

Interactive comment on “Comprehensive Atmospheric Modeling of Reactive Cyclic Siloxanes and Their Oxidation Products” by Nathan J. Janecek et al.

Anonymous Referee #1

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General Comments

This is a strong paper. The methodology is of high quality, the discussion of the results is insightful, and the paper is very well written. Large scale modeling of the atmospheric fate of cVMS has been previously conducted by others using similar methods and the general principles governing atmospheric fate of these chemicals have been discussed. The major technical innovations in this paper are:

- A higher spatial resolution, which allows a better description of concentrations in large urban areas.
- The inclusion of oxidation products in the model, which allows the concentration fields

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of the products to be explored.

The major contributions of this paper to understanding are:

- A more thorough discussion of how cVMS emission patterns and properties affect the horizontal, vertical and temporal variability in concentrations of cVMS and their primary oxidation products. The horizontal and temporal variability for cVMS has been discussed earlier, but not in this depth. The vertical variability for cVMS is novel, as is the discussion of the cVMS oxidation products.

- A comparison of the model results is made with a larger and more diverse set of measurements than has been presented previously attempted, lending more confidence to the modeling, in particular for D4 and D6.

A disappointment with this paper is that more effort was not devoted to exploring the atmospheric fate of the cVMS oxidation products. Although these model data represent one of the major technical innovations of the work, the vast majority of the discussion is devoted to discussing the native cVMS.

Specific Comments

Page 2, line 4: Here the authors take sides in an ongoing infected scientific/political debate. They support this position by citing papers representing just one side of the debate. This is unnecessary and does not contribute to the credibility of their work.

Page 2, lines 16-17: Here several references are given for work that was published in just one paper, even though that one paper is expressly stated at the beginning of the sentence.

Page 2, lines 24-27: I am surprised by the selection of information presented here, given that the second author has published simulations that give much more detailed insight into the latitudinal gradients, urban-remote gradients, seasonal patterns and sensitivity to processes and parameterizations on a hemispheric scale.

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Page 3, line 4: McLachlan et al. (2010) had no measured data from summer and autumn. Incorrect citation.

Page 4, line 26 and paragraph that follows: It is not clear how dry deposition was modeled. Were the surfaces considered to be infinite sinks? Is this a reasonable assumption for the cVMS? I am not aware of evidence showing that cVMS are rapidly degraded on surfaces, except on soil when it is very dry. cVMS have log octanol-air partition coefficients of about 4-6, which suggests that surface media have a limited ability to soak up cVMS and that a partitioning equilibrium between the atmosphere and surfaces would be reached quickly. In this case, assuming that surfaces are infinite sinks would be a poor assumption. While I doubt that this will modify the conclusions of this study, it is important that the assumptions made in modeling deposition are clearly stated and justified.

Page 6, line 31 and elsewhere: The literature cited by the authors discusses other sources of cVMS emissions besides personal care products. For instance, Brooke et al. (2009c) list emissions of residuals in PDMS as being twice as important as personal care products for emissions of D4 to air.

Page 8, lines 20-22: This assumption depends on the number of measurements that were conducted and the time period over which the measurements integrated. A handful of very short measurements can well give a non-representative picture of “typical” summer concentrations. I suggest that the authors provide some information on the number and length of the measurements.

p. 10, lines 18-20: Why are hourly modeled data compared with daily measurements when it is clear that the different time scales makes the comparison difficult? I suggest that you integrate the modeled data into 24 h periods so that a direct comparison can be made.

p.11, lines 10-16: Why did the authors not compare the levels of the oxidation products instead of comparing the levels of their pre-cursors? The concentrations of the oxida-

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tion products of the cVMS have been calculated, and it should be possible to calculate them for SO₂ as well. Given that one of the innovations of this work was the modeling of the cVMS oxidation products, I do not understand why these data are not used.

p.12, line 11: Has this been proven? It seems like a reasonable assumption, but I did not find proof for it in the paper.

Figures 1 and 2: The concentration intervals represented by the different colors are inconsistent. Could you not use a consistent logarithmic scale?

Figure 3: Information should be provided about the time period (dates) for which model data were collected and for which measured data were collected.

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