Comments on egusphere-2023-1317 (ACP), "Atmospheric photooxidation and ozonolysis of sabinene: Reaction rate constants, product yields and chemical budget of radicals", by Pang et al.

This manuscript reports an experimental study on oxidation of sabinene initiated by OH radical and by O_3. The comprehensive comparison on yields of products between experimental measurements here and previous theoretical calculations suggested some possible new reaction pathways such as the possible diradical pathway in ozonolysis reactions. Publication is recommended.

Comments:

1. From Eq. 4 to Eq. 5, the concentrations of O3 and OH are assumed constant. This is not a proper assumption. Fig 3 and Fig 4 showed the changes of concentrations. Because the concentrations of OH and O3 are available from experimental measurements, it is probably better to simply integrate the concentrations as,

$$\frac{d[\text{SAB}]}{[\text{SAB}]} = -(k_{\text{O3}}[\text{O}_3]_t + k_{\text{OH}}[\text{OH}]_t + k_{\text{dil}})dt$$

$$\ln \frac{[\text{SAB}]_0}{[\text{SAB}]_t} = k_{\text{O3}} \int_0^t [\text{O}_3]_{t'} dt' + k_{\text{OH}} \int_0^t [\text{OH}]_{t'} dt' + \int_0^t k_{\text{dil}} dt'$$

Each integrate can be obtained from the experimental concentrations. A linear regression can be used to obtain k_{O3} and k_{OH}, and contributions of OH and O3 in degradation of sabinene can be obtained.

2. Table 5 Yields of Products: For reaction with OH, the yields from the theoretical study (Wang & Wang, 2018) assumed 100% yield of RO from reactions of ROO + NO. This is probably not correct. There should be a fraction of RONO2 formation.

3. It should be noticed that the theoretical calculations all the time carry uncertainty. The predicted rate coefficients usually have uncertainty, about one order of magnitude when using ROCBS-QB3 energies. The results from theoretical calculations can be considered as the most probable values, or sometimes are biased. Therefore, experimentalists need to be aware of this, and theoreticians need to adjust the barrier heights to match the "reliable" experimental data, which are unfortunately rather limited and not available for most of time. Overall, I would consider reasonable agreement between the experimental measurements here and the previous theoretical calculations.