

***Interactive comment on “Parameterization of N<sub>2</sub>O<sub>5</sub> reaction probabilities on the surface of particles containing ammonium, sulfate, and nitrate” by J. M. Davis et al.***

**J. M. Davis et al.**

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After the Open Discussion period, both anonymous referees provided comments on our revised manuscript which was not viewable by the public, but was described in some detail by Davis et al. (2008a, 2008b, 2008c). The Journal's policy dictates that those referee comments should be treated confidentially, so they are not transmitted here. However, the comments will make some important impacts on our final paper. The purpose of this note is to describe key outcomes of the Confidential Commentary period so interested readers can understand the chronology of events that preceded our final publication.

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## Recommended parameterization of $\gamma$ in advanced air quality models

As described by Davis et al. (2008c), our revised manuscript presented two possible parameterizations of  $\gamma$  on aqueous ammoniated sulfate particles. Our main parameterization makes use of all available laboratory data while our “alternative” parameterization excludes the data published by Kane et al. (2001) – referred to hereafter as KAN01. After reviewing our revised manuscript, both referees and the editor urged us to make a recommendation to readers about which one of our parameterizations should be adopted in air quality models. This proved to be a considerable challenge. On one hand, the trend in  $\gamma$  at high RH reported by KAN01 has not been confirmed by any other researchers even when one considers laboratory measurements on a variety of water-soluble particle types (Anonymous Referee #1, 2007; Davis et al., 2008c). On the other hand, our evaluation of the alternative parameterization against the underlying laboratory data reveals some serious shortcomings because removal of the KAN01 data greatly reduces the structure of the entire dataset. Furthermore, none of the publications by other researchers have attempted to explain why the KAN01 data at high RH should be disregarded.

During the Confidential Commentary period, we learned about a potential flaw in the KAN01 experimental procedure which may explain why their measurements of  $\gamma$  continue to rise with RH above 50% while most other measurements (e.g., MOZ88, HU97, HAL03, BAD06) do not. Unfortunately, this information was not made available during the Open Discussion period so we did not have a chance to solicit feedback from the KAN01 authors. Around the same time, practical deadlines at the U.S. Environmental Protection Agency required us to reach a decision about which parameterization to include in the next public release of the Community Multiscale Air Quality (CMAQ) model. Ultimately, we decided to adopt the alternative parameterization in CMAQ version 4.7. It should be noted that this decision was necessitated by a deadline and made without complete information about the KAN01 laboratory experiments. In an attempt to provide readers with a recommendation (as urged by the editor and anonymous referees) while conveying the uncertainty of our decision, we state in Section 5.2 of the final

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paper that “Until more data are collected at high RH, we recommend the alternative parameterization for use in advanced air quality models such as CMAQ, GEOS-CHEM, and WRF-Chem.”

### **A call for future collaboration**

In all versions of our paper, we included a section that discusses critical gaps in the laboratory data. We hope that section will be a useful guide to experimentalists who are planning their next set of laboratory studies on  $\text{N}_2\text{O}_5$  hydrolysis. Our experience during the Confidential Commentary period has alerted us to a more pressing need: a critical review of the existing laboratory measurements. On behalf of the air quality modeling community, we respectfully request that those individuals who are most familiar with the experimental methods used to measure  $\gamma$  recommend which subset of the available laboratory data should be used and/or what modifications should be made to the existing data when developing future parameterizations of  $\gamma$  for air quality models. If anyone is interested in publicly critiquing the available data, we would welcome the opportunity to collaborate in kind with our statistical tools and numerical models.

### **Structural modifications to final paper**

In response to comments raised during the Confidential Commentary period, some of the text described by Davis et al. (2008a, 2008b, 2008c) has been rearranged in our final paper. Discussion of the lack of RH dependence above 50% on various water-soluble particle types has been moved from Appendix A to a new subsection 5.2 in the main body. Consequently, the text in Section 5.2 referred to by Davis et al. (2008a, 2008c) is now found in Section 5.3. The supplementary material referred to by Davis et al. (2008c) has been incorporated into Appendix A so the final paper has no supplement.

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## References

Anonymous Referee #1: Interactive comment on “Parameterization of  $\text{N}_2\text{O}_5$  reaction probabilities on the surface of particles containing ammonium, sulfate, and nitrate” by J. M. Davis et al., Atmos. Chem. Phys. Discuss., 7, S8004–S8008, 2007.

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Interactive comment on Atmos. Chem. Phys. Discuss., 7, 16119, 2007.

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