Atmos. Meas. Tech. Discuss.,
doi:10.5194/amt-2019-489-RC1, 2020

Atmospheric Measurement Techniques Discussions

Interactive comment on "Development of an Automatic Linear Calibration Method for High Resolution Single Particle Mass Spectrometry: Improved Chemical Species Identification for Atmospheric Aerosols" *by* Shengqiang Zhu et al.

Anonymous Referee #1

Received and published: 3 April 2020

General comments: This paper develops an automatic linear calibration method to calibrate the mass spectra for individual particles measured by newly developed HR-SPAMS. The method improves the current accuracy of mass-to-charge (m/z) measurement for single aerosol particles, based on the testing of laboratory-generated sea spray aerosol and atmospheric ambient aerosol. The authors provided the time series of peaks with small m/z differences and a comparison of particle classification between LR-SPAMS and HR-SPAMS. While this method may be applicable to the scientific community, there are still some limitations. The main criticism is the limited discussion of

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the analysis of newly generated mass spectra by the HR-SPAMS, and the lack of discussion on why only sea spray aerosols were selected. It is certainly TRUE that applying high-resolution data with enhanced mass calibration can significantly affect particle classification (identification). However, it is more important if there is new information obtained from the classification.

Specific comments:

1. Introduction: similar instruments, such as Aerosol mass spectrometer (AMS), also have high-resolution versions. Is the calibration method identical to SPAMS? Inclusion of this in the introduction and discussion would be necessary for completeness.

2. Lines 80-85: In this section, it would be better to state the significance of why the calibration is required for each particle. While the authors noted that the ion peak position is still very susceptible to initial ion coordinate and speed, they did not provide details to show the significance.

3. Line 192: "1,409 ambient particles were successfully calibrated". Why some fraction of particles cannot be calibrated? I think the discussion of such an issue in section 3.3 should be moved here to provide clear reasoning. Such an obvious deficiency should also be stated in the abstract or conclusion.

4. What is the matrix size produced by the HR-SPAMS? Is there a limit for the ART-2a to classify the matrix of particle mass spectra? Such information should be included.

5. Section 4.4: What kind of new information is provided when new matrix is included in the classification? I think it would be interesting if there is new information after the classification of newly calibrated mass spectra.

6. Some peak ions should be added to Fig S5 and Fig S6 for clearance.

7. Conclusion: It would be better to include some atmospheric implications for the identification of additional peaks, in particular, organic peaks. Currently, the authors showed that more particle types can be obtained, but it might not be meaningful enough

for the scientific community.

8. Grammar check or minor comments:

Line 70: LDI?

Line 77: “A SPAMS”

Line 99: “accessed”

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