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

Shunliu Zhao et al.

shunliu.zhao@carleton.ca

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COMMENT: The authors present a description and evaluation of the implementation of an adjoint methodology into CMAQ version 5.0. This method is compatible with all the major components of the CMAQ model, which is a step forward from previously published implementations in recent versions of CMAQ that only included the implementation of the adjoint approach for inert aerosol species. The authors evaluate the adjoint implementation in each of the major modules of CMAQ which allows for better confidence in the approach and also provides useful information about which modules are best suited to an adjoint. This could guide future decisions about which particular model components (such as inorganic thermodynamics) to include as part of the core model. Components better suited for sensitivity analysis might be a higher priority in situations where multiple choices exist and perform similarly in terms of speed and skill.

The manuscript is generally well organized and written. The use of brute-force sensitivity and finite difference as an evaluation approach is novel. One concern is the illustrative example at the end. It is very helpful to have an illustrative example of the type of information the adjoint provides, but the Figures (Figure 14) related to the illustrative example are confusing to interpret. The Figure caption suggests annual monetized health benefits normalized by emissions are presented. However, it is not clear whether the monetized benefits are normalized by national emissions or emissions from that same grid cell. Further, it is confusing to think about monetized health effects in places where no people reside (over the ocean for instance) and also where there are little to no emissions (northern Ontario near Hudson Bay). Perhaps there is a alternative illustration of the type of information the adjoint provides which would be simpler to interpret such as looking at concentrations relative to some source/region and not even get into converting the concentrations to health effects.

RESPONSE: We appreciate the reviewer's comment and concern about the clarity of the illustrative example. While we agree with the reviewer that other examples may be more intuitive and easier to follow, we believe that source attribution of health impacts as location-specific BPTs is one of the most relevant, lucid, and practically significant examples of unique capabilities that the adjoint approach offers in the area of policy analysis. To address the reviewer's concern we have completely revised the section, to better explain the process for adjoint-based source attribution of health impacts, and the meaning of the calculated BPTs.

The reviewer is correct that locations with no population or emissions can have large BPTs. We define the adjoint cost function as the benefit over the entire US domain. What we obtain from the adjoint simulation (with unit conversion in post-processing) is the location-specific BPTs. In other words, the BPT values shown in Figure 14 are not normalized by emissions and only suggest how much benefit we would gain (or how much damage we would cause) if we cut a ton (or add a ton) of emissions of a pollutant at a specific location. As benefits are considered at the national scale (i.e., for the entire contiguous U.S.), emissions at locations with no population or emission could have an impact on health due to transport. As part of revising this section, and to address this specific point, the following is added to the manuscript"

"While the adjoint cost function is defined based on PM2.5 long-term mortality in the US alone, location-specific BPTs also provide a measure of cross-border impact. Finally, we note that BPTs are measures of marginal rather than total societal impact across the U.S., and as such, even areas with little or no emissions may show sizeable BPT estimates."

Finally, the reviewer's points about different science modules and their performance with respect to formal sensitivity analysis are well taken. While we agree with these comments, we would also like to point out that evaluation of numerical approaches and algorithms based on their performance in sensitivity analyses and their differentiability is a new and emerging concept in air quality and atmospheric modeling. Historically, these models have not been developed with differentiability in mind, but with accuracy and computational efficiency as the main drivers. As a result of ensuing practical trade-offs, discontinuities abound throughout CMAQ, as well as in other CTMs. These discontinuities are encountered in most science modules such as (in addition to inorganic thermodynamics) cloud processes, advection, mode-merging, SOA formation, native solvers of gaseous and aqueous chemistry, etc. We believe it will be a gradual but continued effort among the modeling community to address the issue of differentiability in future generations of algorithms used in CTMs.

To emphasize this important point we have added the following to the manuscript (section 3.2.1):

"The example given above is one of numerous cases where FDM was found to be inaccurate or inadequate in evaluating adjoint sensitivities. The inadequacy of FDM in producing accurate sensitivity estimates is due to process nonlinearities, as well as discontinuities that exist throughout CMAQ. This is the case in a number of CMAQ processes such as SOA formation, inorganic thermodynamics, clouds, aqueous chemistry, advection, etc. This issue is not limited to CMAQ alone and exists in all air quality models, as providing a smooth solution for the governing equations may be lost in trade-offs for added computational efficiency, improving stability, or reducing numerical artifacts in the development stage."

And the following to our conclusion:

"We find that the development of adjoint versions of air quality and atmospheric models is often complicated by the abundance of discontinuities throughout these models that make differentiation challenging. Historically, these models have not been developed with differentiability in mind, but with accuracy and computational efficiency as the main drivers. As the development and applications of formal sensitivity analysis tools (such as adjoint models) become more prevalent, there is a need for a gradual but sustained effort by the modeling community to consider differentiability as an additional design constraint in future developments."

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Discussion paper