Neutral and ion-induced H_2SO_4 - H_2O particle formation 3: New improved parameterization

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We have developed new neutral and ion-induced sulphuric acid – water particle formation parameterizations for the use of atmospheric models. The new parameterizations are based on improved Classical Nucleation Theory (CNT) of Merikanto et al. (2016) (see also EAC 2016 abstract by Merikanto *et al*). The model has been validated against CLOUD experiments (Duplissy *et al.*, 2016; EAC 2016 abstract by Duplissy *et al*). The model behaves consistently when approaching both the one-component and the kinetic particle formation limits. When the free energy barrier associated with the critical cluster formation vanishes, we use the kinetic equation for the particle formation rate. The neutral parameterization extends the validity ranges of the Vehkamäki *et al.* (2002) parameterization. Also, unlike in Vehkamäki *et al.* (2002), the ion-induced particle formation rates are now parameterized.
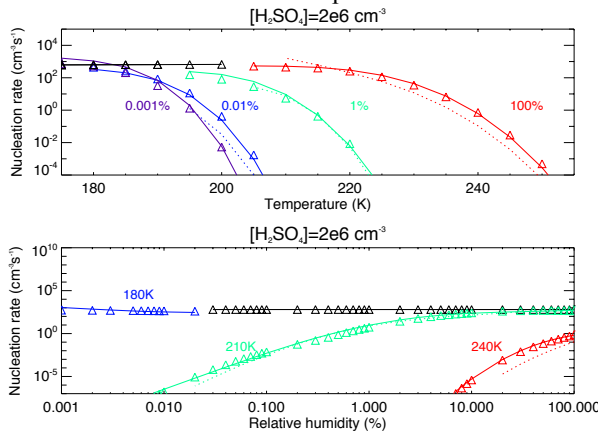

Figure 1. Neutral particle formation rates for a sulphuric acid concentration of $2x10^6$ cm^{-3} as functions of temperatures and relative humidity: old Vehkamäki *et al.* (2002) parameterization (dashed), new theoretical values (triangles) and new parameterized rates (solid lines). The black lines and symbols indicate the kinetic region.

Neutral and ion-induced parameterizations are given for particle formation rate (J $> 10^{-1}$ m^{-3} s^{-1}), radius, composition and number of molecules in the critical cluster. The threshold sulphuric acid concentration above which the kinetic formula applies has been parameterized as well. A parameterization for the threshold acid concentration for the neutral formation rate J $= 1$ cm^{-3} s^{-1} is also given. The neutral parameterizations (see example in Fig. 1) are valid for the temperature range of 165-400 K, relative humidities

ranging from 10^{-3} to 100%, and sulphuric acid concentrations of 10^4 - 10^{13} cm^{-3}. The ion-induced parameterizations (see Fig. 2) are valid for the temperature range of 195-400 K, relative humidities ranging from 10^{-5} to 100%, and sulphuric acid concentrations of 10^4 - 10^{16} cm^{-3}. The low relative humidities attained allow using the parameterizations also at very dry conditions such as on Venus.
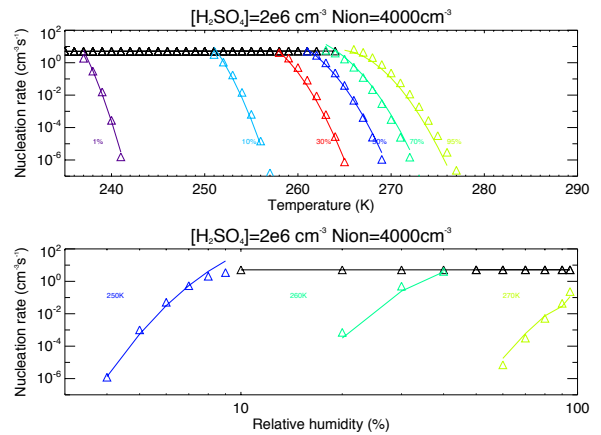

Figure 2. Ion-induced particle formation rates for a sulphuric acid concentration of $2x10^6$ cm^{-3} and ion concentration of $4x10^3$ cm^{-3} as functions of temperatures and relative humidity (see Fig. 1 for lines and symbols).

These parameterizations capture the experimental formation rates and providing reliable predictions outside the experimental range. We recommend using the new model and the improved parameterizations.

Duplissy, J., et al. (2016), *J. Geophys. Res. Atmos.* **121**, doi:10.1002/2015JD023539.

Merikanto, J., J. Duplissy, A. Määttänen, H. Henschel, N. M. Donahue, D. Brus, S. Schobesberger, M. Kulmala, and H. Vehkamäki (2016), *J. Geophys. Res. Atmos.* **121**, doi:10.1002/2015JD023538.

Vehkamäki, H., M. Kulmala, I. Napari, K. E. J.Lehtinen, C. Timmreck, M. Noppel, and A. Laaksonen (2002) *J. Geophys. Res.* **107**, 10.1029/2002JD00.