Comment on gmd-2021-41

Anonymous Referee #2

Referee comment on "Extension of a gaseous dry deposition algorithm to oxidized volatile organic compounds and hydrogen cyanide for application in chemistry transport models" by Zhiyong Wu et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-41-RC2, 2021

This is a generally well-written paper about a difficult scientific topic. The authors document how a well-know dry-deposition model can be extended to treat additional oVOC species. The authors are honest about limitations, and have good explanations for most of the issues. I do have concerns about the assumptions concerning Gns versus Gresidual, as well as some other points as given below. As long as these can be addressed satisfactory then the article, and in particular the changes to the deposition code, will be a useful addition to the literature.

General

The assumption that Gns is "correctly estimated" (L236) when looking at the Gresidual is of course a major problem. As noted by for example Massman (2004), or Cape et al (2009), these non-stomatal terms are very uncertain even for ozone. I would like to see a more thorough assessment of this issue.

Also in this respect, the model assumes that surfaces are either wet or dry. Of course, the real world shows a high degree of variability, and it can be difficult to predict the thickness or coverage of moisture films on leaves (e.g. Wichink Kruit et al., 2008). How can the authors be confident that their Gns is correct when such basic factors as leaf-wetness (and its impacts on aqueous/surface reactions) are so hard to deal with?

I would have liked to see some analysis of the results with RH (or deficit D) as the driving variable, rather than just wet/dry.

I would also have liked to see some indication and better discussion of the uncertainty of the flux measurements. These uncertainties are substantial, and presumably contribute to some of the differences seen in e.g. Fig. 4.

When modeling the deposition of organic compounds, I wonder why water is the only solvent being considered when calculating Rns? Much of the SOA modeling conducted with CTMs assumes indeed that SOA species are absorbed in the organic rather the water

component of the particle. Perhaps complex thermodynamic models (e.g. Zuend et al,2011) are required to cope with the deposition (or bi-directional exchange) of these compounds?

Terminology: I must admit I don't like anybody referring to their own code as "the Model", with capital M, which makes it sound like it is the ultimate reference. Better to say "the model" or "the deposition model" or something similar.

Other comments

L50: The sentence about HCN doesn't seem to fit with the rest of this paragraph, or the oVOC theme in general. Start a new paragraph maybe?

L117-, Do equations 2-3 ascribed to Wu et al. 2018 differ from those of equation 4 which is ascribed to Zhang et al 2002? (It is a little confusing here what is meant by "the Model", when the latter was stated on L108 to be Zhang et al 2003!)

L179-, Fig.1. The authors discuss the discrepancy in HNO3 Vd for hours 19-23. but not why Vd in hours 0-3 is so very different. What happens at midnight that could change Vd?

L196- I agree with ref #1 that this material is background and should come earlier.

L214. Please add a ref to Fig. 2 here, so the reader knows what you are talking about.

L216 claims that "the Jarvis" model is used, but are the Gs equations and parameters as used here (in "the Model") identical to those used in the 1976 Jarvis paper? If not, rephrase

L223. Again, is the stress function used here identical to that from Jarvis 1976? In any case, all such stress functions are very sensitive to the very uncertain methods used to estimate soil water potential (or other metrics, e.g. Buker et al, 2012)

L241-242. The authors say that during night-time the "canopy surface was dry (no dew)", but presumably RH was high and some surface moisture was possible.

L289. The paper states that the measured flux at night-time should better represent non-stomatal surface uptake, but it is is also true that fluxes are very hard to measure at night-time. A brief discussion of this, and its implications, is warranted in the paper. (There are some comments starting on L330 that help in some regard, but these suggest that essentially one cannot trust the night-time Vd calculations; hence no relation with Gns can be established?)

L303. So, what do the chemists tells about the reactivity of PAA versus HAC? I suggest giving some reaction rates and time-scales with OH, O3 and NO3.

L395. Should give the doi

Extra References.

Buker, P. et al., DO3SE modelling of soil moisture to determine ozone flux to forest trees.

Atmos. Chem. Physics, 12(12):5537–5562, 2012. doi: 10.5194/acp-12-5537-2012. URL http://www.atmos-chem-phys.net/ 12/5537/2012/.

Cape J.N., Hamilton R., and Heal M.R., 2009. Reactive uptake of ozone at simulated leaf surfaces: Implications for "non-stomatal" ozone flux. Atmos. Environ. 43: 1116–1123.

Massman W.J., 2004. Toward an ozone standard to protect vegetation based on effective dose: a review of deposition resistances and a possible metric. Atmos. Environ. 38: 2323–2337.

Wichink Kruit, R.J., et al., Measurements and estimates of leaf wetness over agricultural grassland for dry deposition modeling of trace gases, Atmospheric Environment 42 (2008) 5304–5316

Zuend, A. et al. New and extended parameterization of the thermodynamic model AIOMFAC: calculation of activity coefficients for organic-inorganic mixtures containing carboxyl, hydroxyl, carbonyl, ether, ester, alkenyl, alkyl, and aromatic functional groups, Atmos. Chem. Phys., 11, 9155–9206, 2011, www.atmos-chem-phys.net/11/9155/2011/