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Atmospheric Measurement Techniques Discussions

Interactive comment on "FATES: A Flexible Analysis Toolkit for the Exploration of Single Particle Mass Spectrometer Data" *by* Camille M. Sultana et al.

Anonymous Referee #2

Received and published: 16 December 2016

This manuscript provides a description of a flexible analysis toolkit for single particle mass spectrometer (SPMS) data, based in MATLAB, which represents an important and substantial contribution to the SPMS community. The authors have clearly put much thought and work into making the FATES toolkit as adaptable, user-friendly and maintainable as possible. Making the code publicly available is an important step towards transparent and reproducible data analysis. I have no doubt that different implementations and functionality in FATES will grow as it is adopted by the community.

General Comments:

I have two main concerns about this manuscript.

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(1) The use of FATES has been demonstrated only with SPMS data from the author's research group and with only one type of SPMS. For this work to be published the authors must demonstrate clearly the successful implementation of FATES with very different types of SPMS data sets. Related to this point, the authors provide little information on data import and structure for different SPMS data formats. I understand that this information is available in the FATES manual provided on the GitHub page; however, the authors should consider including the manual as a supplement to this paper. The benefits of this (while being, admittedly, somewhat information heavy) will be more specific reference to information contained in the manual in the main text of the paper, and the ability for user's to cite the manual for justification of data analysis choices.

(2) While providing a valuable resource for the SPMS community, this manuscript should also seek to establish some central guidelines or standards for SPMS data analysis and interpretation. The authors indicate the necessity of expert knowledge in determining finalized chemical particle types from a dataset, and provide interfaces to facilitate these decisions. To help ensure the proper and educated use of these tools the authors should provide some concrete criteria by which the identification of chemical particle types should be made in FATES (e.g., criteria for evaluating linkage heights in dendroFATES, guidelines on evaluating cluster similarity using the dot product or other methods, discussion of advantages and disadvantages of different clustering approaches for SPMS data and criteria by which to choose a particular clustering approach). While this information is likely available in pieces in a variety of publications, a discussion of best-practices would really strengthen this work.

Specific Comments:

In general, this manuscript could be written in a more clear and concise manner. Intermingled with a description of the software seems to be sections that read more like an instruction manual. This paper could benefit from more consistency in the way the information is presented.

L95: Do the authors intend to test the compatibility of FATES with MATLAB 2016?

L109 (and other instances): "...a unique, two-column, particle identification (ID)."

Section 2.2: Much of the text in this section describes comparison of run-times for FATES and YAADA. This discussion is a bit difficult to follow and it might be easier if the run-time information was summarized in a table. When another type of SPMS data is included in this paper, similar information could be included provided the data can be analyzed in YAADA.

L318: Related to comment (2), above, how can it be objectively determined that the user should be "satisfied" by the FATES output? At present this seems incredibly subjective, and should be delineated.

Section 4.4: Are there standard procedures for mass-calibrating SPMS data? What is the smallest allowable number of peaks to be used in mass calibration?

Figures: In general, the figures are quite difficult to read.

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