Atmospheric Chemistry and Physics Discussions

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comment on acp-2021-451

Anonymous Referee #2

Referee comment on "Technical note: Adsorption and desorption equilibria from statistical thermodynamics and rates from transition state theory" by Daniel A. Knopf and Markus Ammann, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-451-RC2, 2021

Review of Classical and statistical thermodynamic treatment of adsorption and desorption kinetics and rates

This technical note derives the desorption rates for adsorbed species using thermodynamics and statistical mechanics. The authors do these derivations with two models of the sorbed species: a 2D ideal gas and a 2D ideal lattice gas. The authors demonstrate that these models will retrieve very different values of e.g. desorption energy and timescale. This work is valuable and relevant to the study of atmospheric chemistry.

The authors aim to save space and increase the readability of the manuscript by moving many of the equations to the Supplement. This was a good decision, however the reader who is reliant on the additional information found in the supplement is also the reader who needs to be guided most closely through those equations. The manuscript would benefit from additional text informing readers when equations and assumptions detailed in the Supplement have been brought into the main text. This added text should specify the range of equation numbers over which a derivation has been conducted, and not simply list the equation number of the final result.

237: It seems like the atmospheric chemists most likely to rely on this work are those conducting lab experiments of adsorption and desorption, where coverages may not be small. The authors should provide a quantitative estimate of the level of coverage where they believe the 2D ideal gas is no longer an appropriate model to use.

285: “Supplement Eq. (119ff.)” is likely a broken equation number link?

765 & 792 & 808: Can these derivations be moved to the SI?

Fig 2: extend axes to zero

Fig 5. I recommend labelling each line with its E0des value

Fig. 15. I recommend reducing the number of lines plotted and labelling each line with its desorption rate