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Atmospheric
Chemistry
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Discussions

Interactive comment on "Explicit modelling of SOA formation from $\vec{\alpha}$-pinene photooxidation: sensitivity to vapour pressure estimation" *by* R. Valorso et al.

Anonymous Referee #1

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This paper presents the results of applying a systematic and automated approach to simulating the quantity and composition of SOA formed from the chamber photooxidation of alpha-pinene. The detailed degradation mechanism was developed primarily using the GECKO-A generator (with some manual refinements), and the gas-aerosol partitioning of the evolving product distribution was determined using three established vapour pressure estimation methods. The simulated quantity of SOA is comparable with that observed, but systematically overestimates by a factor of up to about 3 for experiments performed over a range of NOx levels. The extent of overestimation also depends on the vapour pressure estimation method used, although the simulated composition is found to be relatively insensitive to the applied method.

This is an interesting, informative and well-written paper which is appropriate for publication in ACP. It gives a very clear account of a detailed systematic procedure, and provides useful information on a number of aspects of SOA formation from a complex VOC precursor, and its sensitivity to conditions, timescale and vapour pressure estimation method. It demonstrates that the explicit detailed application of methods based on the current state of knowledge allow simulation of SOA mass loadings which are in reasonable agreement with observation, and helps to guide future activities which aim to reduce or explain the level of disagreement. This paper is essentially publishable in its submitted form, but the authors may wish to consider the relatively minor comments below when producing the revised manuscript.

1) Page 10131, lines 7-13: It is stated that some parameters were "set to achieve reasonable agreement between the simulated O3, NO, and NO2 concentrations and the observations, especially for the time profile of alpha-pinene removal". These parameters are stated to include the impact of chamber-specific wall removal of semi-volatile organics, but there actually appears to be no further information on this. Indeed, the "expected" insensitivity of the simulations of O3, NO, NO2 and alpha-pinene to vapour pressure estimation method and therefore the represented extent of the gas-aerosol partitioning of semi-volatile organics (stated on page 10132, lines 16-18) would suggest that the simulations of O3, NO, NO2 and alpha-pinene are probably also insensitive to including wall removal of semi-volatile organics, such that this process cannot be optimized on this basis. Ideally, this point should be clarified – particularly as the final paragraph of section 4.2 suggests that wall removal of product organics was actually not represented.

2) Final paragraphs of sections 4.2 and 6: Some possible uncertainties and contributing factors to the systematic over-simulation of SOA are given. Perhaps the assumption of absorptive partitioning into an ideal liquid phase might be included here, given the results of some very recent studies (Virtanen et al., 2010; Vaden et al., 2011; Cappa and Wilson, 2011). Do the authors feel that the stated uncertainties collectively pre-

clude absolute conclusions about the performances of the vapour pressure estimation methods?

3) The supplementary material shows that the mechanism generated in the present work performs similarly to the MCM scheme in relation to simulation of O3, NO, NO2 and alpha-pinene in the gas phase, at least for one experiment. Given that the MCM gas phase chemistry has previously been evaluated against data from other chambers (Saunders et al., 2003; Pinho et al., 2007), a brief mutually-supporting statement to this effect might be useful in main manuscript.

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