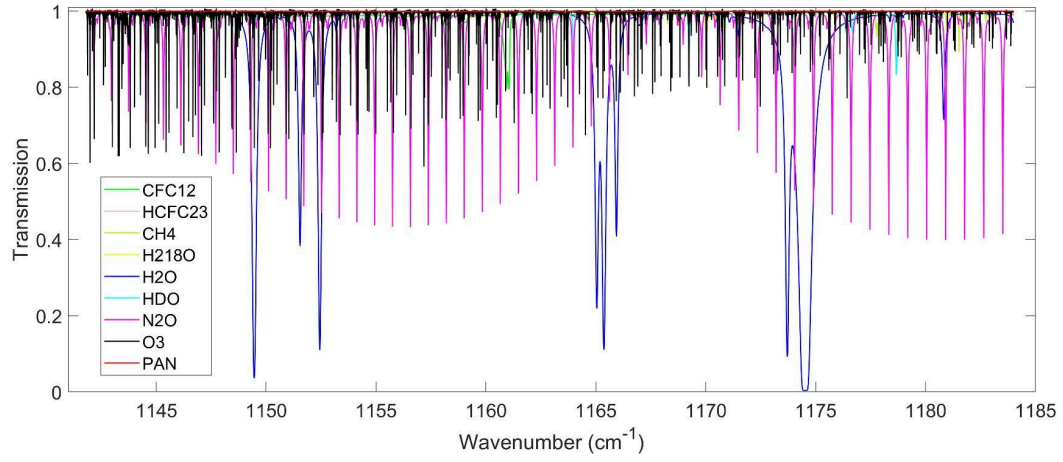


Table S1: FTIR retrieval settings and estimated random and systematic uncertainties (in %) for the tropospheric columns of the species discussed in this work.

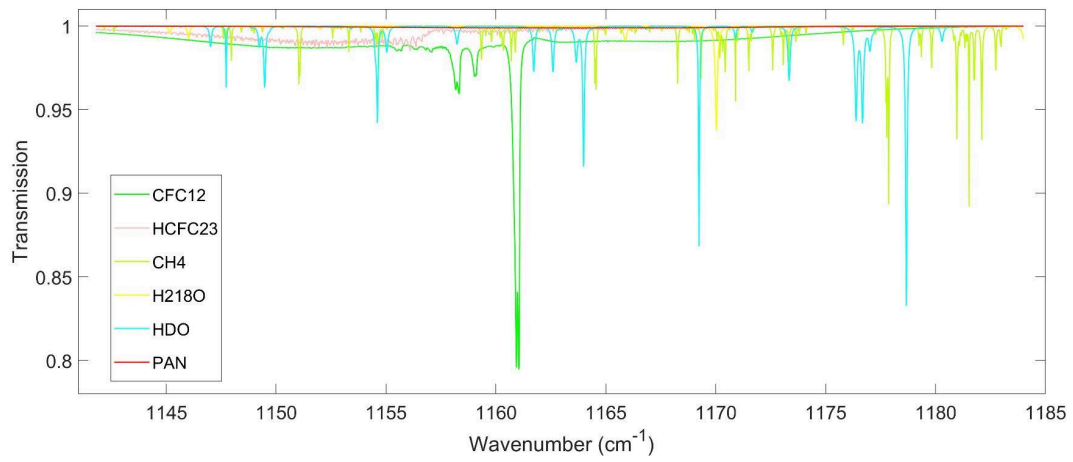
	Spectral windows (cm ⁻¹)	Spectroscopic parameters	Reference	Random Uncertainty	Systematic Uncertainty
HCHO	2763.42–2764.17 2765.65–2766.01 2778.15–2779.10 2780.65–2782.0	Atm16 (= HITRAN 2012 for HCHO)	Vigouroux et al. (2018)	7%	13%
CH ₃ OH	1029.0–1037.0	HITRAN2012, except atm16 for H ₂ O lines	Vigouroux et al. (2012)	2%	17%
C ₂ H ₆	2976.66–2977.059 2983.2–2983.6	C ₂ H ₆ PLL ^a CH ₃ Cl: HITRAN2012 Other species: HITRAN 2008 (modified for O ₃)	Franco et al. (2015)	6%	6%
CO	2057.7–2058.0 2069.56–2069.76 2157.5–2159.15	Atm16 (=HITRAN 2008 for CO)	From https://www2.acom.ucar.edu/irwg , so slightly adapted from Senten et al. (2008).	1.3%	3%
O ₃	991.25–993.8 1001.47–1003.04 1005.0–1006.9 1007.348–1009.0	HITRAN 2020 Except atm20 for H ₂ O lines	Vigouroux et al. (2015)	10%	3%
PAN	1141.8–1184.0	PAN, HFC-23 and CFC-12: pseudo-linelist ^a HITRAN 2012 for other species	This work	6%	20%

^a<http://mark4sun.jpl.nasa.gov/pseudo.html>

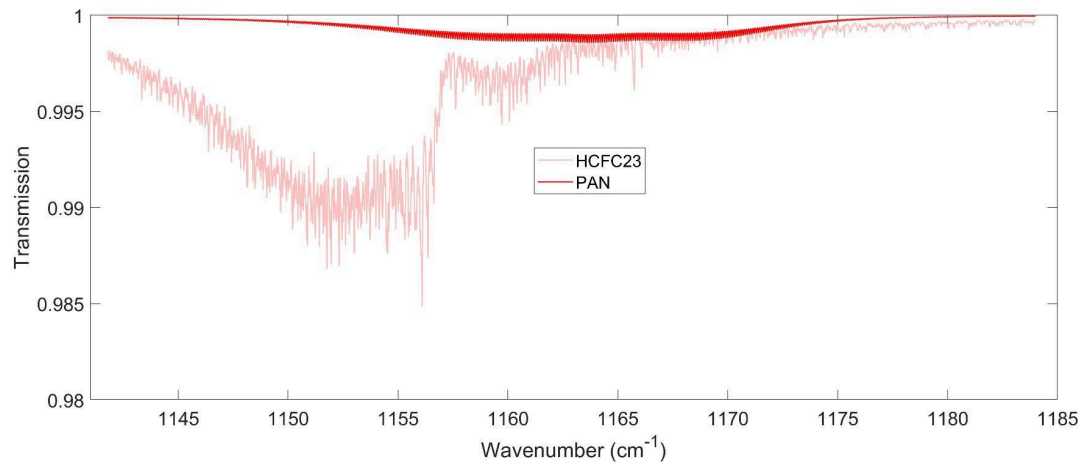
(a)



(b)



(c)



(d)

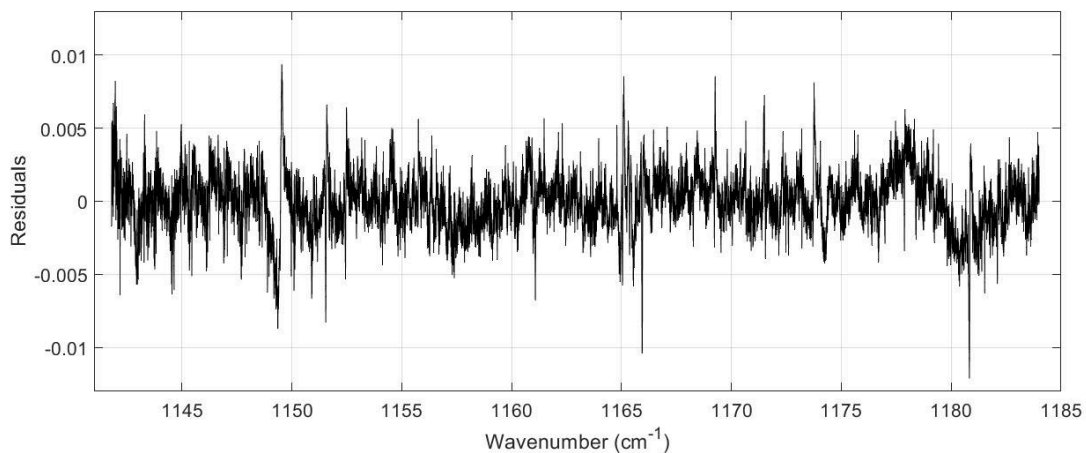


Figure S1. a, b, c) Retrieved spectral signatures for a retrieved PAN column of 5.64×10^{14} molec cm^{-2} . Panel (b) and (c) are zoomed-out versions of panel (a) for different subsets of compounds, to show the relative strength of absorbing gases. (d) Spectral residuals (calculated – observed) for the same spectrum.

Table S2: Seasonal averages of observed meteorological parameters at Maïdo and statistical evaluation (correlation coefficient (R), root mean square error (RMSE) and mean bias) of modelled meteorology against these observations.

	January				July			
	Average	R	RMSE	Mean bias	Average	R	RMSE	Mean bias
Temperature (K)	288.5	0.76	1.34	-0.25	283.1	0.77	2.31	-1.18
Relative humidity, %	74.3	0.67	14.6	1.7	59.4	0.53	23.3	5.1
Solar radiation, W m^{-2}	267.3	0.82	211	4	222.5	0.94	99	-10
Wind direction, °	117.9	0.79	62.5	-9.5	146.9	0.71	61.6	-1.23
Wind speed, m s^{-1}	3.2	0.57	1.83	0.89	2.78	0.31	1.90	0.11

Table S3. Average concentrations of species ($\mu\text{g m}^{-3}$) measured at the air quality stations.

#		Daytime (8:00 - 16:00 LT)			Nighttime (20:00 - 03:00 LT)		
		NO ₂	NO _x	O ₃	NO ₂	NO _x	O ₃
1	Terrain de Sel	7.79	20.32	/	4.83	7.29	/
2	Centre Pénitentiaire	9.17	29.79	/	9.03	17.62	/
3	Lislet Geoffroy	4.67	8.59	/	5.98	7.43	/
4	Sarda Garriga	6.01	18.97	/	7.76	8.73	/
5	Joinville	4.04	8.14	27.15	5.77	7.74	18.77
6	La Marine	2.59	5.84	24.25	4.77	6.06	12.98
7	Plateau Caillou	4.84	10.14	30.93	5.84	7.33	20.01
8	Grand Fond	3.19	6.93	23.75	7.87	10.68	13.84
9	Paradis	5.07	11.89	27.48	8.82	12.95	12.70
10	Route des Tamarins	8.49	44.11	/	11.02	50.20	/
11	Boulevard Banks	17.11	55.90	/	13.93	31.08	/
12	Luther King	8.69	33.39	28.43	10.04	23.03	11.18

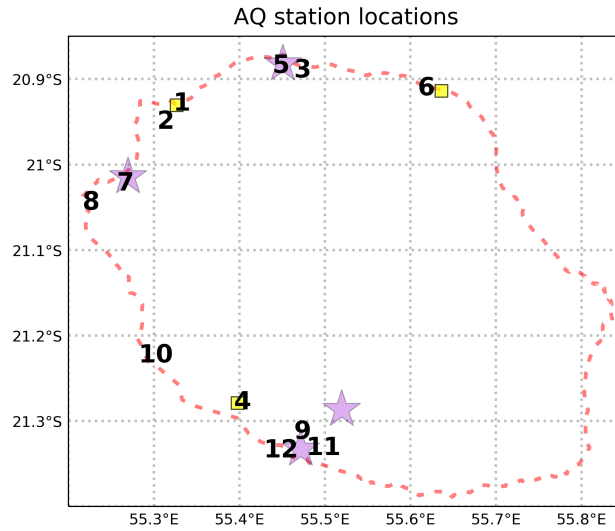


Figure S2. Geographical locations of 12 stations in Table S3. The purple stars and yellow squares represent the most populated cities and power plant locations, respectively, similar to Fig. 2 in the main paper.

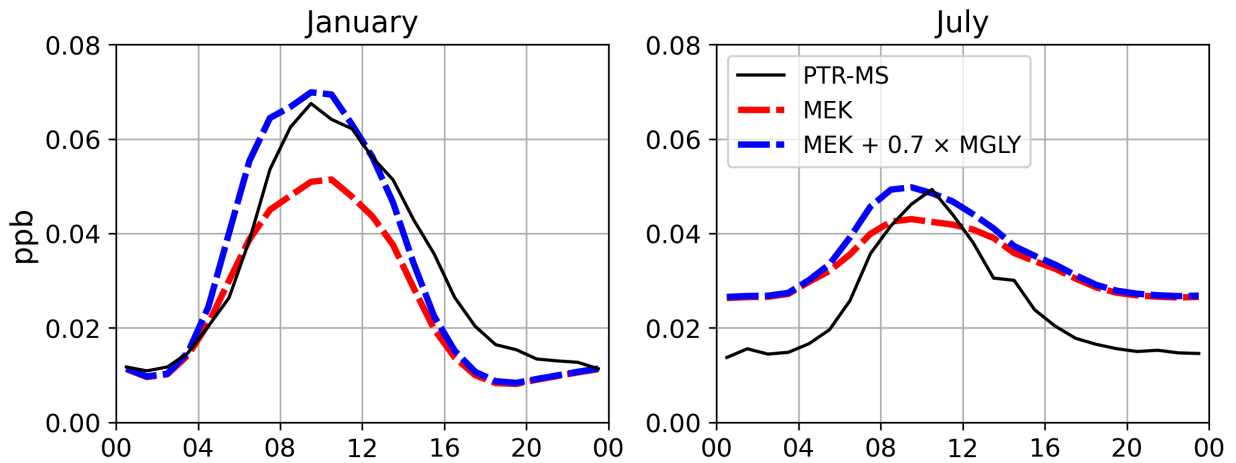


Figure S3. Average diurnal cycle of measured and modelled MEK, omitting (red) and including the MGLY interference (blue).

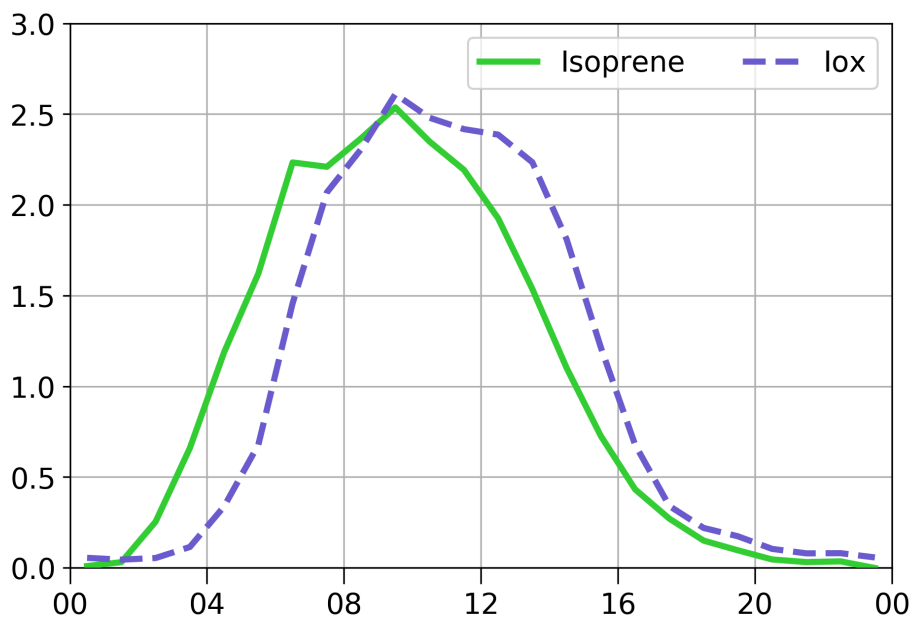


Figure S4. Average diurnal cycle of observed isoprene (green) and lox mixing ratios (purple), normalized by their respective means, for the month of January.

Table S4: Statistics of model performance (correlation coefficient (R), root mean square error (RMSE) and mean bias) against PTR-MS observations. The runs listed are labeled using the shorthand in Table 4. Note that for isoprene, only daytime hours were considered in the statistical evaluation (6AM - 6PM).

	R									
	January					July				
	R0	S2	S3	S4	S5	R0	S2	S3	S4	S5
Formaldehyde	0.650	0.637	0.634	0.623	0.661	0.761	0.762	0.757	0.754	0.790
Methanol	0.706	0.700	0.722	0.704	0.706	0.674	0.671	0.673	0.674	0.675
Acetaldehyde	0.569	0.560	0.562	0.558	0.705	0.457	0.427	0.453	0.450	0.663
Acetone	0.361	0.364	0.392	0.359	0.022	0.585	0.426	0.594	0.586	0.325
Isoprene	0.627	0.653	0.631	0.632	0.647	0.672	0.673	0.690	0.668	0.668
MVK/MACR/ISOOH	0.663	0.659	0.559	0.662	0.658	0.622	0.63	0.245	0.563	0.627
MEK/MGLY (m/z 73)	0.793	0.792	0.698	0.777	0.741	0.629	0.463	0.542	0.614	0.463
Monoterpenes (m/z 137)	0.322	0.344	0.059	0.338	0.339	0.416	0.412	0.142	0.412	0.408
Monoterpenes (m/z 81)	0.391	0.403	0.113	0.4	0.397	0.417	0.422	0.244	0.415	0.419
Acetic acid	0.787	0.782	0.77	0.772	0.786	0.644	0.635	0.646	0.643	0.649

	RMSE (ppb)									
	January					July				
	R0	S2	S3	S4	S5	R0	S2	S3	S4	S5
Formaldehyde	0.551	0.557	0.553	0.581	0.581	0.258	0.254	0.266	0.26	0.267
Methanol	0.361	0.439	0.768	0.362	0.361	0.378	0.488	0.768	0.381	0.383
Acetaldehyde	0.111	0.109	0.112	0.112	0.154	0.092	0.096	0.092	0.092	0.121
Acetone	0.119	0.12	0.116	0.119	0.194	0.084	0.421	0.086	0.084	0.098
Isoprene	0.149	0.144	0.148	0.148	0.145	0.043	0.043	0.042	0.043	0.043
MVK/MACR/ ISOOH	0.115	0.116	0.138	0.118	0.116	0.039	0.039	0.136	0.035	0.039
MEK/MGLY (m/z 73)	0.018	0.021	0.022	0.019	0.026	0.017	0.040	0.017	0.018	0.015
Monoterpenes (m/z 137)	0.021	0.021	0.124	0.021	0.021	0.016	0.016	0.085	0.016	0.016
Monoterpenes (m/z 81)	0.011	0.011	0.108	0.011	0.011	0.014	0.014	0.069	0.014	0.014
Acetic acid	0.226	0.227	0.217	0.234	0.237	0.174	0.17	0.167	0.175	0.181
	Mean bias (ppb)									
	January					July				
	R0	S2	S3	S4	S5	R0	S2	S3	S4	S5
Formaldehyde	-0.394	-0.396	-0.376	-0.441	-0.45	-0.12	-0.112	-0.102	-0.136	-0.186
Methanol	0.177	0.304	0.575	0.176	0.172	0.199	0.368	0.557	0.201	0.202
Acetaldehyde	-0.073	-0.069	-0.073	-0.073	-0.128	-0.014	-0.008	-0.013	-0.013	-0.099
Acetone	-0.051	-0.053	-0.047	-0.051	-0.148	0.035	0.398	0.04	0.035	-0.032
Isoprene	-0.051	-0.046	-0.046	-0.042	-0.048	-0.008	-0.007	-0.007	-0.008	-0.008
MVK/MACR/ ISOOH	-0.010	-0.011	0.042	-0.024	-0.012	0.021	0.021	0.093	0.015	0.021
MEK/MGLY (m/z 73)	-0.001	0.003	-0.011	-0.001	-0.019	0.010	0.035	0.008	0.010	-0.004
Monoterpenes (m/z 137)	0.017	0.017	0.109	0.017	0.016	0.008	0.008	0.072	0.008	0.008
Monoterpenes (m/z 81)	-0.002	-0.002	0.091	-0.001	-0.002	-0.011	-0.011	0.053	-0.011	-0.011
Acetic acid	-0.177	-0.177	-0.168	-0.182	-0.187	-0.126	-0.12	-0.12	-0.127	-0.134

Table S5. Sources of acetaldehyde over Réunion Island (tons/month), including anthropogenic and biogenic emissions (R0), and secondary photochemical formation from precursor species in January and July.

Source	January	July
Anthropogenic emission	144	144
Biogenic emission	21	7
C ₂ H ₆ + OH	27.2	10.7
C ₃ H ₈ + OH	1.2	0.6
C ₃ H ₆ + OH/O ₃	20.3	8.5
BIGENE + OH	17.9	7.8
BIGALK + OH	6.1	2.3
MVK + O ₃	0.04	0.03
MEK + OH	5.5	2.3
C ₂ H ₅ OH + OH	23.0	13.3

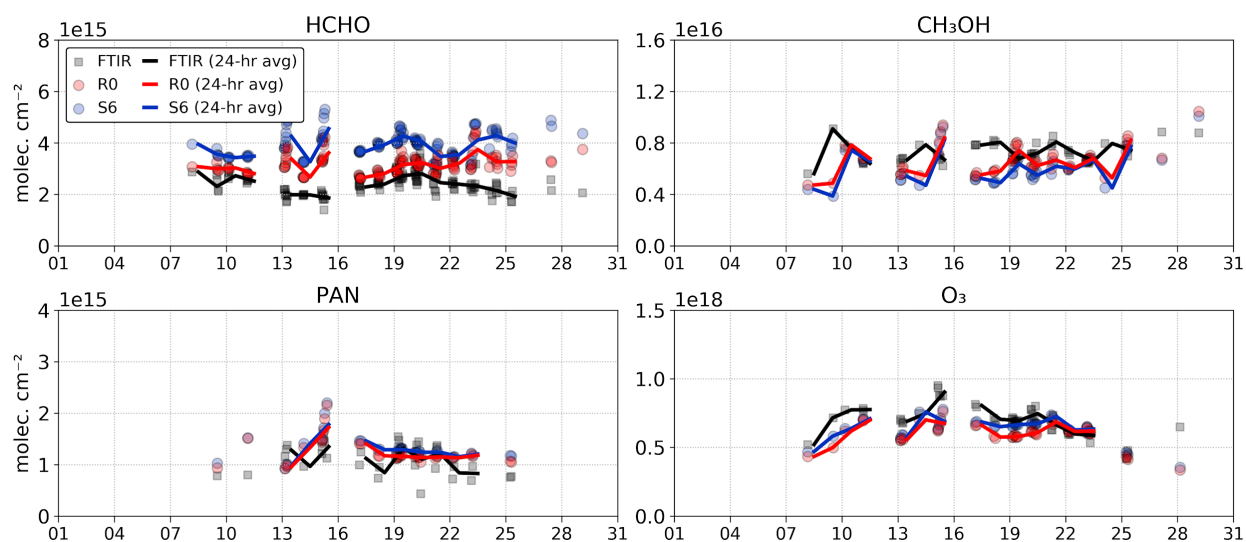


Figure S5. Time series of FTIR-measured and modelled HCHO, CH₃OH, PAN and O₃ tropospheric columns in January 2019. S6 includes NO_x emissions from lightning, which has a moderate influence on these four species, while the others shown in Fig. 15 are essentially unchanged (CO and C₂H₆).

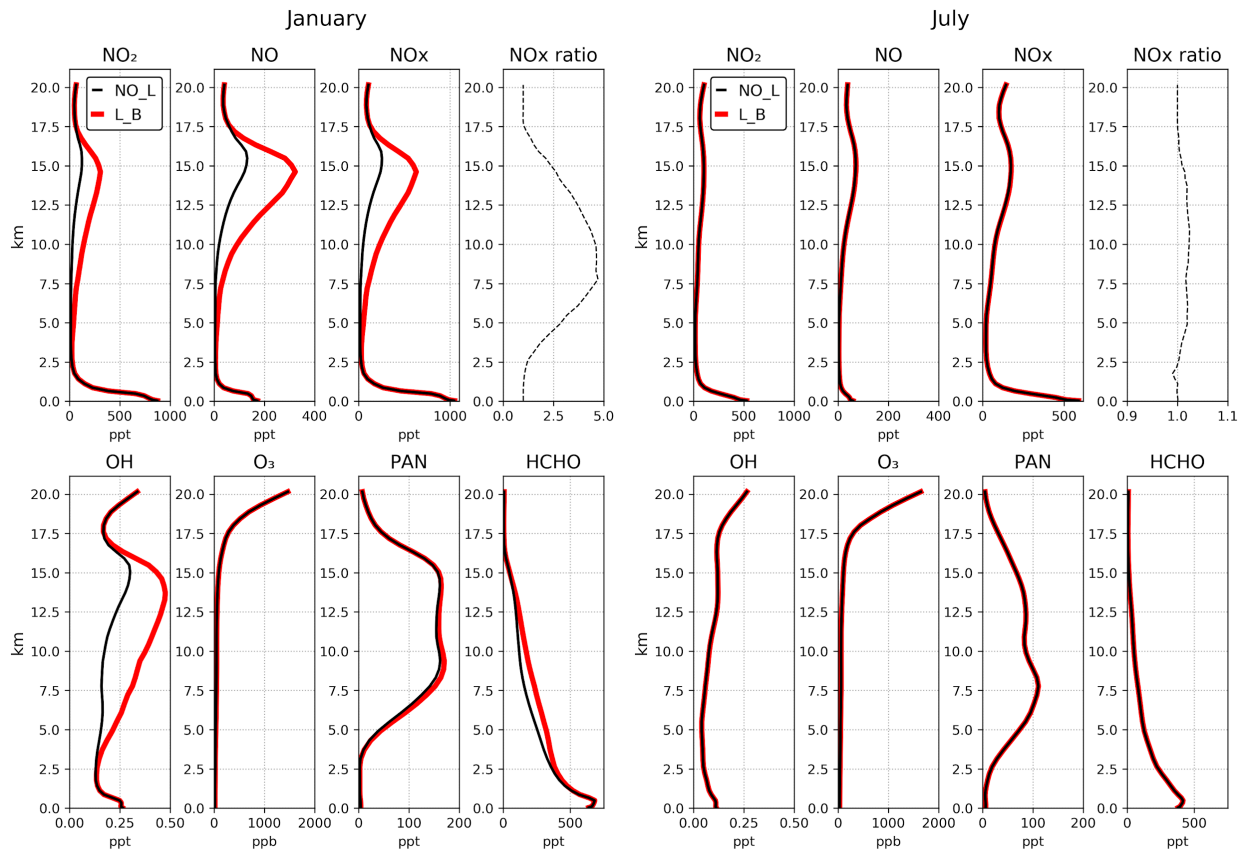


Figure S6. Monthly-averaged vertical profiles for NO_2 , NO , NO_x , OH , O_3 and PAN from WRF-Chem simulations using the R0 settings, with lightning turned off (black line, NO_L) and lightning turned on with the Barten et al. (2020) settings (red line, L_B). The NO_x ratio is obtained by dividing L_B NO_x by NO_L NO_x .

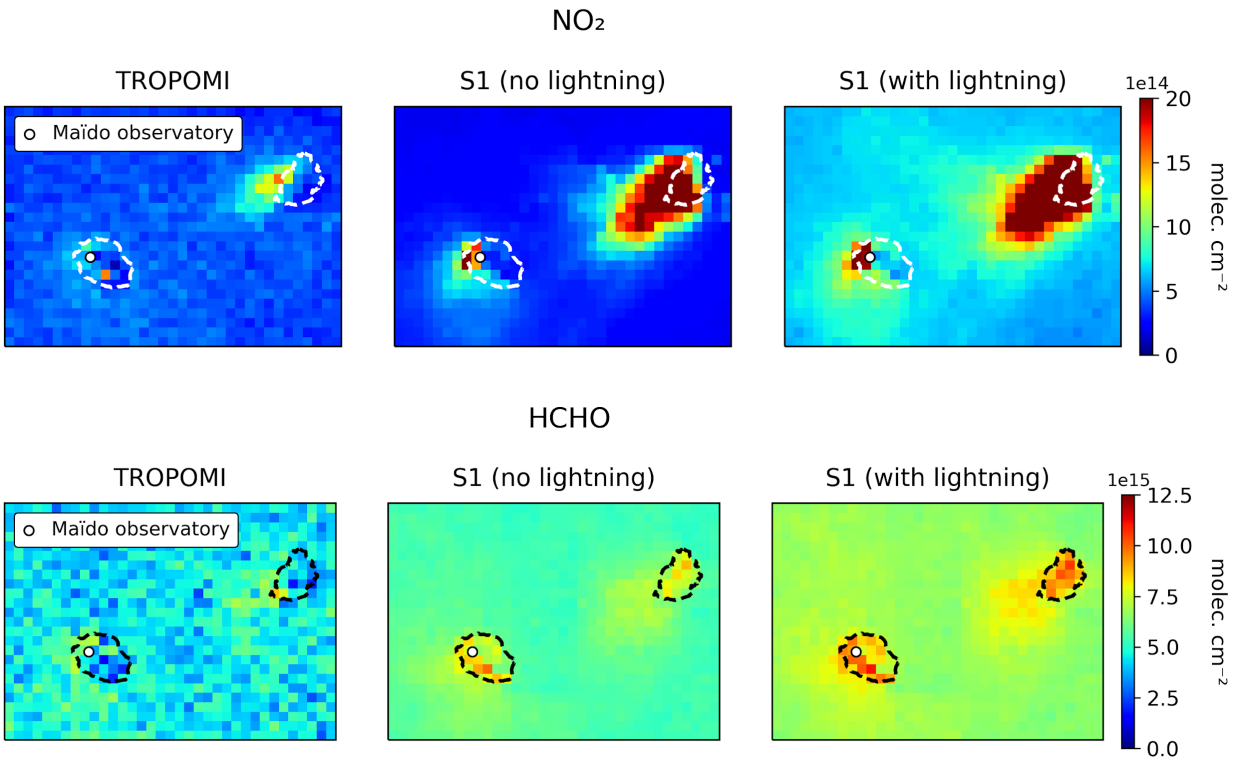


Figure S7. Monthly-averaged NO₂ and HCHO columns from TROPOMI and WRF-Chem simulation S1 for January, regridded to 0.1° resolution. S1 simulation was conducted without lightning (middle panel) and with lightning (right panel).

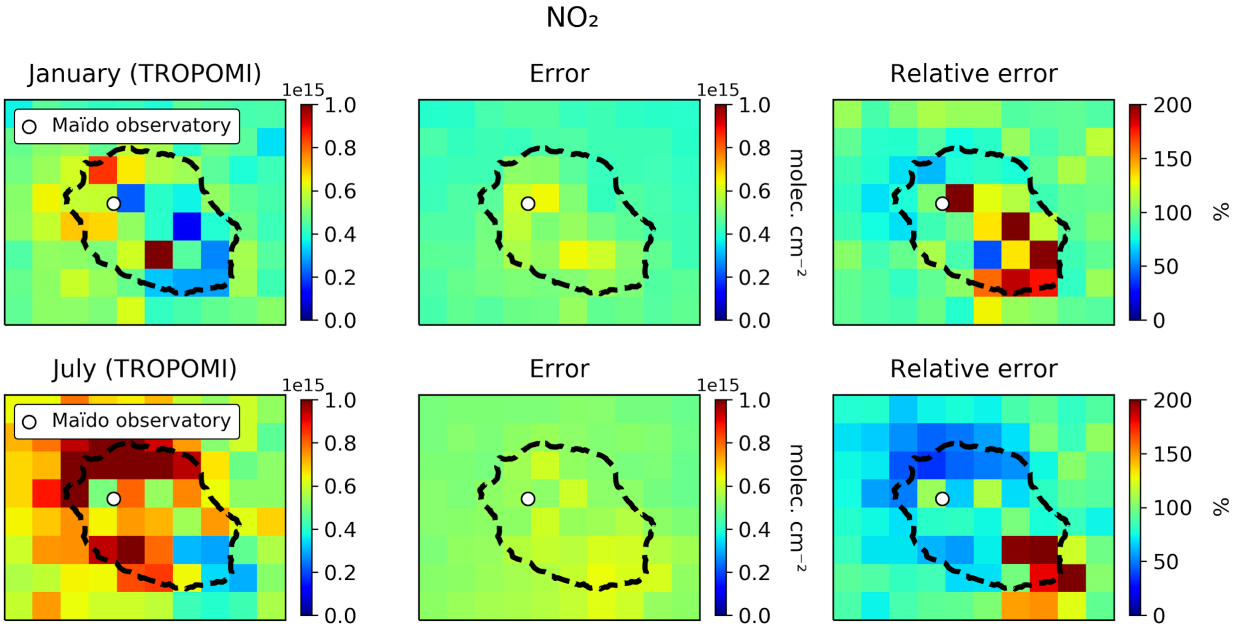


Figure S8. Monthly-averaged TROPOMI NO₂ column (left) and uncertainty (middle) in January and July, regridded to 0.1° resolution, in molec. cm⁻². The relative error is also shown (% , right panel). The NO₂ error excludes the component due to the vertical profile assumption in the retrieval, given that averaging kernels are used in the model comparisons with TROPOMI data.

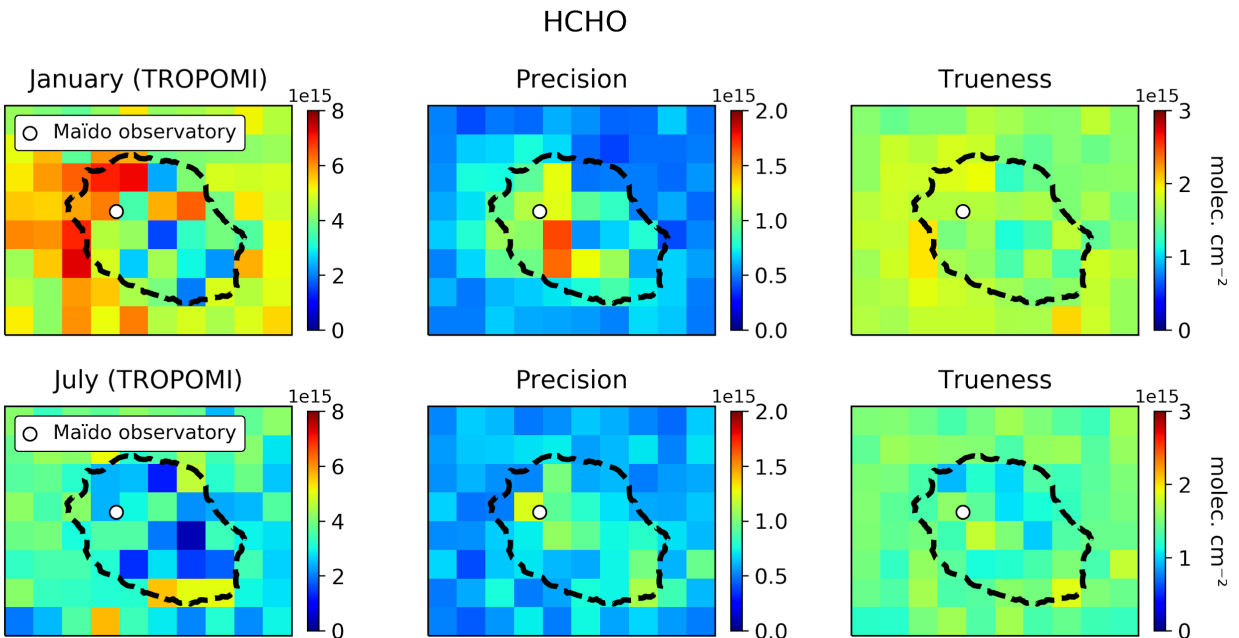


Figure S9. Monthly-averaged TROPOMI HCHO columns at 0.1° resolution (left), precision (mean pixel-level precision from TROPOMI divided by the square root of the number of data) and trueness, for January and July (molec. cm⁻²). The HCHO trueness excludes the component due to the vertical profile assumed in the retrieval, given that averaging kernels are used in the model comparisons with TROPOMI.