

Interactive comment on “Kinetics and mechanism of the uptake of N₂O₅ on mineral dust at 298 K” by S. Seisel et al.

S. Seisel et al.

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We thank all contributors to this interesting discussion, which is - as the editor said - an old important, intense, and unresolved dispute.

In our final response we would like to stress one point again, which seems to us the most important.

We decided to calculate the uptake coefficients on the basis of the geometric (projected) surface area of the sample since this value is the closest to the surface area used in atmospheric models.

As long as the actual surface area of a particle or a sample is not known some kind of reference state has to be used in order to transfer heterogeneous rate constants

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into dimensionless uptake coefficients. The BET surface area represents an upper limit of the reactive surface area, whereas the geometric surface area is a lower limit. In atmospheric models the available surface is usually calculated on the basis of the particle diameter, which results in a geometric surface area. Relating uptake coefficients to the same reference surface as used in atmospheric models would facilitate the implementation of these values into the models and reduce possible errors.

It has to be noted that if bulk samples, as in our study, are used the uptake coefficients based on the geometric (projected) surface area may be overestimated by a factor of 2-3 due to the roughness of the surface. The surface of a sample containing small particles placed onto a sample holder may be approximately described by a number of hemispheres with the diameter of the particles. This surface area of the sample is than the sum of the surface areas of all hemispheres which is exactly twice the projected surface area of the sample or the geometric surface area of the sample holder. The roughness of an individual particle on the sample holder can be neglected since an atmospheric particle exhibits the same roughness and therefore the additional surface will be cancelled out.

As Vicky Grassian said in her comment, it would be desirable to study heterogeneous reactions in more complex environments, that is e.g. humidity, mixture of gases, individual particles.

We fully agree with this statement. A heterogeneous reaction of a gas with a realistic surface is extremely complex, especially under atmospheric conditions. In order to understand such a process completely elementary reactions steps have to be known as well as the influences of humidity, temperature or other gas compounds present. All this information cannot be obtained from one single experiment.

In Knudsen cells or flow tubes such a reaction can be studied under idealized conditions with the goal to obtain fundamental kinetic parameter and reactions mechanisms. By using experiments as proposed by Vicky Grassian the degree of freedom of the

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system under study can be gradually increased. Finally, the reaction system can be studied under simulated atmospheric conditions in large aerosol chambers. All these results together will provide the necessary amount of data to completely describe a complex heterogeneous reaction.

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