Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2020-1186-RC1, 2021

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Influence of atmospheric conditions on the role of trifluoroacetic acid in atmospheric sulfuric acid-dimethylamine nucleation" *by* Ling Liu et al.

Anonymous Referee #1

Received and published: 4 January 2021

Liu and co-workers investigated the influence of different atmospheric conditions on the role of trifluoroacetic acid (TFA) in sulfuric acid (SA) – dimethylamine (DMA) nucleation process using the Density Functional Theory combined with the Atmospheric Cluster Dynamics Code, which is based the previous study on that TFA can participate in SA-DMA-based nucleation under the local atmospheric temperature and nucleation precursor concentrations of Shanghai, China. This study reports the enhancement of particle formation rate by TFA and the contributions of SA-DMA-TFA cluster to the cluster formation pathways can be especially significant in cold and polluted areas, which can not only clarify the different roles of TFA in SA-DMA-based nucleation under broad atmospheric conditions, but also can reveal the potential implications of the usages of

Printer-friendly version

Discussion paper

Freon alternatives on NPF under a wide range of atmospheric conditions. In general, the manuscript is well written and is of broad interest to the readership of Atmospheric Chemistry and Physics. I can recommend publication in Atmospheric Chemistry and Physics after the following comments have been addressed.

Specific Comments: Lines 22-24: “Although sulfuric acid (SA) – dimethylamine (DMA) nucleation mechanism has been identified in the urban city of Shanghai, China (Yao et al., 2018), the nucleation mechanisms are not fully understood and species contributing to NPF under different environments remain to be studied” Please further elaborate why the nucleation mechanisms are still not fully understood even though the SA-DMA nucleation mechanism has been identified in Shanghai. Lines 29-30: “. . ., PFCAs are generally believed to be an important class of environmental contaminants present in various environments” Please provide relevant references for the atmospheric importance of PFCAs. Section 3.1: From Figure 1, it seems that the (SA)3Âů(DMA)4Âů(TFA)1 clusters can be set as boundary clusters. Are there other clusters that can be set as boundary? The detailed boundary clusters that can grow out of the simulated system by Atmospheric Cluster Dynamics Code and the reasons should be illustrated. Line 137: The corresponding temperature and DMA concentration for the 13 times enhancement by TFA should be presented. Line 195 and line 196: The detailed growing way of clusters in SA-DMA-TFA cluster formation pathway should be further illustrated. The reasons for that some clusters involving TFA does not present in the main cluster formation pathway should be elaborated. Supplement, Table S5: Are these simulated results based on the thermodynamic parameters, such as Gibbs free formation energies (ΔG), at the corresponding temperatures shown in Table S5? If so, the ΔG of studied clusters at different temperatures of the studied cities in different months should be presented in the Supplement.

Technical corrections: Line 73: “The collision rate coefficients βi,j between clusters i and j were . . .” should be “The collision rate coefficients, βi,j, between clusters i and j were . . .” Line 83: “where Pref is the reference pressure (in this case 1 atm) where

the formation free energies. . .” should be “where Pref is the reference pressure (in this case 1 atm), at which the formation free energies. . .” Line 86: “3.1 In Influence of temperature and nucleation precursor concentrations on cluster stability and growth trend . . .” should be “3.1 In Influence of temperature and nucleation precursor concentrations on the stability and growth trend . . .” Line 135: “. . . temperature in spring and winter is relatively lower than other time all the year-round, respectively.” should be “. . . temperatures in spring and winter are all relatively lower than other time all the year-round.” Supplement, Line 1 and Line 3: The “ΔG” should be in italic, such as “ΔG”.

Interactive comment on Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2020-1186, 2020.

Printer-friendly version

Discussion paper