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Interactive comment on "Assessment of a multi-species in-situ FTIR for precise atmospheric greenhouse gas observations" by S. Hammer et al.

Anonymous Referee #1

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C1532

Review of Hammer et al: Assessment of a multi-species in-situ FTIR for precise atmospheric greenhouse gas observations

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This manuscript describes the performance of the 'UoW' FTIR trace gas analyser, in particular focusing on the compatability with the WMO-GAW goals for greenhouse gas measurements and quantifying (and correcting, either empirically or via instrumental improvements) cross-sensitivities between measured species and sample conditions. They conclude by making valuable (for current and potential users) recommendations about calibration strategies for the instrument.

Overall, this paper does a thorough job of following through on its title by assessing the performance of the FTIR analyser. It is highly suited to publication in the AMT Special Issue arising from GGMT2011. I do, however, recommend some, mostly minor, changes. There are a number of minor English language corrections necessary, and the paper could benefit from tightening up in areas. I recommend its publication after addressing these issues.

General Comments

- I find the Conclusions and Outlook section addressing the calibration gas consumption and recommendations for number of frequency of calibrations to be particularly useful for users of the instrument. It would be interesting to contrast this to the needs for other instruments that adhere to the WMO-GAW criteria. It would also be nice to recap on the perceived frequency necessary for performing the cross-sensitivity quantification experiments, which is mentioned elsewhere.
- At the end of Sect. 3.3, for example, it is stated that the ILC targets are considered to determine whether the sensitivity is significant. While that may be true over the typical range of variation quoted, how do these effects cumulate? Does that mean that the effects for these gases are ignored, or are the corrections still applied?
- It would be nice to include a table listing the typical variability of sample conditions (temperature, pressure, flow...) for easy reference. This could also list the standard operating conditions (c.f. Sect. 2.3).
- p3660, L25-27: why would the sample pre-treatment compensate for the temperature difference? Is it the treatment itself, or the residence time in the dryers? If the Nafion is housed outside the thermo-controlled enclosure can this be relied upon to compensate for temperature differences in reality? How important is the role of the laboratory conditions on the temperature stability introduced by the Nafion?
- p3662, L18: What is the lifetime of one magnesium perchlorate cartridge? Is it a recommendation of this paper to maintain the H2O between 2 and 10 μ mol mol⁻¹? Otherwise what governs the operational range, and therefore the range that is examined here? Do the authors have any idea how the cross-sensitivity with respect to H2O behaves outside this range that might feed through to making a recommendation for the operational H2O limits? At what point (i.e. H2O mole C1534

fraction) does the cross-sensitivity to H2O start to limit the ability of the instrument to reach the WMO-GAW standards?

- While I appreciate that the linearity of the instrument has, in general, been established, I would expect that three calibration standards are necessary to adequately define the line and/or assess the linearity. After all, one can define a line with only two points - if one of those happens to be incorrect then your line will be misdefined. I would think that some redundancy is necessary. The conclusions mention this, but it could also be addressed earlier (end of Sect. 4).
- p3667, L25-28: Do the authors know why there is disagreement between the Griffith Allan variance results and those presented here? Is it instrument specific? Is this important?

Technical Comments

- Abstract: There is an inconsistency about whether or not acronyms are defined e.g. ILC is, but WMO-GAW, FTIR are not.
- Introduction: p3646, L21 (and numerous other places) the use of which is incorrect. Please check this throughout the manuscript. As a rule, 'which' should either be preceeded by a comma or a preposition. In many cases it could be replaced by 'that', requiring no preceeding comma. The following is an explanation of the difference between using 'which' and 'that'.
 - "The painting, which was hanging in the hall, was stolen"
 - "The painting that was hanging in the hall was stolen"

Both mean that a painting hanging in the hall was stolen. The former simply offers a property of the painting - this does not mean that it was the only painting

in the hall. The latter, on the other hand offers a unique description identifying the painting - it was the one hanging in the hall.

Another exception occurs when addressing a question, e.g. when answering the question: "Which calibration strategy is better?" one could reply "We could not determine which calibration strategy was better"

There are numerous instances of the misuse of the word 'which' that I will not specifically mention.

- p3648, L23: Further on → Hereafter?
- p3648, L27: The wording at the end of this sentence sounds a bit awkward. I suggest rephrasing to "the hardware modifications resulting from the first year's findings are also introduced" (note the plural with modifications).
- p3649, L7: what does the (5.0) mean when referring to the high purity nitrogen? For those not familiar with the grades, it would be nice to list the purity (99.999% ?) or at least refer to it as 'grade 5.0'.
- p3649, L15 c.f. p3650, L11: Please be consistent with the spelling of analyser/analyzer.
- p3649, L17: Would be nice to have the name (magnesium perchlorate) as well as the chemical formula.
- p3649, L18: either by-passed or bypassed, but not by passed.
- p3651, L3 and L23: I think the 'the' before SOC is unnecessary.
- p3651, L3: suggest replacing 'compartment' with 'enclosure' for consistency
- p3651, L22: Delete 'on' at the end of the sentence.

C1536

- p3652, L3: ability of completely exchanging the sample → ability to completely exchange the sample OR ability for the sample to be completely exchanged
- + p3652, L10: results in 0.03 \rightarrow results in a 0.03
- p3653, L3: minute \rightarrow minutes
- p3653, L19: which \rightarrow that
- p3654, L1-4: How valid is this assumption? It would be nice to at least refer to the fact that this assumption will be addressed in later sections.
- p3655, L15: delete 'do'
- p3656, L2: 'cylinder filling' while I can appreciate what this means, it could be better expressed. Perhaps 'Each time a cylinder was filled, it was checked for drifts by GC analysis before and after use', or something similar.
- p3656, L10-11: ?? This sentence requires rephrasing for clarity.
- p3656, L17: As reference \rightarrow As a reference
- p3656, L23: Incorrect English. Suggest rephrasing to '0.1 or 0.05 μ mol mol⁻¹, respectively, for CO₂ in the Northern and Southern Hemispheres.'
- p3656, L25: repetition of 'determined' delete one instance.
- p3657, L3-4: The way this is phrased is confusing, given that the second range is within the first. I suggest rephrasing to state that the second range, or a sub-range, (around operating pressure) is tested in finer pressure steps.
- p3657, L7: 'residual pressure sensitivity' you've just gone to the trouble of defining this acronym, why not use it?!

- p3658, L14: later used thermocouple \rightarrow thermocouple used later ?
- p3658, L15: at least on \rightarrow on at least
- p3658, L21: what is 'the whole system'?
- p3658, L27: move 'was' to after 'experiments'
- p3659, L24-26: You choose a linear fit over a step change. Is there any physical reason to prefer this?
- p3660, L9-10: was the sample flowing or static after the evacuation?
- p3660, L27-29: investigations ... is \rightarrow investigation ... is OR investigations ... are
- p3662, L7-8: differently pronounced \rightarrow shows different behaviour?
- p3662, L15-16: suggest rephrasing this sentence to: 'They may, however, become relevant if water and water isotopologues are to also be measured with the instrument.' It might be nice to have a reference here too, because the fact that the instrument can potentially perform H2O and H2O-isotopologue measurements has not been introduced in this paper, unless I have missed it. I notice that it is mentioned in passing earlier (p3649, L19) it could also be expanded there, maybe just a part sentence saying that this is possible with the instrument, and referring to a publication with details.
- p3663, L3: means \rightarrow methods
- p3663, L24: what about H2O production from the Ascarite, via the 2NaOH + CO2
 → H2O + Na2CO3 reaction? Do you see any effect from this, or counteract this
 is any way?
- p3665, L11: This sentence needs rephrasing to avoid the misuse of respectively. C1538
- p3667, L1: the (laboratory?) temperature oscillated...
- p3667, L20-22: You previously discussed the choice of timestep (p3651, L15), so this is both redundant, but also raises other reasons from what was mentioned earlier. I suggest mentioning all reasons (or removing those not applicable) in one place, and one place only.
- p3668, L16-17: What question about calibration frequency?
- p3668, L21 (and repeated afterwards): suggest calling these 24- and 48-hourly. To me two-daily sounds strange.
- p3669, L22: regular, e.g. daily calibration might help reducing... → regular, e.g. daily, calibration might help to reduce...
- p3670, L1: What does 'One outlier appeared due to a wrong calibration measurement' mean? Was the wrong tank measured? Was the value simply an outlier? Please explain.
- p3670, L23: define MPI-BGC
- p3670, L26: replace mid with middle (both instances)
- p3671, L5-6: Which step change? Suggest that you explain with reference to the fig when this occurred.
- p3671, L17: Suggest that you define the periods that are considered 'stable' and 'less stable'. Perhaps with a horizontal bar in Fig 10 corresponding to one of these.
- p3672, L10: by a factor 2 → by a factor of 2. Should this actually be sqrt(5)? In the following line, should this be 100% larger, as you are calculating relative to the target measurements?

- p3672, L12-13: Different from other IRFs → Different from the IRF for other gases??? (just for clarification, as opposed to the possibility that this might refer to other instruments)
- p3673, L16: not observed anymore \rightarrow no longer observed.
- p3673, L17: 0.1° only \rightarrow only 0.1°
- p3674, L20: not sure about the wording in brackets
- p3675, L19: formally not \rightarrow not formally
- p3675, L25: a few $\mu \text{mol mol}^{-1}$ of H_2O, only \rightarrow only a few ...
- p3676, L18: left over \rightarrow remaining
- p3676, L22: to use \rightarrow using (or 'the use of')

Other: it would be nice to acronyms defined in the figures when they are used.

- Fig. 1: is it possible to have arrows defining the direction of gas flow?
- Fig. 7: our? primary laboratory cylinders.

Fig. 8: it is really hard to see the grey points behind the coloured symbols. It would be nice if something that stands out more could be used.

Fig. 9: some residual German (Mai) in the x-axis label!

C1540