Atmospheric and Watershed Modelling of Trifluoroacetic Acid from Oxidation of HFO-1234ze(E) Released by Prospective Pressurized Metered-Dose Inhaler Use by Shivendra G. Tewari et al.

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This paper is a resubmission of "Atmospheric and watershed modelling of HFO-1234ze(E) emissions from prospective pressurized metered-dose inhalers usage" after public peer review on egusphere. The revised paper shows significant improvements to the original and takes on board many of the reviewers comments. Due to the content of the paper being scientifically valuable as not many studies have been published on pressurised metered dose inhaler emissions, and the improvements made, the paper merits publication in ACP after the minor corrections outlined below.

General comments

The addition of the final section on limitations of the study, into the production of trifluoroacetic acid (TFA) from the atmospheric oxidation of HFO-1234ze(E), outlines clearly the limitations that help to contextualise the results within the wider scientific landscape.

The inclusion of the additional atmospheric oxidations routes, notably the ozonolysis of HFO-1234ze(E) and the photolysis of trifluroacetylealdehyde (TFAA) to produce HFC-23 (CF_3H) greatly improves the paper, despite these routes having little impact on the overall results of the paper. The addition of this information helps to contextualise the results and mechanisms being reported. For completeness, it would be beneficial to outline what the "several other TFAA degradation pathways have been suggested in the literature" (lines 72-73 of the revised manuscript) are. This inclusion isn't imperative as it does not relate to the production of TFA; however, it demonstrates that the authors are aware of the full routes and contextualises the oxidative pathways.

The inclusion of the author derived HFO emissions based on the sales data is a welcome inclusion in the supplementary information. It is acknowledged that the inclusion of the sales data is potentially commercially sensitive, despite the data being country aggregates for all producers of pMDIs. The method used to derive these emissions is explained within section 2.2, so there is suffice information on the provenance of the data.

Specific comments

Whilst I understand why the Dutch drinking water threshold for TFA is cited on line 26 to contextualise the Rhine values, especially as the mouth of the Rhine is in the Netherlands, it isn't clear to me why the values for the Cauvery are compared to this threshold.

Some of the naming of references in the text seem to be incorrect and might be caused due to the use of a reference management software. These should be checked and corrected. Examples of erroneous naming in citations include: line 38 "(Organization, 2022)" instead of World Meteorological Organization, line 42 "(Union, 2024)" instead of Official Journal of the European Union.

The authors have addressed a previous comment by the reviewers on the inclusion of ozonolysis as an atmospheric oxidative pathway for HFO-1234ze(E). They have rightfully acknowledged the temperature dependence of the ozonolysis reactions, which are not included in the McGillen et al (2023) paper (lines 47 – 54 of the revised manuscript). Moreso than the temperature dependence, one would expect OH-initiated chemistry to dominate over ozonolysis due to the reaction rates. An acknowledgement of this limitation in the production in HFC-23 from HFO-1234ze(E) would be beneficial to show why the authors have not looked into the production of HFC-23 in this paper.

There is no description of how the modelled deposition data from GEOS-CHEM is superimposed onto the basin boundaries used for the watershed modelling. It would be good to include the information that was provided as a response to one of the reviewers on this topic in section 2.4

Technical comments

Line 56: add in "known" between 15,000 and chemicals to read "… PFAS are a group of nearly 15,000 known chemicals…".

Line 59: There are some PFAS compounds that take tens of decades to decompose. It might be better to show this rather than stating "many years".

Line 65: Add in "known" between 2,000 and chemicals to read "… presently, there are nearly 2,000 known chemicals that have…".

Line 107: Subtitle "Anthropogenic, Natural, and HFO-1234ze(E) emissions" does not make sense. Suggest altering to "Anthropogenic and Natural Trace gas, and HFO-1234ze(E) emissions".

Lines 109 – 111: Try to avoid using double parentheses, better to list species as "… reactive gases (sulfur dioxide, SO_2; nitrogen oxides, NO_x; ammonia, NH_3; …".

Table 1 footnotes: Adsorption spelt incorrectly on line 3 of the footnotes. Additionally, units of L/kg need to be changes to L kg^{-1}.

Line 309, replace "Gg/yr (or kiltons/year)" with Gg yr^{-1} (or kilotonnes yr^{-1}).

Figure 3 units are not consistent with the rest of the paper – shown as $kg/m^2 \bullet yr$ instead of kg m^{-2} yr^{-1}.

Line 484: Remove “i.e. 4.736 x 0.04 x 10^{-3}” as this does not add any extra information to the paper than the preceding value.

Line 493 – 494: It would be pertinent to reference the limitations of this study, or at least the following section, on the results.

Lines 506 – 510: Again, these results are based on the limitations of the study that should be acknowledged (or at least signed posted to the section on limitations) rather than stating something outright as it is misleading.

Supplemental data: Unts in the table need to be changes to Gg $month^{-1}$. Additionally, the number of significant figures need to be thought about here. Captions are needed for the two plots below the table that show propellant emissions released per month in the UK and Brazil, as well as month names.