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Atmospheric Chemistry and Physics Discussions

Interactive comment on "ANISORROPIA: the adjoint of the aerosol thermodynamic model ISORROPIA" *by* S. L. Capps et al.

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Prof. D. Dabdub

The paper presents the adjoint of ISORROPIA . . . this review adds new specific comments and emphasizes further aspects that would help clarify the manuscript.

We thank Prof. Dabdub for his overall enthusiastic support of ANISORROPIA and the thoughtful review. Our responses to all the issues raised are presented below.

General Comments

One point that stands out is the issue with . . . for non-convergence sensitive to those criteria? Also, how would those criteria affect computational expenses?

This is an excellent point. We have carried out an extensive analysis of the errors. They arise primarily i) during highly concentrated solutions, where the solution ionic strength tends to exceed an maximum limit, and, ii) from the three cases that involve the post-convergence application of Newton-Raphson. Nevertheless, sensitivity tests show that error occurrences can be reduced to 10% without significant increases in disagreement of the adjoint, CVM sensitivities and CPU time by raising the IONIC upper limit to 200. Figures 2, 4, 5, 6 and 7 are revised to include data produced with these adjusted threshold values.

Discussion now clarifies the role of convergence criteria in Section 3 and the effect on computational efficiency in Section 3.3.

Another point is the lack of discussion on implementation of ANISORRPIA in a CTM. The last statement in the abstract is misleading. Even if it might be true, it is not directly addressed in the paper. In addition, the last statement in section 1 does not correspond with the work presented in the manuscript.

The scope of the paper is more consistently defined by the revision of Section 2.1 and the removal of the last sentence in the abstract.

Finally, I strongly second Jim Kelly's comment on section 2.1. It includes an extensive description of mathematical background that seems disconnected from the rest of the paper.

Section 2.1 is revised to describe a cost function in species-space only rather than introducing the inverse modeling framework. The Introduction and Conclusions sections are modified accordingly.

Specific Comments

In page 23481, line 7, the use of [X] is confusing as there is not any X in the preceding equation. The same goes for page 23487, line 16.

The text in each location is revised to refer to one of the species used in the equations.

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In page 23484, lines 20-21: There is no comment on how ANISORROPIA performs at low temperatures (268-288 K) compared to higher temperatures. This is important since many high PM events occur in winter.

The range of 268 – 308 K is now included in the revised Figures 2, 4, and 5 as well as the corresponding discussion.

The axes in Figures 6 and 8 are misleading, as the other reviewers pointed out. It seems that the axes titles correspond to the values with the same alignment, but the reader cannot be sure that the values in the axes are correctly laid out.

The axes labels were switched due to a labeling error in the graphics program. This issue has been corrected and the discussion revised.

In figure 6, for 90% relative humidity, there are some ripples and curves that are difficult to explain. Is this related to convergence issues? Or is this related to the treatment of 10 different regimes? In this last case, would it add value to the discussion to add graphically the boundaries of the possible regimes existing in that ternary system?

Redundant data were included in the ternary diagram and gave rise to some of the ripples. This has now been corrected and included in the revised manuscript.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 23469, 2011.