

1 **Supplementary information for**

2

3 **Trifluoroacetic acid deposition from emissions of HFO-1234yf in India, China,**  
4 **and the Middle East**

5 Liji M. David\*<sup>1,2</sup>, Mary Barth\*<sup>3</sup>, Lena Höglund-Isaksson<sup>4</sup>, Pallav Purohit<sup>4</sup>, Guus J. M. Velders<sup>5,6</sup>,  
6 Sam Glaser<sup>1,7</sup>, and Akkihebbal. R. Ravishankara\*<sup>1,2</sup>

7 <sup>1</sup>Department of Chemistry, Colorado State University, Fort Collins, CO 80523, USA

8 <sup>2</sup>Department of Atmospheric Science, Colorado State University, Fort Collins, CO 80523, USA

9 <sup>3</sup>Atmospheric Chemistry Observations and Modeling Laboratory, National Center for  
10 Atmospheric Research, Boulder, Colorado

11 <sup>4</sup>Air Quality and Greenhouse Gases Program, International Institute for Applied Systems Analysis  
12 (IIASA), Schlossplatz 1, 2361, Laxenburg, Austria

13 <sup>5</sup>National Institute for Public Health and the Environment (RIVM), PO Box 1, 3720 BA  
14 Bilthoven, The Netherlands

15 <sup>6</sup>Institute for Marine and Atmospheric Research Utrecht, Utrecht University, The Netherlands

16 <sup>7</sup>Currently at Tufts University, Medford, MA

17 *Address correspondence to:* [liji.david@colostate.edu](mailto:liji.david@colostate.edu), [barthm@ucar.edu](mailto:barthm@ucar.edu), and  
18 [a.r.ravishankara@colostate.edu](mailto:a.r.ravishankara@colostate.edu)

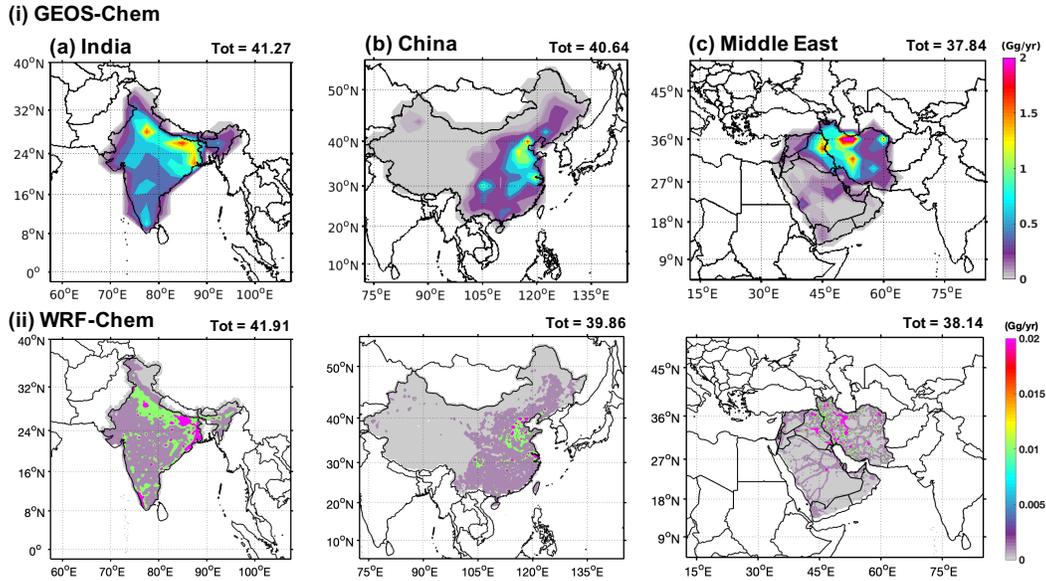
19

20 **Contents of this file**

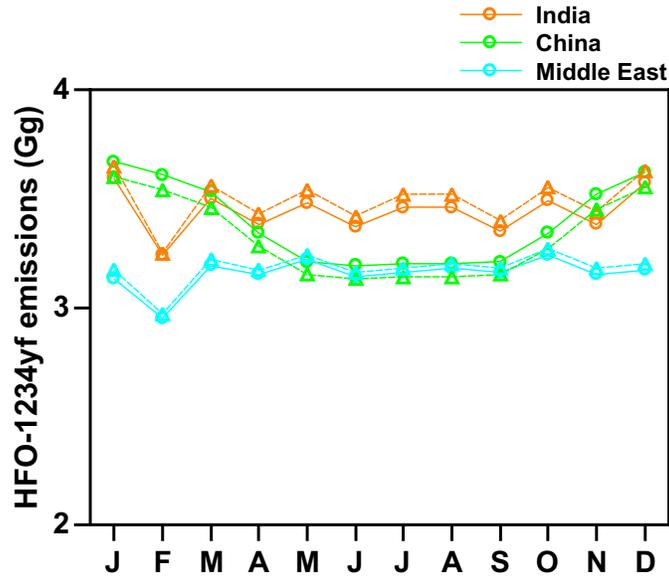
21 Figures S1 to S14

22 Tables S1 to S2

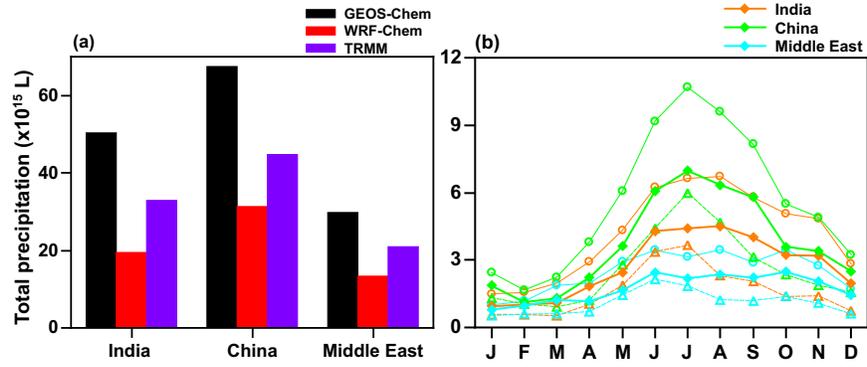
23



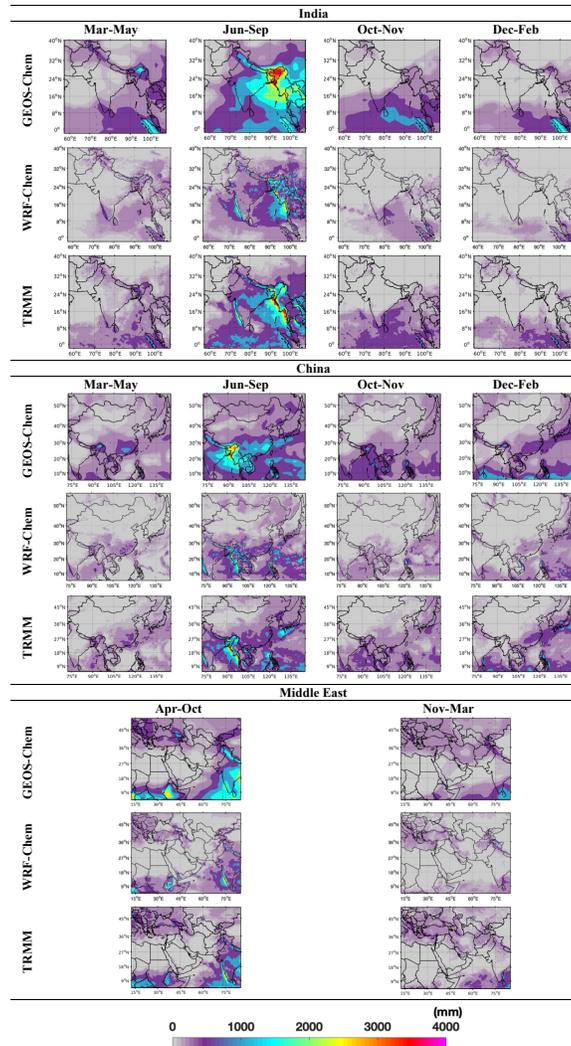
24  
 25 **Figure S1.** Annual spatial distribution of HFO-1234yf emission in the three regions in (i) GEOS-  
 26 Chem and (ii) WRF-Chem. Grid total HFO-1234yf emissions are also shown in each figure in Gg  
 27  $\text{yr}^{-1}$ . The color bars are in Gg  $\text{yr}^{-1}$ . The emissions ranges in GEOS-Chem and WRF-Chem are  
 28 different because the grid sizes are much smaller in the latter than the former.  
 29



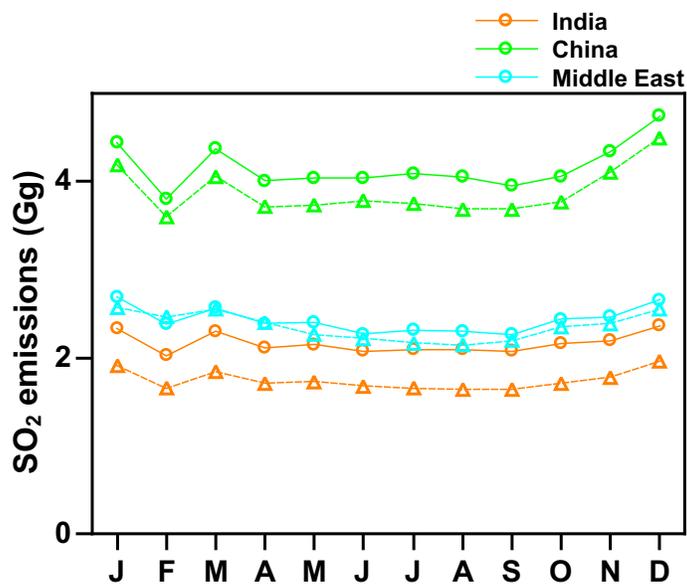
30  
 31 **Figure S2.** Monthly variation in HFO-1234yf emissions in GEOS-Chem (solid line with open  
 32 circles) and WRF-Chem (dashed line with open triangles) in the three regions – India, China, and  
 33 the Middle East.  
 34



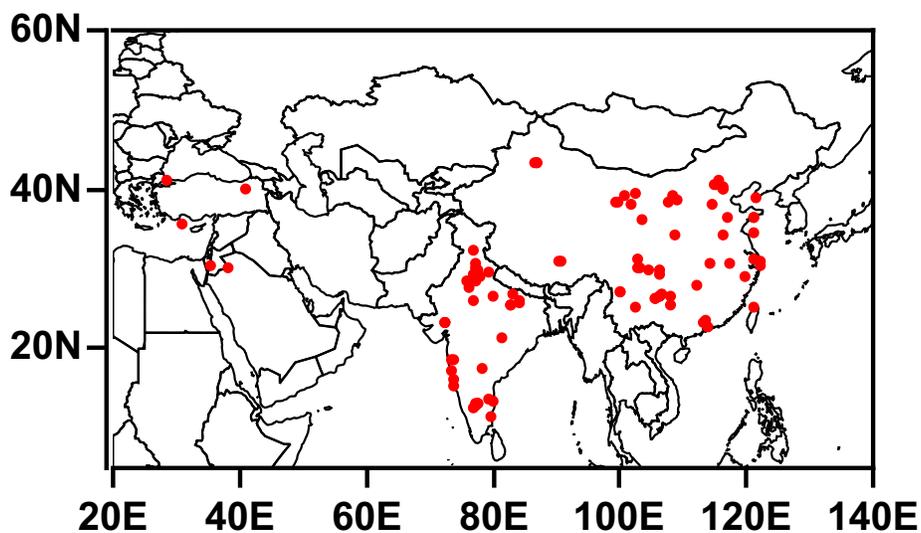
35  
 36 **Figure S3.** (a) Annual and (b) monthly total precipitation in GEOS-Chem and WRF-Chem in the  
 37 three domains. GEOS-Chem results are solid line with open circles, WRF-Chem results are dashed  
 38 line with open triangles, and TRMM observations are solid line with filled diamonds.  
 39



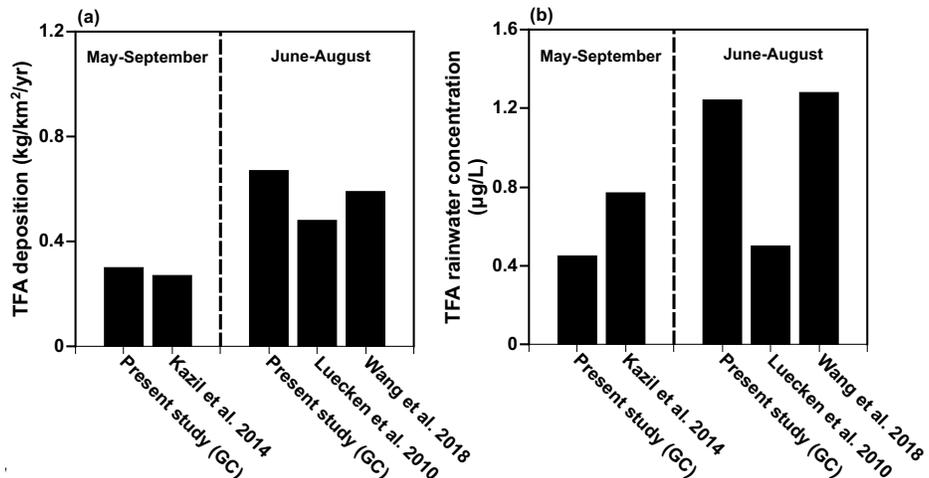
40  
 41 **Figure S4.** Seasonal total precipitation (mm) maps in the three domains from GEOS-Chem, WRF-  
 42 Chem, and TRMM observations.  
 43



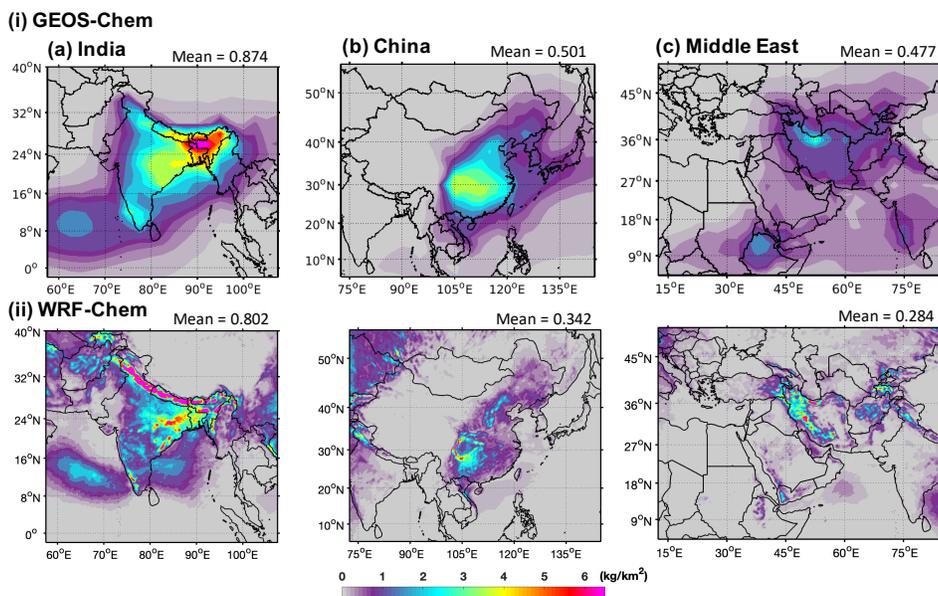
44  
 45 **Figure S5.** Monthly variation in SO<sub>2</sub> emissions in GEOS-Chem (solid line with open circles) and  
 46 WRF-Chem (dashed line with open triangles) from India, China, and the Middle East.  
 47



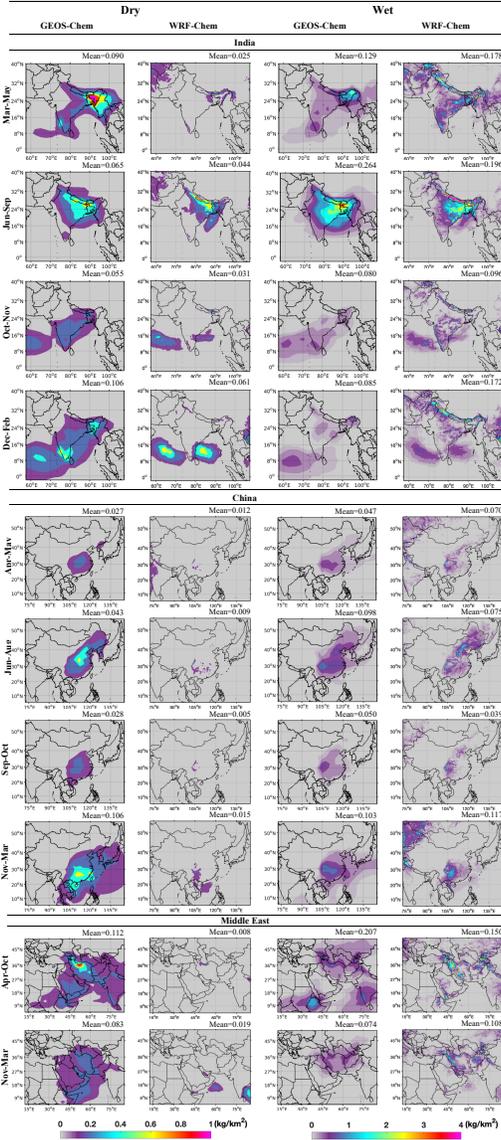
48  
 49 **Figure S6.** The location of sulfate rainwater concentration observations in the three domains for  
 50 2000-2015.  
 51



52  
 53 **Figure S7.** Comparison of TFA deposition and TFA rainwater concentration over the continental  
 54 U.S. from the present study with the previous studies in summer. The emissions are normalized to  
 55 15.21 Gg yr<sup>-1</sup>.  
 56

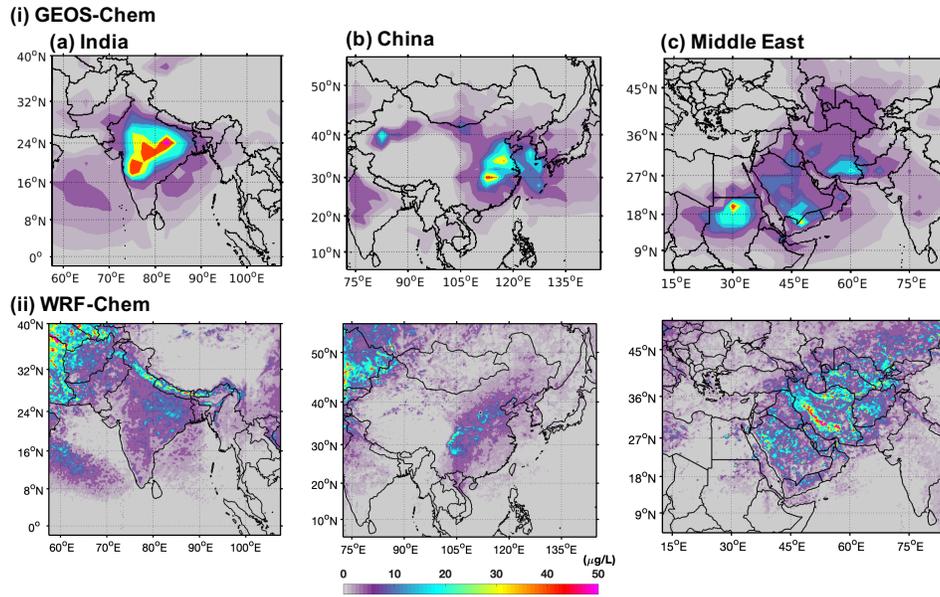


57  
 58 **Figure S8.** GEOS-Chem and WRF-Chem simulated annual total deposition rates of TFA ( $\text{kg km}^2$   
 59  $\text{yr}^{-1}$ ) from dry and wet deposition in India, China, and the Middle East domains. The number at the  
 60 top of each panel gives the mean deposition rates within the domains.  
 61



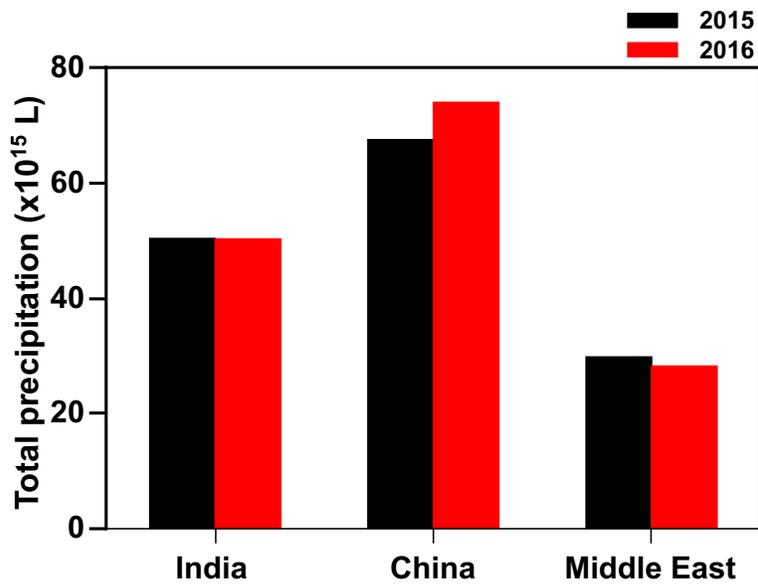
62  
63  
64  
65  
66

**Figure S9.** GEOS-Chem and WRF-Chem simulated seasonal variation in total deposition rates of TFA from dry and wet deposition in India, China, and the Middle East domains. The number at the top of each panel gives the mean dry and wet deposition rates ( $\text{kg km}^{-2}$ ) within the domains.



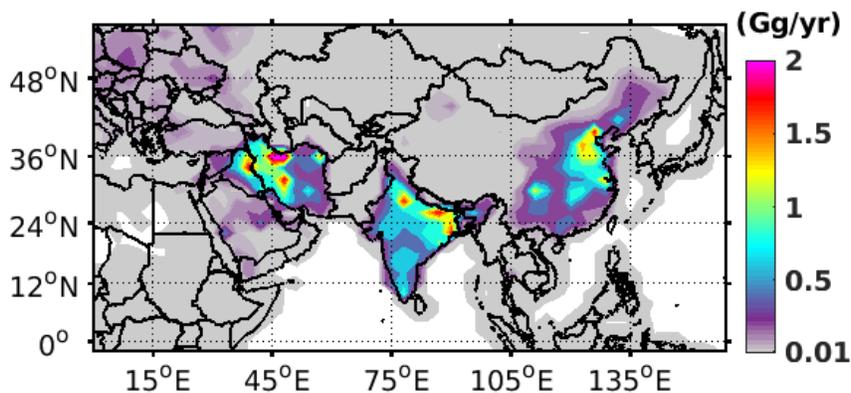
67  
68  
69  
70

**Figure S10.** Contour maps of annual mean TFA rainwater concentrations in GEOS-Chem and WRF-Chem in the three domains.

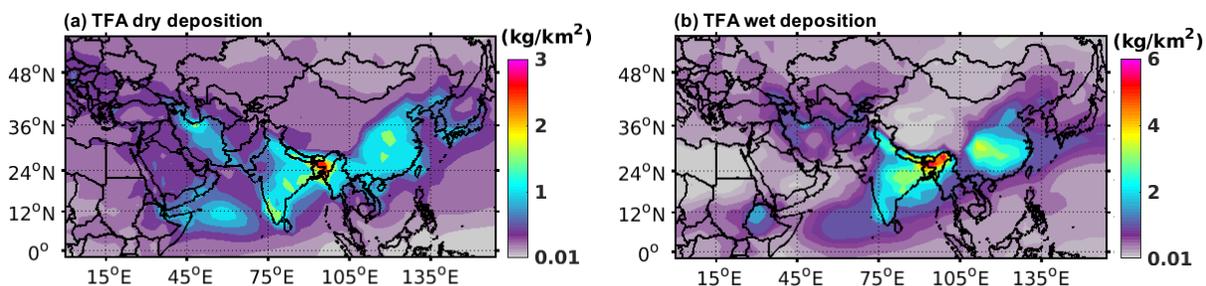


71  
72  
73

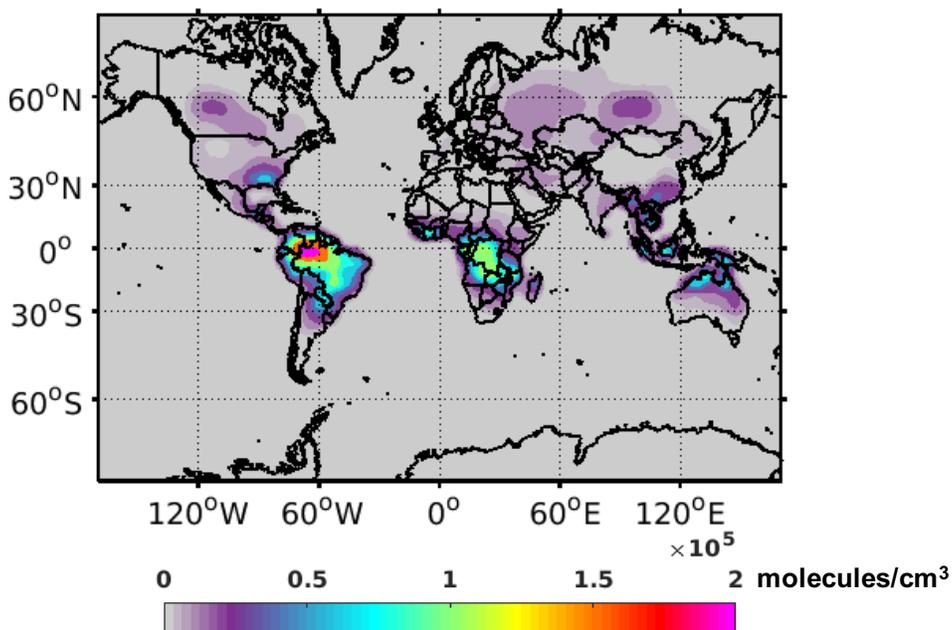
**Figure S11.** Annual total precipitation in 2015 and 2016 from GEOS-Chem in the three domains.



74  
 75 **Figure S12.** Annual spatial distribution of total HFO-1234yf global emissions as simulated in  
 76 GEOS-Chem.  
 77



78  
 79 **Figure S13.** Annual total TFA (a) dry and (b) wet deposition from global HFO-1234yf emissions  
 80 as simulated in GEOS-Chem.  
 81



82  
 83 **Figure S14** Mean surface Criegee intermediate concentration for seven months (January-July)  
 84 simulated using GEOS-Chem.  
 85

86 **Table S1.** The model physics and chemistry options used in WRF-Chem.

Domain	India	China	Middle East
WRF Version	4.1.3 (released November 2019)		
Simulation period	11/01/2014 – 12/31/2015		
Meteorology	Global Forecast System at 0.5° Observational nudging every 6 hours		
Horizontal resolution	30 km		
Grid points (x, y, z)	205×197×40	315×260×40	297×242×40
Microphysics	Morrison two-moment scheme		
Short/Longwave radiation	Rapid Radiative Transfer Model (RRTM)		
Land-surface	Noah Unified Land Surface Model		
Boundary layer	Yonsei University		
Cumulus scheme	Grell-Freitas		
Chemical initial and boundary conditions	CAM-Chem and GEOS-Chem		
Chemistry and Aerosol Scheme	MOZART-GOCART		
Biogenic emissions	MEGANv2.04		
Anthropogenic emissions	EDGAR-HTAP		
Wildfire emission	FINNv1.6		

87  
88 **Table S2.** Seasonal TFA deposition (dry and wet) calculated from GEOS-Chem and WRF-Chem  
89 in India, China, and the Middle East domains.

Seasons	GEOS-Chem		WRF-Chem	
	Dry	Wet	Dry	Wet
<b>Gg</b>				
<b>India</b>				
Mar-May	0.798	1.14	0.190	1.37
Jun-Sep	0.423	1.73	0.259	1.17
Oct-Nov	0.740	1.11	0.402	1.19
Dec-Feb	0.972	0.773	0.543	1.39
<b>China</b>				
Apr-May	0.607	1.07	0.263	1.27
Jun-Aug	0.629	1.45	0.124	0.956
Sep-Oct	0.681	1.20	0.124	0.781
Nov-Mar	0.717	0.711	0.116	0.687
<b>Middle East</b>				
Apr-Oct	0.632	1.17	0.038	0.730
Nov-Mar	0.656	0.554	0.167	0.736

90