

## ***Interactive comment on “Photochemical grid model implementation of VOC, NO<sub>x</sub>, and O<sub>3</sub> source apportionment” by R. H. F. Kwok et al.***

### **Anonymous Referee #2**

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### **GENERAL COMMENTS**

This paper describes the implementation of the O<sub>3</sub>-VOC-NO<sub>x</sub> version of the Integrated Source Apportionment Method (ISAM) in the Community Multiscale Air Quality (CMAQ) model and then shows results from an example application and comparisons with results from a source-sensitivity method ("brute-force" method). This paper is a companion paper to an earlier paper by three of the authors on the implementation of the PM<sub>2.5</sub> version of ISAM in CMAQ. The O<sub>3</sub>-VOC-NO<sub>x</sub> version of ISAM is similar in some respects to the Ozone Source Apportionment Technology (OSAT) method previously implemented in the CAMx air quality model, but the ISAM method is more detailed, particularly for VOC species, and it can be applied to deposition as well as to ambient concentrations.

This is a well-written paper that describes a significant new analysis method for air quality modeling. The method itself is clearly described as is the relationship of this source-apportionment method to other source-apportionment and source-sensitivity methods. The illustrative example that is provided shows the power and usefulness of the method, and the similarities and differences between the ISAM results and the brute-force results appear to be reasonable.

I have made a number of specific comments and suggestions below related to clarity and completeness that I would ask the authors to consider. I have also included a number of editorial comments and corrections.

## SPECIFIC COMMENTS

1. The authors should consider expanding the title slightly to "Photochemical grid model implementation and application of VOC, NO<sub>x</sub>, and O<sub>3</sub> source apportionment" (cf. line 9 of Abstract and Kwok et al. (2013) title).
2. Line 14 (p. 5801) of Section 3.1 mentions lateral boundary conditions and initial conditions. Are contributions from the upper boundary also considered (this question was motivated in part by Supplemental Fig. S1j and lines 12-13 on p. 5807)?
3. Lines 23-24 on page 5802 of Section 3.1 provide a very brief mention of dry and wet deposition, although a number of figures in the Supplement show deposition results. It would help the reader to interpret these figures if it were stated in Section 3.1 which CB05 species dry deposit and which CB05 species wet deposit. For example, Supplement Fig. 7 shows O<sub>3</sub> total deposition results (dry+wet). Does CMAQ consider O<sub>3</sub> wet deposition? And Supplement Fig. 12 shows non-zero total deposition for only four VOC species; is this due to dry deposition only or to wet deposition only or to both, and are the other VOC species assumed not to dry deposit or wet deposit?
4. I was surprised that Section 3 did not include any discussion of the computational costs of ISAM-O<sub>3</sub>, including the actual and percentage increase in the number of tracer

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fields and the increase in simulation time. This is very relevant information to a user.

5. There are a few details that could be added to the beginning of Section 4: Which CMAQ version was used? What was the model top and what were the elevations of the lowest few model levels? Which WRF version was used? What was the WRF horizontal grid spacing? Were the CMAQ and WRF grid map projections the same? What were the GEOS-Chem grid characteristics (e.g., horizontal grid spacing, number of vertical levels, model top)? Which gas-phase chemistry mechanism did GEOS-Chem use, and if VOC species mapping was required, what was it?

6. The second paragraph of Section 4 describes the 11 tracer sectors that were considered in this example study. Figure 1 then shows spatial tiles for nine of these sectors for one time. For completeness would the authors consider expanding this figure by adding one more row of three tiles to show the OTHR, ICON, and bulk O<sub>3</sub> fields?

7. Table 2 shows that the OTHR sector contributes 15.8

8. I did not understand Supplement Figure S5 and how it relates to Figure 2. Does Figure S5 show time series for 6 different sites in the Riverside area plus time series for 6 different sites in the Sacramento area (the caption is unclear)? What is the spatial size of these subnetworks? Does Figure 2 show an average time series over multiple sites or a time series for an individual site, and if the latter, are these different sites from those shown in Figure S5? Some expanded discussion in Section 4.1 could address these questions.

9. Section 3.1 describes an "NO<sub>y</sub>" family of nine CB05 nitrogen species. In the "NO<sub>x</sub>" portion of Section 4.1, I was confused as to whether what is being analyzed in Figures 6 and 7 is NO<sub>x</sub> = NO + NO<sub>2</sub> or NO<sub>y</sub>. If the former, then does the NO<sub>x</sub> deposition considered in Supplement Figures S8 and S9 only correspond to NO<sub>2</sub> dry deposition or do any of the results presented in the manuscript relate to NO<sub>z</sub> species? I also noted that the maximum daily O<sub>3</sub> total deposition is about 80 g/ha (Figure S7), that the maximum daily VOC total deposition is about 20 g/ha (Figure S11), but that the maximum daily

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NO<sub>x</sub> total deposition is only about 1 g/ha (Figure S9) – is this reasonable?

## TECHNICAL AND TYPOGRAPHICAL CORRECTIONS

p. 5792, l. 4 Perhaps "Source-based apportionment techniques" (as a general comment on the manuscript, compound adjectives are sometimes hyphenated but more often they are not, and this is done inconsistently; consider the many uses of both "zero out" and "zero-out")

p. 5792, l. 8 Perhaps "track source emissions through ..."

p. 5792, l. 25 "... are either to be accounted for pollutant levels in a given scenario" – awkward phrase; same comment for p. 5811, l. 23

p. 5793, l. 28 Perhaps "... Zhang et al., 2009) and contributions from specific ..."

p. 5794, l. 7 "... compared directly with source sensitivity apportionment approaches"?

p. 5797, l. 4-6 Instead of  $N$  in all 3 equations, perhaps  $N_{O_3}$ ,  $N_{VOC}$ , and  $N_{NO_x}$

p. 5797, l. 20 "emissions sources that contributed"

p. 5801, l. 13 "deposition"

p. 5802, l. 14, 18 Could mention the number of VOC and NO<sub>y</sub> tracers (i.e., "14 CB05 VOC species", "nine nitrogen compounds in CB05")

p. 5803, l. 5 "is the Jacobian matrix"

p. 5803, l. 14 The use of  $P$  to denote "production" was introduced on p. 5795 (l. 25), but this convention is not followed in this line or in a few other places (e.g., p. 5803, l. 24; p. 5804, l. 4)

p. 5804, l. 6 "Milford"

p. 5804, l. 13-14 Perhaps "the total  $PO_3$  and  $DO_3$  terms"

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p. 5805, l. 7 Perhaps "Following the ozone production apportionment, subsequent apportionment ..."

p. 5806, l. 1 Perhaps "... from a 2007 year-specific annual GEOS-Chem"

p. 5806, l. 12 Perhaps "contributed" rather than "taken up"

p. 5806, l. 13 Perhaps "... the leading NO<sub>x</sub> emissions sectors by mass were ..."

p. 5806, l. 21 "at 16:00 LT"

p. 5807, l. 20 "Together with Supplement Fig. S5, which shows ..., Fig. 2 demonstrates"

p. 5807, l. 24 Perhaps "... was used to provide an alternate estimate of source ..."

p. 5809, l. 2 Perhaps "... shows notable inflow of O<sub>3</sub> from the boundaries, as shown more clearly in the stacked bar charts in Fig. 4"

p. 5809, l. 14 Perhaps "contributes" rather than "attributes"

p. 5811, l. 5, 9 Insert references to Supplement Figs. S13a,c and S13b,d as well; also, since the discussion refers to the BIOG, BCON, and ONRD sectors, you could swap Figs. S13 and S14 to maintain the same order.

p. 5811, l. 24-25 Perhaps "Implementation of O<sub>3</sub> tracking capability in CMAQ-ISAM for the CB05 gas-phase mechanism adopts ..."

p. 5812, l. 14 Should be "complements"

p. 5813-5818 Missing references:

\* Chameides et al. (1988)

\* Finlayson-Pitts and Pitts (1986) [tangled up with first Foley et al. entry]

\* Henderson et al. (2011)

\* Pfister et al. (2013)

\* Lu et al. (1998)

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- \* Milford et al. (1994)
  - \* Sillman et al. (2000)
  - \* Tonnesen (1999)
  - \* Tonnesen and Dennis (2000a,b)
- p. 5813-5818 References not cited in text:
- \* Andreani-Aksoyoglu et al. (2002)
  - \* Baker and Foley (2011)
  - \* Choi et al. (2014)
  - \* Guenther et al. (2006)
  - \* Haagen-Smit and Fox (1954)
  - \* Kleinman et al. (1994)
  - \* U.S. Environmental Protection Agency (2011a)

p. 5813, l. 18 "Jama-J. Am."

p. 5813, l. 20 "Chameldes"

p. 5817, l. 23 "Naitonal"

p 2 of Supplement "June 10"

## Figures

- \* The captions for Figures 3, 6, and 8 do not give the averaging period; they could also indicate that the data points correspond to all 8374 surface grid cells.
- \* Figure 2 shows time series for the entire simulation period but Figures 4, 7, and 9 only consider the last 5 days and no explanation is given.
- \* The yellow NNRD label in Figures 4, 7, and 9 does not show up very well; could a darker shade of yellow be used?
- \* The mention of bulk total deposition in the Figure 4 caption is confusing and unnecessary.

\* Some figure captions refer to "biogenic BIOG" and some to "BIOG3 vegetation (BIOG)".

\* In the upper labels for Figures S7, S9, and S11-S14, perhaps "Daily-total domain-average".

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Interactive comment on Geosci. Model Dev. Discuss., 7, 5791, 2014.

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