

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 #2

Received and published: 19 May 2008

General Comments

The manuscript of Cantrell reviews methods for linear least-squares fitting of data and provides practical advice for researchers who wish to use such methods. The review by Cantrell does not present new scientific findings and is not a rigorous mathematical or statistical treatise. Rather, it provides operational information to guide users on which routines to use. References for the routines are also provided for the interested reader. This paper will be useful to researchers and is an appropriate contribution to Atmospheric Chemistry and Physics.

Specific Comments

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- Referee #1 would like to see the publication of this manuscript. I concur with this assessment.

- I also concur with the comments of Referee #1 suggesting that the manuscript should discuss the need to test whether a linear relationship between x and y exists in cases where r^2 is small.

- By demonstrating the use of different routines on sample data (on formaldehyde and peroxy radical concentrations), Cantrell provides a useful tutorial for readers. However, one element that is lacking in this discussion is how the errors (or uncertainties) in the measurements and model are incorporated into the uncertainty in the slope and intercept, i.e., the solution to equation (2) (for the case of the σ ; standard σ ; least-squares method). For example, on page 6421, lines 1-2, Cantrell states that the fits mostly have slopes of unity within the combined measurement-model uncertainties. What is the uncertainty in the slope, and how does this uncertainty vary with the different routines? (See also point 1 made in the comment by T. Brauers.) Furthermore, the author is encouraged to discuss the assumption that uncertainties calculated in linear least-squares routines are normal (i.e., Gaussian), and that the uncertainty estimates for the slope and intercept are considerably more complicated if the measurement errors are non-Gaussian or correlated.

- In section 5, how were data points below the detection limit treated? Were these data points included in the calculations or were they just set to zero? (If they were included, was it assumed that these values were described by a uniform probability distribution between zero and the detection limit?)

- The impact of outliers discussed in the manuscript is a common issue confronted by researchers. A more rigorous treatment of how to treat outliers would be welcome; the process used by Cantrell to investigate the effect of outliers is somewhat ad hoc. However, while such a treatment would be welcome, this reviewer cannot suggest a specific process that would be better.

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- For Section 5, it would be useful to know the correlation coefficient for the formaldehyde dataset and for the peroxy radical dataset.

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

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