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Atmospheric Chemistry and Physics
Discussions

# *Interactive comment on* "Modelling Atmospheric Mineral Aerosol Chemistry to Predict Heterogeneous Photooxidation of $SO_2$" *by* Zechen Yu et al.

**Anonymous Referee #2**

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This manuscript represents a model for evaluating the importance of dust in sulfate formation, particularly in adding the kinetics and mechanism of heterogeneous photocatalytic reactions of $SO_2$ on mineral dust in the model. It is essential to consider the photooxidation of $SO_2$ in order to improve the accuracy of sulfate formation modeled in the atmosphere. Therefore, this study is of substantial interest. However, some major points should be carefully considered before it is published.

Major comments:

(1) The indoor chamber data shows that, in the absence of ATD particles, $[SO_4{}^{2-}]_T$ at 55% RH is two times larger than that at 19% RH (Table 1 L1A, B and C), but when RH increases to 80%, the enhancement of $[SO_4{}^{2-}]_T$ is not distinct. Additionally, in the

presence of ATD particles, $[SO_4{}^{2-}]_T$ is unexpectedly lower than that in the absence of ATD at 55% RH (Table 1 L3 and L1B), contrary to that at 80% RH (Table 1 L4 and L1C). However, these observations are not discussed in the manuscript and shown in the model.

(2) In addition to react with $SO_2$ and $NO_2$, OH radicals produced on the surface of particles under UV conditions can undergo heterogeneous reaction with particles as well as self-reactions, resulting in the significant decrease of OH radicals participate in the oxidation of $SO_2$ and $NO_2$, and subsequently overestimating sulfate and nitrate formation in the model. Furthermore, in addition to compete OH radicals with $SO_2$, the presence of $NO_2$ can also react with $SO_2$ on the surface of particles to promote sulfate formation at high RHs as like in aqueous phase. However, these mechanisms were not considered in dust phase in the model (Table S1).

(3) In Figure 3, it seems that modeled results are not in agreement with experimental observations at scenarios (a) without ATD particles and (b) low loadings of dust particles, especially for time-changing trends, meaning that the gas and aqueous phase reaction of $SO_2$ may be not well considered in the model. The authors should give explanations or speculations for this discrepancy in the manuscript.

(4) The authors estimated gas-particle partitioning constant of $NO_2$, $K_{d,NO2}$, based on the relationship between the Henry's law constants of $NO_2$ and $SO_2$ (Eq. 15), but $K_{d,O3}$ is obtained from literature results (Eq. 14). Is it reasonable to estimate $K_{d,NO2}$ according to Eq. (15)? And why $K_{d,NO2}$ and $K_{d,O3}$ are set based on different method since previous studies have investigated the heterogeneous reaction of $NO_2$ on mineral dust as well? Moreover, in Section 3.2.1 the authors considered the influence of RH on $K_{d,SO2}$, however, the expression of $K_{d,NO2}$ and $K_{d,O3}$, which is also closely related sulfate formation in the model, was not shown as a function of RH.

Minor comments:

Page 4 Line 27 "The detail description" should be "The detailed description"

Page 4 Line 21 The indoor chamber data of this study was obtained from our recent laboratory study (Park and Jang, 2016), however, $[SO_4{}^{2-}]_T$ values shown in Table 1 is different with Park and Jang (2016) reported. For example, Table 1 D1, L1 B and L8 in the manuscript corresponding to Table 1 D1, L1D and L8 in Park and Jang (2016), respectively.

Page 7 Line 19 and 21 “$SO_4{}^2$–$NH_4{}^+$–$H_2O$” should be “$SO_4{}^{2-}$–$NH_4{}^+$–$H_2O$”.

Page 11 Line 17 Give more detailed description about $k_{auto}$o and $k_{OH,O2}$ derived from the indoor chamber data.

Page 14 Line 21 “L7 and L8 in Table 1” should be “L6 and L7 in Table 1”.

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