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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A new diagnostic for tropospheric ozone production" *by* Peter M. Edwards and Mathew J. Evans

Anonymous Referee #1

Received and published: 20 July 2017

This paper presents a novel analysis of ozone production in terms on the spin states of the bonds in the precursor species. This is an interesting and original concept, and is a commendable attempt to generate a diagnostic of ozone production that has a sound physico-chemical basis, and one that provides more process insight than the standard methods based on NOx cycling. The paper is worthy of publication, but needs revision to address a number of weaknesses and to enhance its value to the scientific community.

General Comments

The background theory behind the diagnostic could be presented more clearly. While the concept of electron spin is well understood in the physical chemistry community, it is necessary to provide a brief introduction for a wider audience, along with references

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Discussion paper

to literature where readers can learn more.

The paper addresses the rate of ozone production, but discussion focuses solely on long-term integrated ozone production on an annual global scale. It is not clear how applicable the new diagnostic is to smaller regions and shorter timescales where the assumption of steady state (line 141) may be less appropriate, and where emissions may be less important than transport. What is needed to extend the diagnostic to these smaller spatial and temporal scales? The potential for analysis of regional budgets is alluded to on line 307, but no detail is provided.

The strengths and limitations of the approach should be set out more clearly. What additional insight does the new metric provide and how might this be applied to real problems (e.g., to the sensitivity of ozone production to assumptions of VOC speciation, to simplification of isoprene chemistry, or to treatments of deposition processes?) How does the approach compare with previous attempts to generate diagnostics, e.g., though the concept of photochemical ozone creation potentials (POCPs) for individual VOCs? There is little reference to earlier approaches in the field.

Specific Comments

Figure 4: please explain how the contributions of the R and F terms presented in the figure are derived. It is easy to see for the standard diagnostic, where the terms sum linearly to the total PO3, but it is not as clear for the new diagnostic as the terms are no longer independent of each other (as defined in Eq. 1).

The meaning of the horizontal dashed lines in Figure 4 is not clear.

l.270: How many simulations were performed for these sensitivity studies? Please state this in the text.

Figure 7 is not well conceived. It is not clear why a log-NOx scale is used, given that the relationships expected are not exponential (neither line drawn here is expected to be straight, as would quickly become evident at larger or smaller NOx levels). Perhaps

plot OH vs CH4 bond emission directly, and label the points with the NOx level?

Figures 8 and 10 would be more effectively presented through the use of a bar chart, so that the relative changes can be seen more clearly.

Supplement: The "errors in chemistry scheme" need some explanation, and these entries should be at the bottom of the table, as it doesn't aid the reader's comprehension to put them at the top.

The supplement needs more detail on the implementation of the approach. It would be difficult for anyone to replicate in a different model without more information about the reaction classification. It would be helpful to provide a worked example of how the multiple in the Table is arrived at, and this could be included in the supplement.

Typos and minor issues

The English grammar needs a little work in places, particularly where the subject of a verb is inappropriate (e.g., "GEOS-Chem fixes CH4 concentrations..." on line 318 would be clearer as "CH4 concentrations are fixed in GEOS-Chem...")

l.133: add the before top

l.251: grammar in first sentence needs correcting.

l.358: MO2 should be written as CH3O2 for consistency with line 356, and it would be helpful to do this throughout the text, e.g., line 427/8.

Numbers less than 10 without units are better presented as text than numerals.

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