Author Response

Revised Submission: egusphere-2025-4222 - Curve fitting algorithm for multimodal particle size distributions – a theoretical basis

RC1: The work is done and presented well. There are no major questions about the quality of the work. The main question this reviewer has is "why"? The manuscript is about fitting functions to a multimodal particle size distribution. This is basic data analysis and all major scientific software suites include this capability. An argument was made that the presented work simplifies the process so that the user does not have to learn how to find the peaks (which in itself could be problematic since now there's a black box doing the analysis). However, the code is written in R (using existing R packages for analysis - so again, where's the novelty?) which limits its usefulness to those using R (as opposed to e.g., Python or Matlab). As such, there is little scientific merit to be reviewed here. In conclusion, this manuscript does not offer anything novel to meet the standards of AMT and qualify as a full research paper. The manuscript could be re-submitted as a technical note or the focus could be shifted to analyzing the data from SPL using the R functions described.

The authors thank RC1 for their careful review of the manuscript and for their constructive comments. While several major scientific software packages include capabilities for fitting multimodal particle size distributions (MPSDs), we are not aware of a readily accessible and flexible implementation that can accurately characterize the wide range of ambient and laboratory measurements considered in this work. One of the primary motivations for developing this algorithm was the lack of an openly available and broadly applicable MPSD fitting framework identified in the literature. We agree that automated peak identification is an obstacle for users to develop experience with manual peak selection. However, for large datasets, manual analysis is impractical, as previously discussed by Mäkelä et al. (2000).

R was selected as the implementation platform because of its strong statistical capabilities and use within the aerosol sciences community. In keeping with the open-access objectives of this work (as shown in the supplement), the algorithm has been designed to be transparent and readily adaptable to other programming environments, such as Python or MATLAB as mentioned. We further argue that this open-access framework addresses accessibility limitations commonly associated with other instruments or models such as IGOR or IDL.

We appreciate the suggestion that the work may be more suitable as a technical note. However, as this article type is no longer offered by AMT, we believe the latest revision is the most appropriate format in presenting a method focused manuscript and its evaluation.

RC2: The work done by Rapp et al. is presented clearly and coherently and I have no major issues with the writing itself or the structure of the manuscript. However, I cannot recommend its publication as a research paper and would recommend its resubmission as a technical note. While the method presented in the manuscript could be of use to some, it is not novel enough for a full research article and the study itself presents little new additional research. In addition, it is only available for R, which undoubtedly limits the number of potential users.

The authors thank RC2 for their careful review of the manuscript and helpful comments. We appreciate the suggestion that the work may be more suitable as a technical note. However, as this article type is no longer offered by AMT, we believe the latest revision is the most appropriate format in presenting a method focused manuscript and its evaluation. Regarding user limitations to R, a primary focus of this work was open access and accessibility (see supplement) such that it could be readily implemented into other programming languages.

Other comments:

1. Fig. 1 and 2: the fit seems to be poorer for smaller diameters. The limitations imposed by size or low concentrations and their implications on the interpretation of the fitted modes could be discussed.

While the size constraint was already included in section 4.3, we included a brief description on low concentration limitations. This is further supported in the comparison to other fitting methods as suggested in Comment 2.

2. No comparison with other mode fitting methods is presented. Some comparative results would increase the value of the study.

We thank the reviewer for this constructive comment and have included a comparison (Sect. 3.4) with the DO-FIT model which was frequently referenced in the manuscript (Hussein et al., 2005). We also adjusted locations throughout the manuscript referencing this inclusion.

Both models were run in a tri-modal configuration on the entire SPL dataset as described within the manuscript. This comparison includes a comparison of accuracy metrics (Table 2), fitting properties across lognormal spaces (Figure 7), and prediction error comparison (Figure 8).

3. The study is focused on introducing a R-based curve fitting algorithm for modal aerosol size distributions. The paper would be more useful were some actual examples of using the algorithm given. In addition, detailed description of the outputs of the algorithm should be provided.

Examples and descriptions of the implementation of the algorithm were included in the supplement which was designed as a user-manual. We have added a sentence at the end of the algorithm description section (Sect. 2.7) directing readers to the supplement.

References

Hussein, T., Dal Maso, M., Petäjä, T., Koponen, I. K., Paatero, P., Aalto, P. P., Hämeri, K., and Kulmala, M.: Evaluation of an automatic algorithm for fitting the particle number size distributions, Boreal Environ. Res., 10, 337, 2005.

Mäkelä, J. M., Koponen, I. K., Aalto, P., and Kulmala, M.: ONE-YEAR DATA OF SUBMICRON SIZE MODES OF TROPOSPHERIC BACKGROUND AEROSOL IN SOUTHERN FINLAND, Journal of Aerosol Science, 31, 595–611, https://doi.org/10.1016/S0021-8502(99)00545-5, 2000.