.g. instruments with larger cavities?
We can expect that with a larger cell, there will be more inertia and hence a larger temperature dependence. However, within one type of instruments, we also observe some instruments with a significantly larger dependence than the others.

P10 L9-10: Please state what the meteorological sensors need to be compliant against? ATC specifications document? Also, are the meteorological data submitted to the same database as the GHG data?
The meteorological sensors need to comply with the list in the specification documents and indeed the meteorological data as well as the diagnostic data (flow rate, room temperature) are submitted to the same database.

P11 L16: Replace “Belgium and France” with “Belgian and French”.
P11 L28-30: This sentence isn’t clear and I cannot decipher what the authors mean. Please rephrase to give clarity.
We will rephrase for clarity. We wanted to say that some sites use two systems: the rotary valves to switch between the calibration and target gases and solenoid valves to choose between air at different levels and cylinder gases.

P11 L32-33: Has a study ever been done by ICOS on the representativeness of using buffer volumes? As I understand it, one of the main advantages of using optical instruments is the added information that can be gained from the short-term variability in mole fractions. Would it be better to not use buffer volumes to futureproof the data at these sites for when numerical models can ingest high frequency data and simply smooth data based on statistical filters, as used at other sites and networks?
We have studied the representativeness of using buffer volumes. The results have been presented at the Monitoring Station Assembly meetings.
The advantage of buffer is to have a better hourly representativeness while using discrete data for a multisampling height site.
As of now, only fours sites have chosen to use the buffer volumes.

P13 L11-13: What were the sources of leaks for GAT and STE? It is not often that papers include lessons learned information, which is often very useful to other stations in diagnosing problems of their own.
Unfortunately, we do not know the source of the longer stabilization time. At both sites, several interventions happened over time. This is also a lesson to learn on the ATC side, that we must make sure that the PIs are aware of the Step2 report recommendations and that they are followed up through.

P13 L19: As American English has been used throughout the manuscript, please remove the th from after 15 (both occasions) as this is only included in British English.
P14 L30: As far as I am aware, there are two methods for a Nafion counter purge: using a dry gas, such as zero air or N2, or the Welp et al. (2013; 10.5194/amt-6-1217- 2013) method of reflux mode (i.e. taking a small portion of dried air post-Nafion and using it as the counter purge gas but ensuring it is at a lower partial pressure than the sample gas). Which method is currently recommended by ICOS when using a Nafion to dry samples?
We recommend to use the reflux method described in Welp et al (2013) which avoid using consumable gas.

P15 L4: Full name used for Jungfraujoch instead of a trigram. Please replace with JFJ to be consistent.
P15 L20: Grammatical error, please change to – "In this paper we have presented the process used to label ICOS atmospheric stations.".
P15 L28: Replace "oftentimes" with "often".

Table 1: Please include a reference to the ICOS atmospheric station specification document in the caption. In the table, it is not clear that the column "Gases, periodical" relates to flask measurements. Please add in more information in the column caption or in the table caption to clarify this. In addition, was atmospheric pressure at the highest inlet height ever discussed as a useful parameter for modellers to see the pressure differences between the top and bottom inlets of towers?
No added value was found in having different measures of the atmospheric pressure. For modelers, we do measure the temperature gradients, useful to evaluate the inversion.

Table 2: I am assuming that the thresholds cited in this table are specific to a certain type of instrument, i.e. CRDS seeing as these instruments are mostly used within the network for CO2 and CH4 analysis. In addition, please could you include the H2O threshold used for calibration gases, as referred to on P5 L25-26.
The thresholds here are instrument specific and can change within the same type of instruments but indeed the thresholds written here work well for most of the CRDS instruments. For CO, they work as well for OA-ICOS, being even very conservative.

Table 3: Please can you ensure that the writing of magl is consistent with figures (often written as m agl). This also applied to masl.
Table 4: The ambient air percentage for KRE looks erroneous (5069 %).

All figures: Please include lists of full site names, with acronyms in parentheses, of any site included in the figure. In addition, if any instrument number is included or a cylinder D number, please give an explanation. If species are mentioned, ensure that any numbers are subscripted, e.g. CO2, not CO2.
Figure 1 caption: Suggest changing to = " One month of target gas injections for CO2 (ppm), shown as the difference of calculated vs. assigned mixing ratios. Short term target data is plotted in green, whilst long term data is in brown. The calibration dates are shown by the light orange open circles.

Cylinder number (D******), mean values (± X), point-to-point variability (Ptp) and difference to the assigned value (Diff) are displayed above the figure."
Figure 2 caption: Notwithstanding that the figure is there to show locations to connect a cylinder to run the leak tests outlined in section 2.3.3., a key for the different parts shown in the figure would be useful for reader comprehension.
Figure 3 caption: Please indicate what the values in the 2nd and 3rd columns represent.
Figure 4 caption: Please indicate why there are duplications of LIN (as explained in the manuscript text).
Figure 6 caption: please indicate how the deviation of measurement from assigned values is calculated.
Figure 12 caption: The MHD Marine Smooth Curve isn't explained, please include a brief description of the methods used to derive the curve.
Figure 13: To make the insert clearer, consider adding a black border around to isolate it from the main figure. In addition, add in a list of the sites, with the acronyms in parentheses, as well as giving the years for the colours of when sites were first labelled.
Figure 15: It is currently hard to read the site acronyms and instrument numbers, please reduce the text size slightly so that there are some gaps between each site,like in Figure 16.
Figure 17: There is no bottom tine to the top plot.
Figure 20: What is the difference between ATC MetroLab HB 2016-05 and ATC Mlab Droplet?
HB stands for humidity bench while the Droplet is for the droplet test described in the text. The humidity bench allows a much more controlled and precise sensitivity test. We will detail the caption to give more clarity.