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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A study of volatility by composition, heating, and dilution measurements of secondary organic aerosol from 1,3,5-trimethylbenzene" *by* Kei Sato et al.

Anonymous Referee #1

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This paper investigates the volatility of SOA produced from the photooxidation of 135-trimethylbenzene through the combination of composition analysis by LC-MS, evaporation upon heating (TD-AMS), and isothermal dilution in the smog chamber. The estimated VBS varied substantially due to the limitations of each approach. This paper is an extension of a recent study from this research group on alpha-pinene SOA into anthropogenic SOA. SOA formation from aromatic hydrocarbons is regaining attention in recent years as it may involve the formation of highly oxygenated molecules (HOMs) via auto-oxidation. This paper presents an impressive set of data and is generally well written. However, I found some discussions confusing or missing details. The following are my specific comments, which I am sure the authors can address.

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1. C* from LC-MS was calculated using the linear fit to MW versus logC* relationship shown in Figure S3. The molecular structures of each compound are taken from MCM and previous experimental studies (Table S3). The corresponding logC* values were calculated using SPARC. I do not understand why you would use only one line to represent the relationship between MW and logC* since C* strongly depends on MW and O/C. In Figure 3, they show that O/C varies widely from ∼0.3 to ∼0.9. Thus, applying one line to all of the data does not seem reasonable. Since empirical formulae are available from LC-ToF-MS analysis, I do not see the need for the single-line calibration that neglects O/C distribution (Figure S3). Am I missing something? Since Li et al.'s molecular corridor parameterization accounts for the number of C, H, O, and N, I believe Li et al. parameterization is much more appropriate than the "linear fit" of this study (Figure S3 and Figure 4ab).

2. Therefore, I think this statement in P.32 needs more considerations. "The results from the method by Li et al. were higher probably because the TMB photooxidation products had lower volatilities than a wide range of organic compounds referred to in the analysis of Li et al." Li et al.'s dataset included ELVOC with logC0 down to even -10 or less. It seems unlikely that TMB products had lower volatilities than what was considered by Li et al.

3. Please provide more details on the equilibrium time-scale calculations. I don't see a definition of the "effective saturation ratios" (SR_eff). P.11, L.14-15 refers to eq. 2 in Saleh et al., but the equation is SReff = 1 -exp(-t/tau). I suppose it is meant to be eq.1 in Saleh et al. that defines SReff. Since eq. 1 and 2 in Saleh et al. are quite simple equations, I think it should be shown in this manuscript.

4. Similarly, I would like to see more details on volatility estimation using the PTR-MS. Although the text refers to Inomata et al. (2014), there should be a brief description of the procedures. Did the analysis assume a certain value of the heat of vaporization?

5. The error bars in Figure 3cd are based on assumed "maximum uncertainty of 20%

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for the total EIC peak intensity" and error propagation analysis. Is there any basis for choosing 20%? As authors must be well aware, the sensitivity of ESI-MS is highly compound specific.

6. Figure 2: Is this a result of direct infusion to ESI-MS? Please clarify.

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