

Interactive comment on “PyCHAM (v1.3.4): a Python box model for simulating aerosol chambers” by Simon Patrick O’Meara et al.

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Addendum to Response to referee comments on the manuscript “PyCHAM (v1.3.4): a Python box model for simulating aerosol chambers”

Motivated by the referee comments during the initial review of this manuscript, the authors were pleased to find that two modifications to the PyCHAM programme reduced processing times for by up to a factor of 500. The first modification is to change from the Assimulo BDF solver to the scipy BDF solver, the second is to integrate the problem for gas-particle partitioning of water prior to integration of other processes (gas-phase photochemistry, gas-particle partitioning of non-water component(s) and gas-wall partitioning of all components).

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Including this change we have repeated all the simulations presented in the paper and found no change in model results. The significant acceleration in processing time greatly increases utility for users; for example, the time for the 32 size bin 60 s time step simulation presented in Table 5 now takes 4 minutes rather than 44 hours. We therefore request that referees consider the revised manuscript, for which the relevant changes are detailed below.

Change Number Change Detail 1 The model version is updated to 2.1.1 in the manuscript title 2 Line 120: Reference of Assimulo ODE solver replaced by reference to SciPy ODE solver 3 Line 293: processing times for the gas-phase photochemistry problem updated 4 Table 5: processing times updated 5 Line 660: discussion around processing times revised to be consistent with Table 5: “Whilst the processing times in Table 5 are reasonable, it is appreciated that higher resolutions and more complex chemical schemes may be used. Future work will investigate use of a just in time compiler, which offers a portable solution to python acceleration.”

6 Line 688: removed comment about long processing times decreasing utility

Interactive comment on Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2020-234, 2020.

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