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Atmospheric Chemistry and Physics Discussions

ACPD

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Interactive Comment

Interactive comment on "Modelling the reversible uptake of chemical species in the gas phase by ice particles formed in a convective cloud" *by* V. Marécal et al.

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The article by Marecal et al. presents simulations of gas adsorption onto ice along trajectories through a convective storm. The work is a preliminary study for implementing the gas adsorption process into a 3-dimensional cloud chemistry model. The work is interesting in that it compares results from two approaches, the commonly used Langmuir equilibrium method and the kinetic trapping theory.

The paper is well written and the only major comment is whether it is better suited for *Geoscientific Model Development* rather than ACP. There are some points that need clarification and explanation before consideration for publication.

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Specific Points or Questions

1. P. 24368, lines 8-10 state that the ice crystal shape is diagnosed at each grid point and time and that the shape depends on the temperature and relative humidity. I thought the ice crystal shape would also depend on its history. So if it was created in the -25C region and then lifted to the -38C region, it would still have the shape of the -25C regime. I may be mistaken, but I would like to hear the authors' comments in regards to ice crystal shape.

2. P. 24370, lines 1-4. I always find it helpful to see a sounding of the meteorological conditions because a sounding gives context to both the 3D cloud simulation and the particle trajectories.

3. Section 2.4. In the description of the air parcel trajectories, it would help to be more clear. My understanding is that the cloud model is run, 7 trajectories are found, and winds, temperature, humidity, water and ice water mixing ratios are recorded. Then this information is used as input to a box model that calculates trace gas adsorption. Another approach would be to use the winds, temperature, and humidity as input to a cloud parcel model which calculates its own cloud drop and ice crystal distributions.

4. P. 24378, lines 20-27. I find it remarkable that acetic acid (CH3COOH) adsorbs more readily than formic acid (HCOOH). I think that is due to the partition coefficients, but why does that happen?

5. p.24379, line 11 states that the uptake coefficient is well correlated with the ice mixing ratio. I think it is stating that the uptake of HCl decreases when the ice mixing ratio increases – correct? Would the correlation be obvious from a scatter plot and what is the correlation coefficient? What is the explanation for this correlation – is it size of particles (e.g. with liquid drops, the higher surface area to volume ratio of small drops allows for more dissolution than large drops), or perhaps the history along the trajectory?

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6. One thing I am wondering is if the history of the cloud physics processes along a trajectory plays a role in these calculations – this is related to point 3 above. If an air parcel is lifted from cloud base, forms cloud drops and then ice crystals that then grow by deposition or aggregation, does the amount of trace gas in the different cloud particles (drop, crystal, aggregate) reflect the cloud physics? For example, does the trace gas in the ice crystal get transferred to the larger particle during aggregation? If not, how would the results differ from what is reported?

Technical Details.

1. Throughout paper: The variable A is used as part of the gas adsorption partition coefficient (p. 24374, line 3) and for surface area of an ice crystal. Please differentiate between these two parameters.

2. p.24379, lines 1-4 should be part of the previous paragraph

3. p.24379, line 3, should be “Assessment”

4. p 24381, line 18 should be “trace gas”

5. p 24382, line 17 should have “accommodation”

6. p 24387, line 24 should be “is used. The effect of saturating the ice”

7. p 24388, line 6 explain what RUN1M is here because it is the conclusions (for readers who do not read the whole paper)

8. p 24388, line 16 should be “gas phase for the lifetime”

9. p 24389, line 17 should be “can depend on”

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 24361, 2009.

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