

Löher et al. describe the characterization of a new atmospheric simulation chamber built at the University of Bayreuth. The authors describe the design, photolysis, chemistry, and wall interactions of the chamber for purposes of gas-phase mechanism studies. The authors also describe SPME and PTR-ToF-MS techniques deployed to study important intermediates of VOC oxidation. The authors study the OH oxidation of toluene as a testbed for the new chamber and to demonstrate the capabilities of the system in quantifying product yields.

The paper is very well-written and organized and provides all of the necessary information to understand the performance of the BATCH reactor. I view this manuscript as a reference point for future studies utilizing the BATCH reactor, as is typical for other chamber and/or flow tube description papers published in AMT or similar journals. The manuscript also provides some nice science describing the chemistry of toluene and yields for relevant products. I only have one substantive comment and a small number of minor comments and suggestions. I support publication.

Main comment

Section 4.1.2. The authors parameterize measured wall losses using simple equations. How does this parameterization compare against theoretical considerations or other efforts to quantify wall losses using chemical information? There are a number of papers that have investigated vapor wall loss and developed a number of parameterizations (e.g., Yeh and Ziemann, Ye et al. 2016, McVay et al. 2014 to name a few). These are estimated using C^* , which in itself is related to molecular weight by the ideal gas law. How do these relate to the functions described here? And why the square root of the vapor pressure? Some context and description of previous parameterizations would be helpful.

I can see how this is a valid approach for the toluene system, but is it the intention of the authors to use this more broadly for other systems? If so, I would think that it may be necessary to discuss this in more detail and how this parameterization compares to other forms (as noted in comment above). This parameterization seems very simple compared to previous efforts to characterize wall loss rates, but I may not be aware of all of the various efforts.

<https://www.tandfonline.com/doi/full/10.1080/02786826.2016.1195905>

<https://www.tandfonline.com/doi/full/10.1080/02786826.2015.1068427>

<https://pubs.acs.org/doi/10.1021/es502170j>

Minor Comments

Lines 101-112: This is a very nice discussion about the utility of derivatization. Can the authors point to some relevant studies on the aromatic systems that have used

derivatization to quantify the yields of aldehydes, acids, etc.? I think this would be helpful to place in context why derivatization is a powerful technique and relevant to the studied toluene system.

Lines 125-132: I would also point towards papers that have studied the SOA and product yields from the second generation products (e.g., cresol, Schwantes et al. 2017). This would be relevant to the discussion that follows about multi-generational formation of glyoxal.

Line 154: This is very impressive temperature range I may have missed this in the text, but what are the dimensions of the containment room? How quickly does it take to reach the desired temperature set point? Is it possible to do dynamic temperature changes during experiments? My take is that this system is about the same size as that described by Osseiran et al. and contained in a similar temperature-controlled vessel. Is that correct? As a note, it might be nice to have a picture of the chamber in a TOC graphic to get a sense of the scale.

<https://www.sciencedirect.com/science/article/abs/pii/S1001074220301170>

Line 168: Is this the footprint of the Teflon chamber? Can the third dimension be provided to get a sense of the full size at max volume (300 L)?

Line 250: Perhaps useful to note the estimated mass that could be collected on the SPME fibers for a typical experiment (e.g., the toluene system)?

Line 256-262: Later in the text, the authors note that the stability of ISTDs were tracked for a week using PTR-ToF-MS. I would include that discussion here.

Lines 382-385: Was there an order that experiments were conducted? I.e., were NO_x-free experiments conducted prior to those where NO was injected? If not, is there uncertainty associated with possible NO_x sources from the walls? Previous studies have shown that walls act as a NO_x source once NO or NO₂ are introduced as reactants (e.g., Rohrer et al.), so I feel that this should be referenced here.

<https://acp.copernicus.org/articles/5/2189/2005/acp-5-2189-2005.html>

Line 419: Do wall losses include possible line losses?

Line 502: For consistency with the previous comparison, I would recommend phrasing that the experimental photolysis rate is “21% higher” than the calculated value.

Line 525-527: This sentence tends to suggest that HONO is not contributing, but this is a little speculative without HONO or measurements of NO / NO₂ at low detection limits. I would suggest leaning on the conclusion that H₂O₂ is the main source of OH radicals and leave out the mention of HONO.

Lines 529-531: Here, and elsewhere, it would also be helpful to see the photolysis and OH lifetimes for each species. This would help the reader to gauge how much loss of these species might be expected after they are formed relative to OH or other processes and complement the loss distributions shown in Fig. 11.

Figure 8: It is somewhat difficult to see the dark grey bars relative to the lighter grey bars. Perhaps using a different color would help? Or, dotted vertical lines could indicate new experiments?

Lines 752-753: This may be the case for chamber studies, but previous studies investigating field observations of isomer distributions (e.g., C8-aromatics, propanal / acetone) have applied isomer-specific sensitivities to interpret PTR signals in very complex mixtures (e.g., biomass burning, Koss et al.). This is also a technique currently used in other mass spectrometers with significant variability in isomer sensitivities (e.g., I-CIMS, Xiong et al.)

<https://acp.copernicus.org/articles/15/11257/2015/>

<https://acp.copernicus.org/articles/15/11257/2015/18/3299/2018/>