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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Development and chamber evaluation of the MCM v3.2 degradation scheme for β-caryophyllene" *by* M. E. Jenkin et al.

Anonymous Referee #1

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This is a valuable paper that synthesizes current knowledge on the atmospheric chemistry of beta-caryophyllene and describes its implementation in the Master Chemical Mechanism which the authors make available to the community. Comparisons with measurements from chamber studies (including new and previously reported experiments) are interesting, as much for their agreements as for a few discrepancies.

The model does reasonably well in many respects, including the prediction of [SOA] for a broad range of studies (last column of Table 1), the time evolution of beta-caryophyllene, NO, NO2 and O3 (Fig. 11, 13), and many specific compounds predicted and observed by mass spectrometry, or at least associated to plausible fragments.

On the other hand, it is sobering to see that even first generation products are over-predicted by a factor of two (e.g. Fig. 15, top panels, noting that left and right scales

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differ). Many other comparisons (e.g. bottom of Fig. 15 and Figs. 16-19) only test the general shape of the time evolution, as model ppb are plotted alongside uncalibrated counts, and so are not quantitative.

Hence my only suggestion: To provide a summary of the model evaluation (beyond simply asserting that the model is generally acceptable, as now stated in the abstract), identifying major successes and discrepancies, somewhat along the lines of what I attempted to list above but that the authors could do much more thoughtfully. This could be done in the Discussion/Conclusion section, and it would also fit well in the Abstract, replacing the current wish list of future studies which seems a bit misplaced and arguable.

Technical suggestions:

Fig. 5 caption (and other figures): "figures" -> "values" or "numbers"

p.2902 and later: exocyclic need not be in quotes.

p.2906/l.3: presumably mean CH3C(O)OO = acetyl peroxy radical, not CH3(O)O2

eq. 2 alignment

p.2911/15-20: The discussion of the source of NO is unclear, Do you mean "minimizing" rather than "optimizing"? Is "subtle" influence small but important, or small and not important? Also, it is well known that NO2 will outgas from teflon surfaces. Are you sure the source was NO rather than NO2?

Table 1: [SOA] needs units

p. 2916/17-22: It's unfortunate that the main SOA product, C131CO2H, was not seen by Li et al. But the MCM prediction should help motivate its future detection.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 2891, 2012.