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Geoscientific Model Development Discussions

# *Interactive comment on* "A Multiphase CMAQ Version 5.0 Adjoint" *by* Shunliu Zhao et al.

**Anonymous Referee #2**

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Summary

This is a very nice model development paper that summarizes a new capability in CMAQ with a potentially wide range of future applications for source attribution, inverse modeling, etc. Having both discrete and continuous adjoints as necessary for different processes along with the use of FDM vs CVM when necessary makes this novel for an air quality model like CMAQ. The authors have systematically broken down the CMAQ model into each of its major atmospheric processes and discussed both the implementation and evaluation of the adjoint technique, along with a policy-relevant illustration at the end.

Major Comments:

Given the motivation for this development to go beyond the earlier version of CMAQ Adjoint for gas-phase chemistry and demonstrate capability to model PM2.5, I find it



extremely limiting that the evaluation scenario used only a 7-day model simulation, and all evaluation is apparently shown only for a single hour (last hour of a day). While I appreciate the resource requirements for a longer time period, with the growth in computing technologies, it would have been valuable if the evaluation was performed for a one-month period at the minimum to ensure that the results are robust. Also, showing the evaluation for a 24-hour average (in addition to the single hour shown mostly) would also be policy-relevant given the short-term form of the health-based standard for PM2.5.

Further, the species used for evaluation is very selected (mostly ASO4J) and not robust and comprehensive. I suggest the authors quantify the evaluation metrics for all major PM2.5 constituents for each process when applicable.

Specific Comments:

Page 2 Line 26: Please add full citation for Constantin and Barrett, 2014 to the list of references. It is missing now.

Page 4 Line 5: Can the authors add a brief description of how the CMAQ adjoint capabilities as described in this study are different from the GEOS-Chem adjoint in Henze et al, 2007 or any other updates since then?

Page 7 Line 6: Should deposition (dry and wet) be added to the list of science processes in CMAQ? I do see later on that the authors justify not developing an adjoint for the deposition process.

Page 10 Section 2.5. This section discusses development of a python-based adjoint forcing pre-processor and mentions ability to calculate local maximum 8-hr average O3 concentration. However, the final policy illustration in Section 4 uses a PM2.5 case study. Please clarify if the python-based pre-processor was enhanced for this application as well, or if a different approach was used for the demonstration case.

Page 11 Section 3: For details about the other inputs used in this study, the reference

is to Turner et al (2015a). But that study used 12km modeling, while this is using 36km. Please clarify and reconcile this apparent discrepancy.

Page 12 Section 3.2.1. Why was AALKJ chosen here for the evaluation of the aerosol module? Can you provide some justification?

Page 13 Line 17: Can you quantify this "acceptable accuracy", or provide a reference?

Page 16 Line 1: If I understand this right, the adjoint agrees with the CVM, with a relative error less than 10%. Isn't this rather high to be acceptable? If so, for an emissions sector that has a 5% contribution, the results are within the error that the adjoint model produces, and hence cannot be meaningfully used for that range? Please provide some context to this 10% so that future users of this technique do not misuse it, and are aware of the limitations. In fact, I suggest that a separate section of limitations be added to point out other such issues.

Page 16 Line 3: "The problem with the FDM has been discussed earlier" Please provide exact Section where it was discussed earlier

Page 16 Section 3.4: Can you provide this information in a table? It may be easier on the reader

Page 17: For the model application case, even though it is illustrative, please provide additional information on the source of meteorology and emissions inputs that were used.

Page 17 Line 3: Change "IO" to "I/O"

Page 17: Line 19: "extrapolating from April to the full year". Should this really be "7 days in April" as stated in Section 3?

Page 17 Line 24: Why NO and not NOx (NO + NO2)?

Page 18 Line 18: The language re code availability seems to indicate that the model is not ready for further dissemination given the need for expanded user testing. Please



clarify.

Figures 1- 8: When you say "final concentration", is the spatial plot for the last hour of one-day? Did that one day have a spinup or is truly the first day of the modeling for this development? Is that same one hour used in the scatter plot, or all hours from the one day? Suggest that all hours for a single day be used in the scatter.

Figure 9: Which grid-cell was used in showing this Jacobian? Can you provide some context for the choice of this grid-cell and if it is representative for the whole domain? It will be helpful to see how these differences propagate through the 7-day period (or at least a month if feasible) that was modeled. Perhaps, show that as a time-series?

Figure 7 Caption: Change "The perturbation size for the FDM is 0.01/0.001/0.0001 ppb for the three figures" to clarify which figure has what size – top to bottom or bottom to top

Figure 7: Can you explain the non-zero values for FDM ranging between 0 – 3000 when ADJ = 0, for all top 3 figures?

Figure 11: What is the impact of this numerical noise in layers aloft in the adjoint of the transport scheme, and how would this affect the model results? I see a note on page 15 Lines 1-2 that "these are not uncommon and desirable fix does not appear possible."

Figure 11 Caption: There is really no "top plots" here. Please reword.

Figure 14 Caption: Should "long-term PM2.5 exposure" really be "7-day PM2.5 exposure"?

Table 1: Please define acronyms such as CADJ, DADJ, etc. What are cells 1 – 6 in this table? There is a lot of information in this table for evaluating the full adjoint, but the discussion of this table is very skinny. For e.g., look at cells #3 and #5. The FDM results range so widely (from 21.21 to -23.2), while both CADJ and DADJ results are much closer. What does this mean?

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