Atmos. Meas. Tech. Discuss.,
doi:10.5194/amt-2017-352-RC1, 2017

Atmospheric Measurement Techniques Discussions

Interactive comment on "Assessing the degree of plug flow in oxidation flow reactors (OFRs): a study on a Potential Aerosol Mass (PAM) reactor" *by* Dhruv Mitroo et al.

Anonymous Referee #2

Received and published: 21 December 2017

This manuscript describes a modeling-measurement comparison of residence time distributions in a PAM-style oxidation flow reactor (OFR). The authors show that under their experimental setup determining the true reactor RTD requires deconvolution of the plumbing external to the reactor. It is shown that for various changes in the gas introduction and exit configuration (single tube, sparger, rings), the RTD is indistinguishable. A CFD simulation shows that despite the RTD suggesting a well-stirred reactor, the flow pattern is quite different with central jetting, recirculation and dead zones. An additional CFD simulation showed that with a cone on the inlet, the flow pattern is similar and not plug-flow.

The paper is generally well-written and explores an understudied and important aspect of OFRs which are rapidly becoming more widely used in atmospheric lab and field studies. Therefore, I recommend publication after a few minor-to-moderate revisions described below.

General/Main Comments:

- The authors seemed to have missed some very relevant recently-published work on RTDs and some of the effects on kinetics and VOC reactions (see details below) which provide additional context for framing this work.

- The "Potential Impacts" section could use substantial improvement. The OH reactivity (OHRext) usage seems inaccurate and the discussion following is therefore unclear (see details below). Also, this section seems a bit abstract and underdeveloped, in that it doesn't convey how these issues may actually impact real experiments and applications that people are using OFRs for. I would recommended framing and expanding the points made to discuss how they might affect results for typical applications. I.e. SOA yields or compositions, gas-product formation, aerosol chemical or physicochemical transformation (e.g. hygroscopicity), etc. Given that the manuscript is intended for publication in an atmospheric-focused paper, a stronger connection to how this study will help advance measurements related to the atmosphere is important.

- Indeed, the experimental setup used in this study requires backing out the substantial delays and smearing of the gas delivery and measurement systems. The authors do a nice job of working out and explaining a method to accurately extract the true OFR RTDs. However, in practice wouldn't it be best to minimize the plumbing and/or detection delays using a system with a much faster response time? E.g. use of 1/8" tubing, CO_2 gas, and LICOR CO_2 detector could achieve response times of probably only a few seconds, couldn't it? It would be useful to discuss/recommend the best experimental practices to most easily and accurately extract the parameters that other OFR users could then apply to their systems, based on what was learned in this study.

Detailed Comments:

- P5, L97: Ortega et al. 2015 should be updated to ACP 2016.

- P5, L97-104 (and latter part of the intro such as P6, L126-128) seems to be missing some of the recent literature related to measured/modeled RTDs and chemical effects in PAM-type OFRs that would provide better context of what has/hasn't been done in terms of modeling/characterizing OFR flow (especially PAM-type most relevant to this work). These include (but may not be limited to): Peng et al. 2015 (which the authors cite earlier) expands substantially on the Li et al paper and discusses how different flow RTD assumptions (plug, laminar, measured) affect OH exposure (see Section 3.5, Figs. 9, 10, S11, S12, S16, Table S1); Ortega et al. ACP 2016 (cited elsewhere) shows FLUENT CFDs of with/without the inlet plate installed (Section 2.2, Fig. S1); Palm et al. ACP 2017 (www.atmos-chem-phys.net/17/5331/2017/) shows RTDs from FLUENT CFDs without the inlet plate installed for the PAM OFR for different particles sizes and compared to the Lambe et al 2011 RTD. (Section 2.2, Fig. S1); Palm et al. ACPD, 2017 (https://doi.org/10.5194/acp-2017-795) shows some modeled chemical differences (in VOC decays) for different RTD flow assumptions (Figs. 1, 2, S6).

- P7, L161: consider reporting SO2 tank concentration.

- P8, L182: delete "create" or "allow"

- P10, L218: add hyphen for first-order

- P10, L224-225: What is meant by "however those simulations required significant computer time to resolve mesh sizing"? Do the authors mean to say it would take too much time to run (or justify running) for this study?

- P18, L395-397: Again, more detailed modeling work from other publications on effects of differing RTDs and flow assumptions missing here.

- P18-19: "Potential Implications" section. The use of OHRext appears to not be accurately used. OHR is not an exclusively intensive property of a compound (as seems to

be implied in the text) but rather depends on the concentration and OH rate constants of the compounds present that can react with OH. Also OHR is a measure of the (inverse) OH lifetime, not its reaction partners. Maybe the authors really mean the OH lifetime of different compounds? i.e. kvoc+oh x [OH].

- P19, L412-16: It's not clear why compounds that react faster with OH would be more prone to be lost to the reactor walls. It seems that the opposite is stated above. Also not clear how rapid mixing would help that situation.

- P19, L406-407. Add "a" before phenomenological or make "model" plural.

- P19, L412: Statement: "This configuration would suit a laboratory experiment with slow kinetics, where concentrations can be made high enough to where wall losses aren't an issue." This statement may be very misleading. Simply increasing concentrations in many cases does not decrease the relative importance of wall effects since they are often first-order losses and the walls may not necessarily establish equilibrium and relevant timescales. Please revise to precisely state what is meant here, or possibly delete if not relevant.

- P20, L442: add "the" or "a" before "focus"

Figures:

- Fig. 1: Higher resolution on detailed photos needed. This may have just been the pdf conversion that shouldn't be an issue if high-resolution pictures provided for final publication. Otherwise, the thorough photographic documentation is a nice inclusion.

- Fig. 1b "internals" photo: black label too hard to read on dark background. Try white or yellow and move to the right.

- Fig. 2: all text too small (axes labels, tick label). Also x-axes labels on two plots on left are hiding behind data

- Fig. 4. Units for velocity missing. Also, the colorbar and labels are too small.

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2017-352, 2017.