Supplementary Information for *Atmospheric fates and global warming potential of HFO-1234ze(E) and its degradation product trifluoroacetaldehyde (CF_3CHO)*

Beth Killen[1], Jenny A. Fisher[2,3], Christopher S. Hansen[1], Paul B. Krummel[4], Martin K. Vollmer[5], and Scott H. Kable[1]

[1]School of Chemistry, UNSW Sydney, NSW 2052, Australia

[2]College of Science and Engineering, James Cook University, Douglas, QLD 4811, Australia

[3]Environmental Futures, University of Wollongong, Wollongong, NSW 2522, Australia

[4]CSIRO Environment, Aspendale, Victoria, Australia

[5]Laboratory for Air Pollution / Environmental Technology, Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland

February 24, 2026

This Supplementary Information provides additional details that support the main manuscript. It includes: Supplementary Text S1: Comparison of AtChem2 and GEOS-Chem CF_3CHO sinks, Supplementary Figures S1-S4, and Supplementary Tables S1-S2.

S1 Comparison of AtChem2 and GEOS-Chem CF_3CHO Sinks

Comparing the relative contributions of photochemical loss processes in GEOS-Chem (Figure S4) to those in AtChem2 (main text Figure 3b) reveals some differences between the 3D and box model simulations. Although photolysis dominates in both cases, it accounts for a larger fraction in the box model (80%) than in the 3D model (67%). This difference is likely due to the different time periods covered by each simulation: the box model represents a summer month when photolysis conditions are optimal, while the 3D model uses annual average conditions that include winter months and high-latitude regions where solar radiation is reduced and photolysis rates are much lower. The higher photolysis fraction in the box model also reflects its boundary-layer focus, where deposition is less important than in the full 3D simulation that includes efficient mid-tropospheric wet removal. Despite these differences, the two models both show that the net reaction with HO_2 is of minor importance.

S2 Supplementary Figures

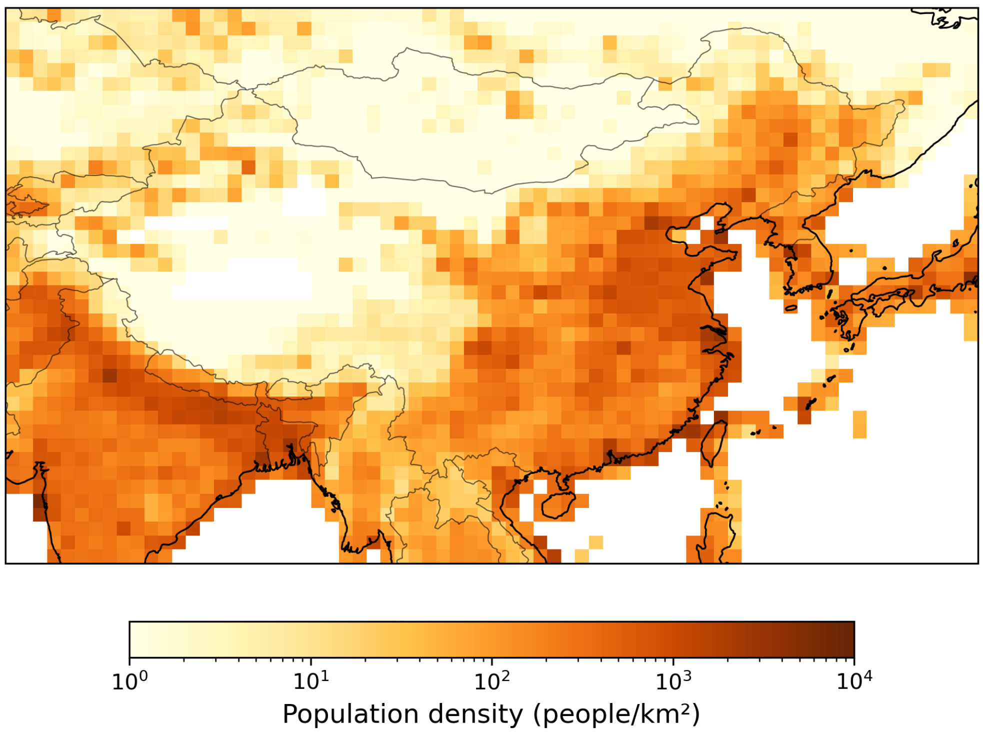

Figure S1: Population density distribution over China used to spatially allocate HFO-1234ze(E) emissions (12.6 Gg yr^{-1}) for Henry's Law sensitivity tests. Emissions are distributed proportionally to 2015 population density (1), following the HCFC-141b replacement scenario from Wang *et al.* (2).

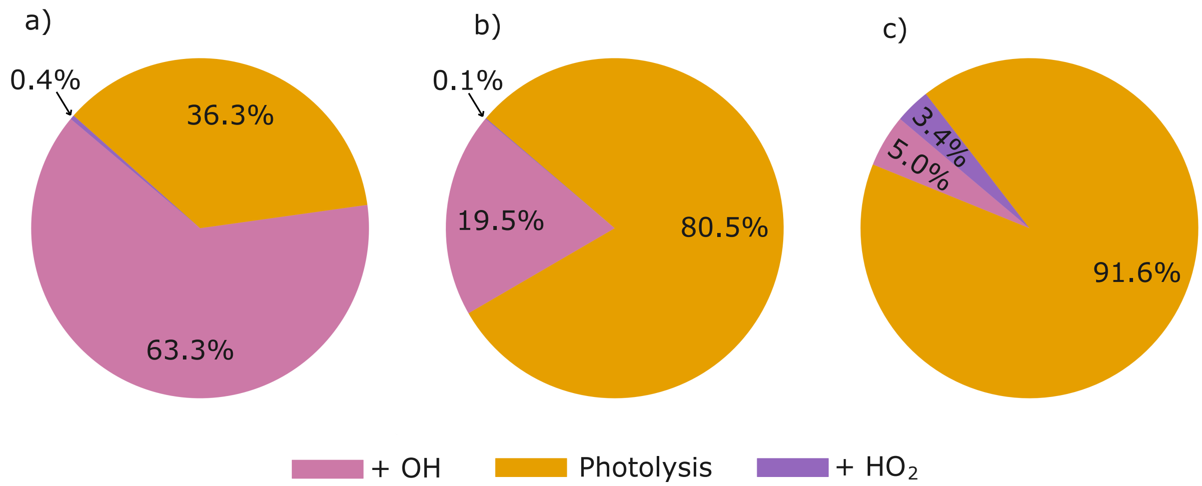

Figure S2: Average percentage contribution of each loss process to total atmospheric removal of CF_3CHO under different conditions. a) with 10x increased HO_2 concentration, b) increasing the rate of the forwards reaction in Long *et al.* (3) by 10, and c) simulating conditions representative of around 5 km altitude.

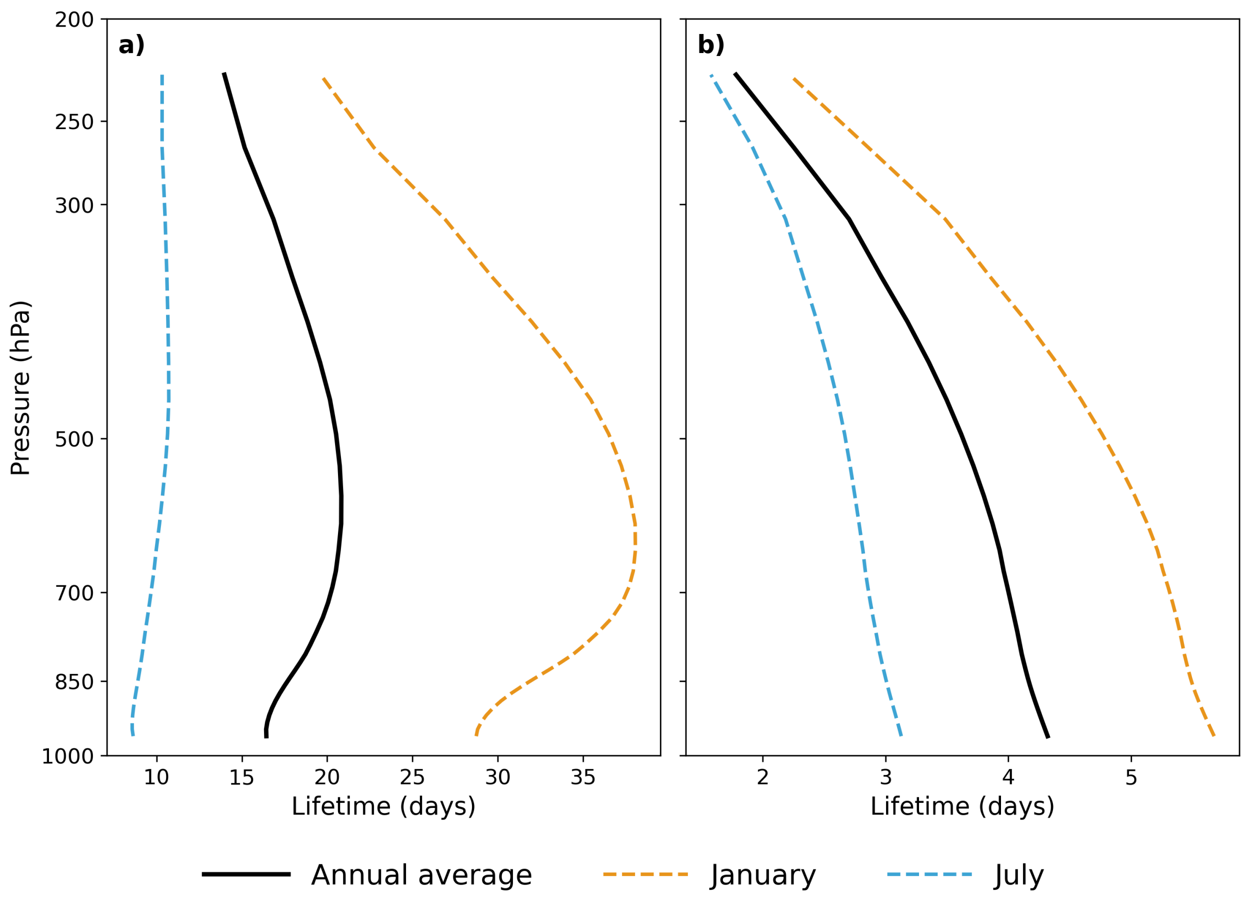

Figure S3: Seasonal and altitudinal variations in the lifetime of a) HFO-1234ze(E) and b) CF_3CHO.

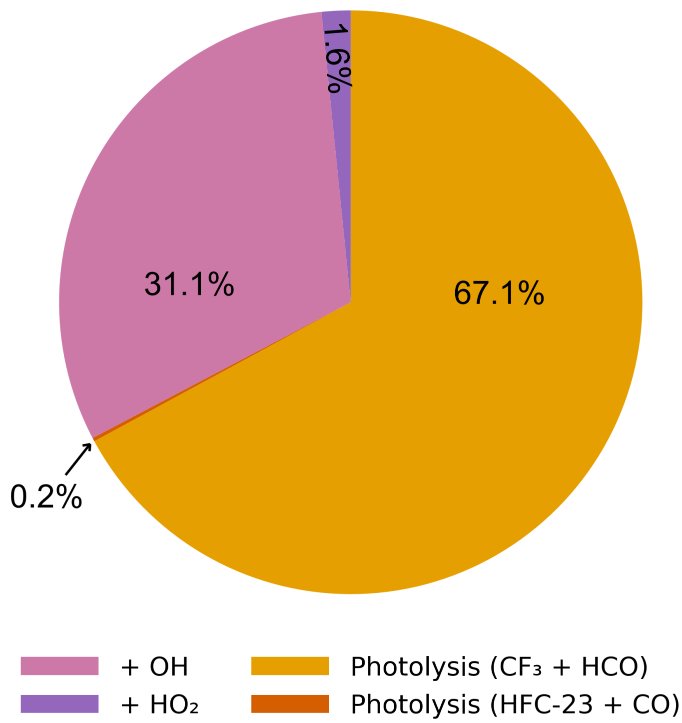

Figure S4: Relative contribution of CF_3CHO photochemical processes only (no deposition) as simulated by GEOS-Chem.

S3 Supplementary Tables

Table S1: Pressure-dependent quantum yields for CF_3CHO photolysis to HFC-23 and CO (R2) at 1 nm resolution (242 - 320 nm) used in Cloud-J photolysis rate calculations. Wavelengths 248, 266, 281 and 308 nm are directly from Van Hoomissen *et al.* (4). All others are interpolated to 1 nm intervals as described in main text Section 2.2.2.

Wavelength (nm)	**QY (650 Torr)**	**QY (100 Torr)**
242	0.395	0.395
243	0.396	0.396
244	0.395	0.395
245	0.394	0.394
246	0.395	0.394
247	0.395	0.393
248	0.358	0.358
249	0.394	0.391
250	0.394	0.389
251	0.393	0.389
252	0.389	0.388
253	0.387	0.387
254	0.386	0.387
255	0.385	0.385
256	0.384	0.384
257	0.382	0.382
258	0.379	0.379
259	0.373	0.373
260	0.367	0.367
261	0.364	0.364
262	0.360	0.360
263	0.352	0.352
264	0.344	0.345
265	0.337	0.342
266	0.407	0.407
267	0.316	0.320

Continued on next page

Wavelength (nm)	**QY (650 Torr)**	**QY (100 Torr)**
268	0.300	0.301
269	0.281	0.281
270	0.264	0.267
271	0.247	0.256
272	0.225	0.247
273	0.202	0.235
274	0.181	0.219
275	0.160	0.202
276	0.140	0.184
277	0.122	0.167
278	0.105	0.151
279	0.094	0.137
280	0.084	0.123
281	0.056	0.114
282	0.055	0.097
283	0.044	0.086
284	0.036	0.075
285	0.030	0.066
286	0.025	0.057
287	0.020	0.050
288	0.017	0.043
289	0.014	0.037
290	0.011	0.032
291	0.009	0.028
292	0.007	0.024
293	0.006	0.021
294	0.005	0.018
295	0.004	0.015
296	0.003	0.013
297	0.003	0.011
298	0.002	0.010
299	0.002	0.008

Continued on next page

Wavelength (nm)	**QY (650 Torr)**	**QY (100 Torr)**
300	0.001	0.007
301	0.001	0.006
302	0.001	0.005
303	0.001	0.004
304	0.001	0.004
305	0.000	0.003
306	0.000	0.003
307	0.000	0.002
308	0.000	0.002
309	0.000	0.002
310	0.000	0.001
311	0.000	0.001
312	0.000	0.001
313	0.000	0.001
314	0.000	0.001
315	0.000	0.001
316	0.000	0.001
317	0.000	0.000
318	0.000	0.000
319	0.000	0.000
320	0.000	0.000

Table S2: Model-observation comparison for HFO-1234ze(E) at AGAGE monitoring sites. Observations are multi year means (2020-2024), and model values are from the 2019 simulation, sampled at each site location.

Site	**Lat**	**Lon**	**Obs (ppt)**	**Model (ppt)**	**RMSE (ppt)**[†]	**Bias (ppt)**	**NMB (%)**[‡]
Zeppelin	78.9	11.9	0.12	0.15	0.06	0.03	28
Mace Head	53.3	−9.9	0.18	0.19	0.07	0.01	8
Jungfraujoch	46.6	8.0	0.26	0.14	0.16	−0.12	−47
Trinidad Head	41.1	−124.2	0.16	0.17	0.07	0.01	7
Gosan	35.4	129.3	0.16	0.76	0.62	0.60	369
Ragged Point	13.2	−59.4	0.02	0.03	0.01	0.01	42
Cape Matatula	−14.3	−170.6	0.01	0.00	0.00	0.00	−33
Kennaook/Cape Grim	−40.7	144.7	0.01	0.05	0.04	0.04	637

[†]RMSE: Root Mean Square Error, $\sqrt{\frac{1}{n}\sum_{i=1}^{n}(M_i - 0_i)^2}$, based on monthly means. [‡]NMB: Normalized Mean Bias, calculated as (Model − Obs)/Obs × 100%.

References

[1] Center for International Earth Science Information Network – CIESIN – Columbia University Gridded Population of the World, Version 4 (GPWv4): Population Density, Revision 11. 2018.

[2] Wang, Y.; Wang, Z.; Sun, M.; Guo, J.; Zhang, J. Emissions, degradation and impact of HFO-1234ze from China PU foam industry. *Science of The Total Environment* **2021**, *780*, 146631.

[3] Long, B.; Xia, Y.; Truhlar, D. G. Quantitative Kinetics of HO2 Reactions with Aldehydes in the Atmosphere: High-Order Dynamic Correlation, Anharmonicity, and Falloff Effects Are All Important. *Journal of the American Chemical Society* **2022**, *144*, 19910–19920, PMID: 36264240.

[4] Van Hoomissen, D.; Chattopadhyay, A.; Montzka, S. A.; Burkholder, J. B. CHF3 (HFC-23) and CF3CHO Quantum Yields in the Pulsed Laser Photolysis of CF3CHO at 248, 266, 281, and 308 nm. *ACS Earth and Space Chemistry* **2025**, *9*, 589–602.