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Atmospheric Chemistry and Physics Discussions

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Interactive Comment

Interactive comment on "Technical Note: Review of methods for linear least-squares fitting of data and application to atmospheric chemistry problems" *by* C. A. Cantrell

Anonymous Referee #1

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It is well-known that many publications and atmospheric chemistry researchers have misused the standard linear least-square fit approach, even with full knowledge of both x and y uncertainties at comparable levels. This is due, at least partially, to the fact that the bivariate linear least-square fit procedures are not commonly available in graph/plot and/or spreadsheet software packages. It is also important to recognize that a higher level of understanding is required to use the bivariate linear least-square fit in terms of the necessity/benefit, inputs (especially the uncertainties), and the interpretations of the results. As indicated in the title, author has clearly shown his effort to provide some guidance and clarification to the atmospheric chemistry researchers and a user-friendly spreadsheet to enable the readers to try the bivairate linear least-square fit with rela-

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Interactive Discussion

Discussion Paper

tive ease . In this manuscript, the author opted to emphasize the practical applications, with actual examples, instead of the rigor of statistics; however, a comprehensive list of references is given for those who are interested in a deeper understanding of the statistical basis. Therefore, this reviewer would like to see the publication of this manuscript with some modifications:

The author showed in figure 3 that the deviation of standard linear least-square fit is larger when the r2 value is smaller. It should be noted here that when r2 is small (e.g., $<$0.5) one should question if a linear relationship exists between x and y. Statistical tests (e.g., t-test, F-test) should be applied to show the statistical significance of the fitted slope and intercept. This should be a necessary part of this manuscript.

The bivairate linear least-square fit requires uncertainties in X and Y as inputs. Often a researcher will use an upper bound as the uncertainty of a measured variable/species. This will have unintended consequences. For example, if one variable can vary by orders of magnitude (e.g., j(O1D), using a uncertainty of 10% of the measurement would unfairly underweight the high values, since the larger absolute uncertainty is associated with the higher value. Many times, high value measurements are considered to be more reliable ones. Thus, the author is encouraged to discuss different way to assign weighting factors to variables and the consequences of different approaches. Finally, it would be worthwhile to mention the use of bivariate linear least-square fit with a constant weighting factor (e.g., 1), especially when uncertainties are not precisely determined. This is one effective approach to get a unique result regardless which variable is placed on the x-axis.

As for the examples given by the author, this reviewer believes that simpler sample data is probably better for the reader to understand the benefit or limitations of the bivariate linear least-square fit. For the two cases given in the manuscript, the author pointed out that the relationship between the model predictions and observations can be complicated as the model bias may be dependent on actual environmental conditions. This is at least partially due to the inadequateness and/or incompleteness of model chemistry

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to describe the actual atmospheric processes . Thus, these examples are somewhat too complicated for this manuscript. Perhaps, a comparison of modeled and observed j-values or NO2 will be more straight forward without invoking other chemical or physical interpretations.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 6409, 2008.