Atmos. Meas. Tech. Discuss., 8, C282–C285, 2015
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Atmospheric Measurement Techniques Discussions

Interactive comment on "PTRwid: a new widget-tool for processing PTR-TOF-MS data" *by* R. Holzinger

Anonymous Referee #1

Received and published: 11 March 2015

The manuscript of Holzinger reports a software tool to post-process raw data recorded by the Proton Transfer Reaction 'Time-of-Flight' mass spectrometer (PTR-TOF-MS) manufactured by Ionicon (Innsbruck Austria). In particular, the manuscript thoroughly describes just the operating conditions of the software rather than presenting a novel measurement technique. Actually, the approach presented here to analyze PTR-TOF-MS raw data is not unique as it follows another approach that has been already published (Müller et al. 2013) and widely tested by a user community of international scientists (https://sites.google.com/site/ptrtof/), while PTR-TOF-MS technology has been already validated as a reliable system for trace gas analysis (Jordan et al. 2009; Graus et al. 2010). As a consequence, it should have been very interesting (and very useful for the scientific community) to compare the performances of the preexisting ap-

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proach developed by Müller et al (2013) with those of the approach presented here by Holzinger, especially when these two different approaches have to post-process the same raw dataset recorded by same PTR-TOF-MS. Moreover, it is not clear what is the real advantage to use the approach presented here rather than the preexisting one of Müller et al (2013), and why there was the real need to develop another software tool instead of implementing the one already in use. However, the application of the software presented here by Holzinger is strongly limited by the fact that best performance are achievable if a single raw data file has been recorded for 30-120 minute long (as the author wrote in lines 20-21, page 3 and in line 14-15, page 5)! Indeed the biosynthesis and kinetics of emission of volatiles organic compounds in plant leaves often happen in 'seconds or minutes' of time spans (Brilli et al., 2011), and also in micrometeorological applications of eddy covariance flux measurements of VOC it is more advisable to record small data file to be merged together in a later step (i.e. 6 minutes; Müller et al. 2010; Ruuskanen et al. 2010; Kaser et a. 2013) rather than big files of 30 (and more) minutes because small files are easy to manage and avoid (important) data loss if one single file resulted corrupted and thus unusable. In addition, I have serious doubts about the use of a library (mentioned as 'masslib') for assigning a name to a chemical compounds identified as a peak in the PTR-TOF-MS spectra; the author should make it clear how the library deals with the fragmentation pattern of VOC and how the use of such library is able to assess protonated ions related to the ion chemistry of PTR-TOF-MS (i.e. inevitable clustering ions with water molecules). In conclusion, since the manuscript presents some inconsistencies and is very technically oriented, I suggest the author to consider publication in a more specialist journal that takes into account the development of software tools as a subject area of interest, after addressing the concerns risen above and the points listed below.

- The manuscript includes too many figures (10 !!!); as some of those appear more like 'screenshots', they could be either merged in a few figures or moved to supplementary information (where there is already a Figure B1, oddly without a Figure A or B2. . ..); by the way in Fig. 3 panels are missing. - Line 10, page 2: it is written: "attributed

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peak", but attributed to what? - Lines 15-19, page 2: I would simply say: "PTR-TOF-MS technology records full mass spectra with high mass resolution that allow differentiating between ions having the same nominal but different exact mass weight". - Lines 4-7, page 3: actually the approach developed by Müller et al. (2013) shape the peaks on then basis of certain 'ions' that are always produced by the PTR-TOF-MS, as the primary ions m/z 21.022 (H183O+) and m/z 39.033 (H2O-H183O+) that do not saturate the detector and result isolated from other peaks (and thus easy to define and model). - Line 4, page 4: the author should consider that "single lab measurements" may run for time spans < than hours! (Brilli et al. 2011). - Line 10, page 5: What "drifts in these parameter" the author does refer to? - Line 14-15, page 5: The author should demonstrate/show to what extent the code presented here can give good performances even though analyzing files recorded for shorter time periods that 30 minutes. - Line 17, page 5 and line 15 page 6: which are the "data containing parameter"? - Line 2, page 6: the author should specify what are the "scans" for? - Line 8, page 6, line 19-20, page 6: the author speaks about "6 times", "range of 20-10000", "8 times", but how all those thresholds have been defined and optimized? - Lines 10-13, page 7: the author should make clear what the parameters "a, t0, m, x" refer to. In particular, the parameter "x" has been reported as "EX" from here to the end of the manuscript! The author should carefully double-check the manuscript to avoid this and other "typing" mistakes occurred throughout the manuscript. - Lines 23-24, page 8: please rephrase ". . .the corresponding TOF-bins of the corresponding. . ." as it sounds very bad. - Lines 12-13, page 9: why and how the values of "90 nanoseconds" and "7 times" have been chosen? - Line 8 and line 17, page 9: consistency is required as first it is written "Figure 4" and then "Fig. 4". - Line 7, page 10: something is missing within the sentence ". . .we consider all peaks the maximum signal. . ." - Lines 9-10, page 10: again, the author should explain how/why values of "800 counts" and "10 times" have been chosen. - Lines 5-19, page 11: this part is puzzling and difficult to follow and should be rephrased (avoiding such inappropriate wording as "routine executes all routines", in line 13). - Line 21, page 11: the abbreviation "ppm" refers here to "TOF bin width" but it confounds

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with another very similar abbreviation indicating concentrations (Part Per Million); I suggest the author to use a surrogate for such index so to avoid misunderstandings. - Line 28, page; line 26 page 14. . .: the author mentions here and many more times throughout the manuscript about a Quadruple-PTR (namely PTR-MS or TD-PTR-MS), that do not require a mandatory post-processing step to elaborate the data as the PTR-TOF-MS. So why has the PTR-MS or TD-PTR-MS has been mentioned? - Lines 15-19, page 14: what exactly are the numbers “487” and “1350” used by the author as constant multipliers? (nevertheless, in English language is “multiplying by” and not “multiply with”). - Line 16, page 14: it written “our off-line TD-PTR-MS method”, but who is the other since Holzinger is the only author of this manuscript? - Line 20, page 15: the author refers to “engineering data”, without providing any explanation of what kind of “engineering” has been done. - Lines 3-26, page 17: the author should clarify the differences between the “attribute formulas” presented here and the one already (published) available on the web (http://www.chemcalc.org/) - Line 21, page 17: it is not clear the connection between “the measured signal” and the “attribute formulas” described in this subsection. - Lines 19-21, page 18: this confirms my concerns about the application of this software tool in long-term (many months) eddy covariance flux measurements of VOC because the time consumed to open the big files will add to that required to post-process the same file thus further slowing down the data analysis and make it unsustainable. - Lines 14 and 19, page 21: what is it “menue”? - Line 18, page 23: “the Utrecht PTR-TOF-MS” is different form those manufactured by Ionicon in Innsbruck (Austria)?

Interactive comment on Atmos. Meas. Tech. Discuss., 8, 1629, 2015.