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Using the Monte Carlo Markov Chain method to estimate contact parameter temperature dependence: implications for Martian cloud modelling

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In the last years several datasets on deposition mode ice nucleation in Martian conditions have showed that the effectiveness of mineral dust as a condensation nucleus decreases with temperature (Iraci et al., 2010; Phebus et al., 2011; Trainer et al., 2009). Previously, nucleation modelling in Martian conditions used only constant values of this so-called contact parameter, provided by the few studies previously published on the topic. The new studies paved the way for possibly more realistic way of predicting ice crystal formation in the Martian environment. However, the caveat of these studies (Iraci et al., 2010; Phebus et al., 2011) was the limited temperature range that inhibits using the provided (linear) equations for the contact parameter temperature dependence in all conditions of cloud formation on Mars.

One wide temperature range deposition mode nucleation dataset exists (Trainer et al., 2009), but the used substrate was silicon, which cannot imitate realistically the most abundant ice nucleus on Mars, mineral dust. Nevertheless, this dataset revealed, thanks to measurements spanning from 150 to 240 K, that the behaviour of the contact parameter as a function of temperature was exponential rather than linear as suggested by previous work.

We have tried to combine the previous findings to provide realistic and practical formulae for application in nucleation and atmospheric models. We have analysed the three cited datasets using a Monte Carlo Markov Chain (MCMC) method. The used method allows us to test and evaluate different functional forms for the temperature dependence of the contact parameter. We perform a data inversion by finding the best fit to the measured data simultaneously at all points for different functional forms of the temperature dependence of the contact angle m(T). The method uses a full nucleation model (Määttänen et al., 2005; Vehkamäki et al., 2007) to calculate the observables at each data point.

We suggest one new and test several m(T) dependencies. Two of these may be used to avoid unphysical behaviour (m > 1) when m(T) is implemented in heterogeneous nucleation and cloud models. However, more measurements are required to fully constrain the m(T) dependencies. We show the importance of large temperature range datasets for constraining the asymptotic behaviour of m(T), and we call for more experiments in a large temperature range with well-defined particle sizes or size distributions, for different IN types and nucleating vapours.

This study (Määttänen and Douspis, 2014) provides a new framework for analysing heterogeneous nucleation datasets. The results provide, within limits of available datasets, well-behaving m(T) formulations for nucleation and cloud modelling.

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