

README file for the dataset associated with the research article titled: Trifluoroacetic acid deposition from emissions of HFO-1234yf in India, China, and the Middle East.

Research article authors: Liji M. David^{1,2}, Mary Barth³, Lena Höglund-Isaksson⁴, Pallav Purohit⁴, Guus J. M. Velders^{5,6}, Sam Glaser^{1,a}, and A. R. Ravishankara^{1,2}

Author affiliations: ¹Department of Chemistry, Colorado State University, Fort Collins, CO 80523, USA, ²Department of Atmospheric Science, Colorado State University, Fort Collins, CO 80523, USA, ³Atmospheric Chemistry Observations and Modeling Laboratory, National Center for Atmospheric Research, Boulder, CO, USA, ⁴Pollution Management Research Group, International Institute for Applied Systems Analysis (IIASA), Schlossplatz 1, 2361 Laxenburg, Austria, ⁵Centre for Environmental Quality, National Institute for Public Health and the Environment (RIVM), P.O. Box 1, 3720 BA Bilthoven, the Netherlands, ⁶Institute for Marine and Atmospheric Research Utrecht, Utrecht University, the Netherlands, ^aCurrently at: Tufts University, Medford, MA, USA

Research article abstract: We have investigated trifluoroacetic acid (TFA) formation from emissions of HFO-1234yf, its dry and wet deposition, and rainwater concentration over India, China, and the Middle East with GEOS-Chem and WRF-Chem models. We estimated the TFA deposition and rainwater concentrations between 2020 and 2040 for four previously published HFO-1234yf emission scenarios to bound the possible levels of TFA. We evaluated the capability of GEOS-Chem to capture the wet deposition process by comparing calculated sulfate in rainwater with observations. Our calculated TFA amounts over the U.S., Europe, and China were comparable to those previously reported when normalized to the same emission. A significant proportion of TFA was found to be deposited outside the emission regions. The mean and the extremes of TFA rainwater concentrations calculated for the four emission scenarios from GEOS-Chem and WRF-Chem were orders of magnitude below the no observable effect concentration. The ecological and human health impacts now and continued use of HFO-1234yf in India, China, and the Middle East are estimated to be insignificant based on the current understanding, as summarized by Neale et al. (2021).

Research article citation: David, L.M, Barth, M., Höglund-Isaksson, L., Purohit, P., Velders, G.J.M., Glaser, S., and Ravishankara, A.R.: Trifluoroacetic acid deposition from emissions of HFO-1234yf in India, China, and the Middle East, *Atmos. Chem. Phys.*, 21, 14833-14849, <https://doi.org/10.5194/acp-21-14833-2021>, 2021.

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Contact: Liji David, liji.david@usu.edu

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Data sources and structure:

Source: Data compiled by Liji David. TFA deposition and TFA rainwater concentration simulated by the models - GEOS-Chem and WRF-Chem.

Spatial coverage: India (2°S-40°N and 57°E-109°E), China (5°N-55°N and 72°E-145°E), The Middle East (3°N-50°N and 12°E-87°E)

Temporal coverage: 2015, 2016

Data description: The TFA deposition and TFA rainwater concentration was calculated in GEOS-Chem and WRF-Chem models over the India, China, and the Middle East domains.

Format of data files: There are 10 data files along with a README file. The data files are described as follows:

1. The file 'dry_wet_deposition_percent_domains.csv' gives the percentage contribution of dry and wet deposition to total annual TFA deposition from GEOS-Chem and WRF-Chem in the three domains.
2. The file 'TFA_deposition_scenarios.csv' gives the total TFA deposited (dry and wet combined) in four emission scenarios for 2020 to 2040 within the three domains.
3. The files 'TFA_rainwater_monthly_IN.csv', 'TFA_rainwater_monthly_CH.csv', and 'TFA_rainwater_monthly_ME.csv' give the monthly variation in TFA rainwater concentration calculated from GEOS-Chem and WRF-Chem in India, China, and the Middle East domains, respectively.
4. The file 'TFA_rainwater_scenarios.csv' gives the mean TFA rainwater concentration in four scenarios for 2020 to 2040 within the three domains.
5. The files 'dry_wet_deposition_percent_2015-2016.csv' and 'TFA_rainwater_2015-2016.csv' give the percentage contribution of dry and wet deposition to total annual TFA deposition and TFA rainwater concentration, respectively, in the three domains for 2015 and 2016.
6. The file 'total_deposition_percent_domains_regions.csv' gives the percentage of total TFA deposition (dry and wet combined) calculated from GEOS-Chem and WRF-Chem models in the three domains.
7. The file 'total_deposition_percent_global_regional_emissions.csv' gives the percentage of total TFA deposition from global and regional emissions in the three domains.

Recommended use: Please read the associated publication to understand our analysis method.

Reference:

1. R. E. Neale, *et al.*, Environmental effects of stratospheric ozone depletion, UV radiation, and interactions with climate change: UNEP Environmental Effects Assessment Panel, Update 2020. *Photochem. Photobiol. Sci.* **20**, 1–67 (2021).