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Supplement of

Constraining the budget of NO_x and volatile organic compounds at a remote tropical island using multi-platform observations and WRF-Chem model simulations

Catalina Poraicu et al.

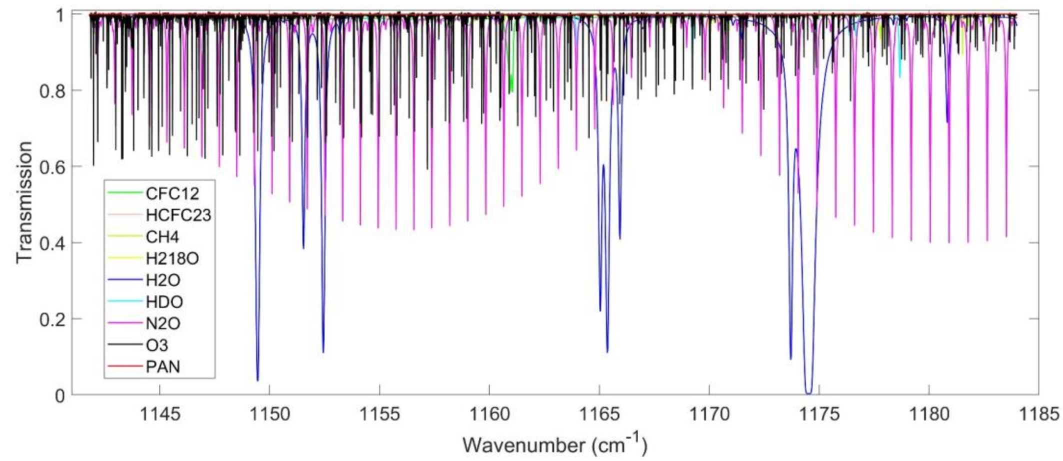
Correspondence to: Catalina Poraicu (catalina.poraicu@aeronomie.be)

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_3OH	1029.0–1037.0	HITRAN2012, except atm16 for H_2O lines	Vigouroux et al. (2012)	2%	17%
C_2H_6	2976.66–2977.059 2983.2–2983.6	C_2H_6 PLL[a] CH_3Cl: 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_2O lines	Vigouroux et al. (2015)	10%	3%
PAN	1141.8–1184.0	PAN, HFC-23 and CFC-12: pseudo-linelists[a] HITRAN 2012 for other species	This work	6%	20%

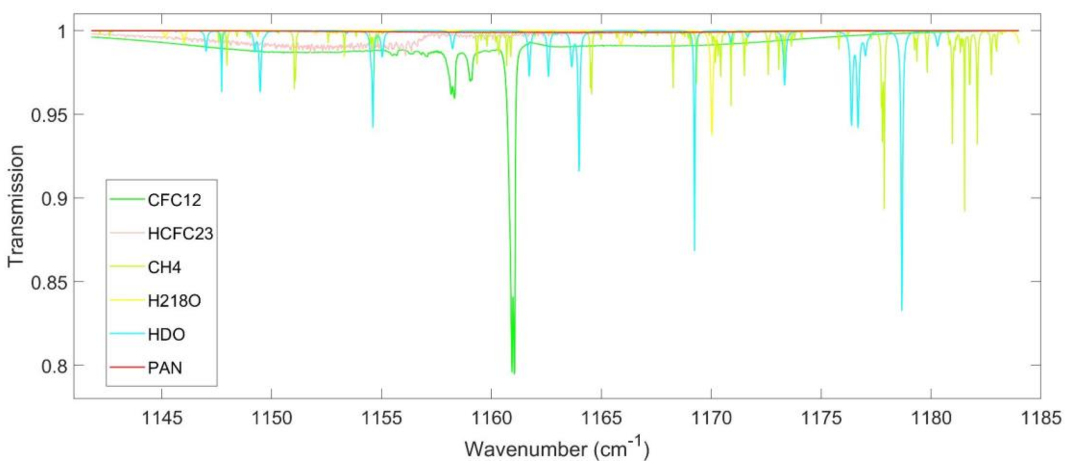
[a]http://mark4sun.jpl.nasa.gov/pseudo.html

(a)



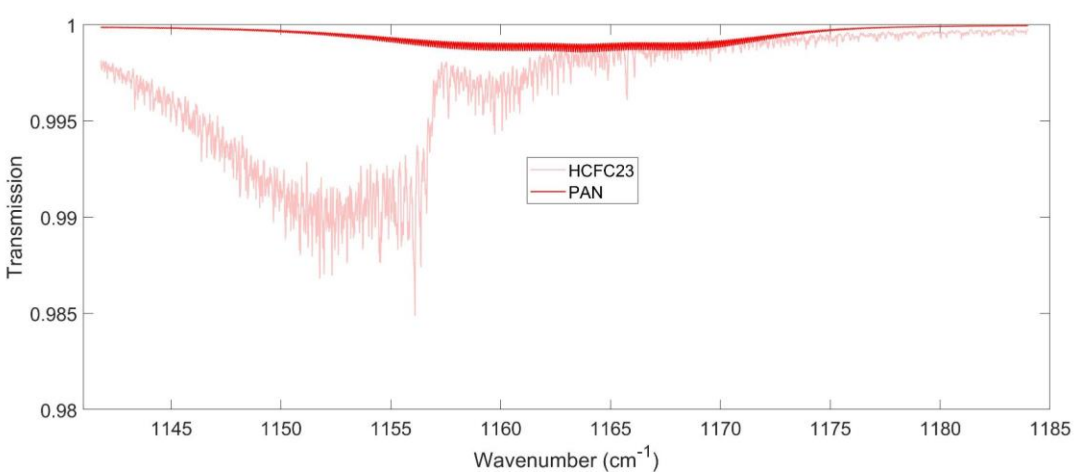
Transmission
Wavenumber (cm^{-1})
0
0.2
0.4
0.6
0.8
1
1145
1150
1155
1160
1165
1170
1175
1180
1185
CFC12
HCFC23
CH4
H218O
H2O
HDO
N2O
O3
PAN

(b)



Transmission
Wavenumber (cm^{-1})
0.8
0.85
0.9
0.95
1
1145
1150
1155
1160
1165
1170
1175
1180
1185
CFC12
HCFC23
CH4
H218O
HDO
PAN

(c)



Transmission
Wavenumber (cm^{-1})
0.98
0.985
0.99
0.995
1
1145
1150
1155
1160
1165
1170
1175
1180
1185
HCFC23
PAN

(d)

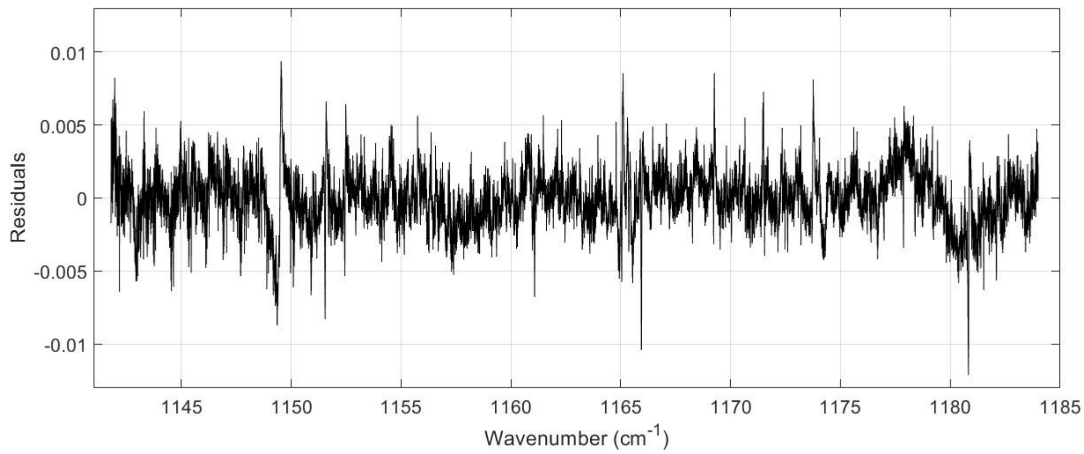


Figure S1. a, b, c) Retrieved spectral signatures for a retrieved PAN column of 5.64×10^{14} molec cm^{-2}. Panel (b) and (c) are zoomed-out versions of panel (a) for different subsets of compounds, to show the relative strength of absorbing gases. (d) Spectral residuals (calculated – observed) for the 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 (µg m^{-3}) measured at the air quality stations.

		Daytime (8:00 - 16:00 LT)			Nighttime (20:00 - 03:00 LT)		
#		NO_2	NOx	O_3	NO_2	NOx	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

Table S4. Statistics of model performance (Perason's correlation coefficient, root mean square error and index of agreement) against NO_2, NOx and O_3 in situ concentrations measured at the air quality stations.

NO_2				
		January		
#	Station	Correlation coefficient	Root mean square error (RMSE) (µg m^{-3})	Index of agreement (IOA)
1	Terrain de Sel	0.116	26.643	0.249
2	Centre Pénitentiaire	0.149	17.500	0.295
3	Lislet Geoffroy	0.357	4.594	0.594
4	Sarda Garriga	0.145	7.097	0.379
5	Joinville	0.351	4.620	0.585
6	La Marine	0.318	5.461	0.524
7	Plateau Caillou	0.396	7.359	0.489
8	Grand Fond	0.393	5.204	0.615

9	Paradis	0.424	10.751	0.470
10	Route des Tamarins	0.304	10.094	0.461
11	Boulevard Banks	0.144	12.312	0.450
12	Luther King	0.157	8.037	0.483
		July		
#	Station	Correlation coefficient	Root mean square error (RMSE)	Index of agreement (IOA)
1	Terrain de Sel	-0.338	39.321	0.202
2	Centre Pénitentiaire	0.491	20.736	0.571
3	Lislet Geoffroy	0.598	9.319	0.759
4	Sarda Garriga	0.634	6.333	0.716
5	Joinville	0.649	7.639	0.770
6	La Marine	0.537	5.668	0.721
7	Plateau Caillou	0.509	7.178	0.662
8	Grand Fond	0.375	8.418	0.553
9	Paradis	0.463	13.575	0.597
10	Route des Tamarins	0.388	18.284	0.571
11	Boulevard Banks	0.542	19.374	0.573
12	Luther King	0.443	15.348	0.541
NOx				
		January		
#	Station	Correlation coefficient	Root mean square error (RMSE)	Index of agreement (IOA)
1	Terrain de Sel	0.053	41.687	0.289
2	Centre Pénitentiaire	-0.037	24.997	0.338
3	Lislet Geoffroy	0.369	7.428	0.580
4	Sarda Garriga	-0.104	20.510	0.202
5	Joinville	0.356	7.038	0.580
6	La Marine	0.223	8.671	0.450
7	Plateau Caillou	0.323	7.948	0.539
8	Grand Fond	0.346	6.521	0.595
9	Paradis	0.142	13.607	0.456
10	Route des Tamarins	0.256	62.468	0.439
11	Boulevard Banks	0.027	41.521	0.420
12	Luther King	-0.118	30.077	0.404
		July		
#	Station	Correlation coefficient	Root mean square error (RMSE)	Index of agreement (IOA)
1	Terrain de Sel	-0.337	53.953	0.185
2	Centre Pénitentiaire	0.446	26.104	0.663
3	Lislet Geoffroy	0.541	17.902	0.618
4	Sarda Garriga	0.521	7.997	0.700
5	Joinville	0.605	10.551	0.747
6	La Marine	0.483	8.433	0.634
7	Plateau Caillou	0.160	22.904	0.477
8	Grand Fond	0.308	12.801	0.517

9	Paradis	0.390	43.760	0.424
10	Route des Tamarins	0.393	51.952	0.425
11	Boulevard Banks	0.530	63.359	0.459
12	Luther King	0.470	41.972	0.457
O_3				
		January		
#	Station	Correlation coefficient	Root mean square error (RMSE)	Index of agreement (IOA)
5	Joinville	0.580	10.981	0.673
6	La Marine	0.466	15.608	0.575
7	Plateau Caillou	0.603	13.241	0.690
8	Grand Fond	0.504	20.806	0.480
9	Paradis	0.630	15.343	0.655
12	Luther King	0.570	22.642	0.544
		July		
#	Station	Correlation coefficient	Root mean square error (RMSE)	Index of agreement (IOA)
5	Joinville	0.645	14.767	0.706
6	La Marine	/	/	/
7	Plateau Caillou	0.517	17.268	0.607
8	Grand Fond	0.558	16.923	0.619
9	Paradis	0.701	18.482	0.675
12	Luther King	0.556	29.163	0.523

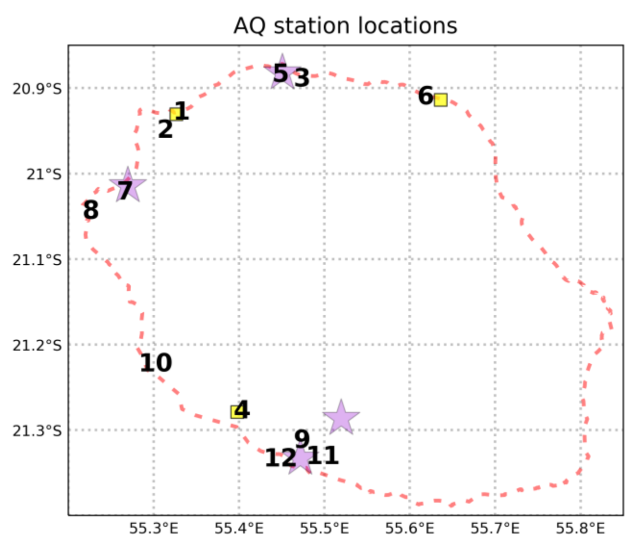


Figure S2. Geographical locations of 12 stations in Table S3. The purple stars and yellow squares represent the most populated cities and power plant locations, respectively, similar to Fig. 2 in the main paper.

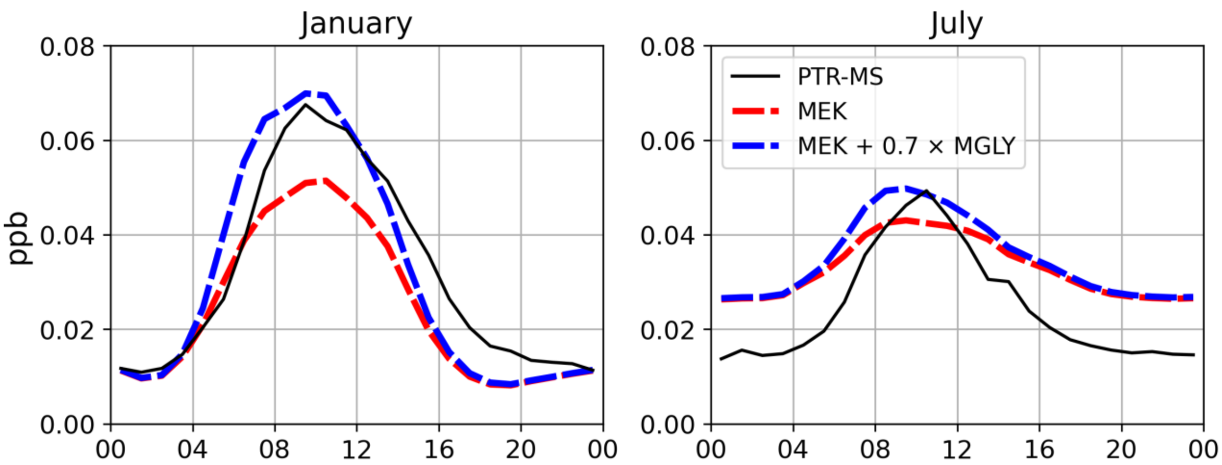


Figure S3. Average diurnal cycle of measured and modelled MEK, omitting (red) and including the MGLY interference (blue).

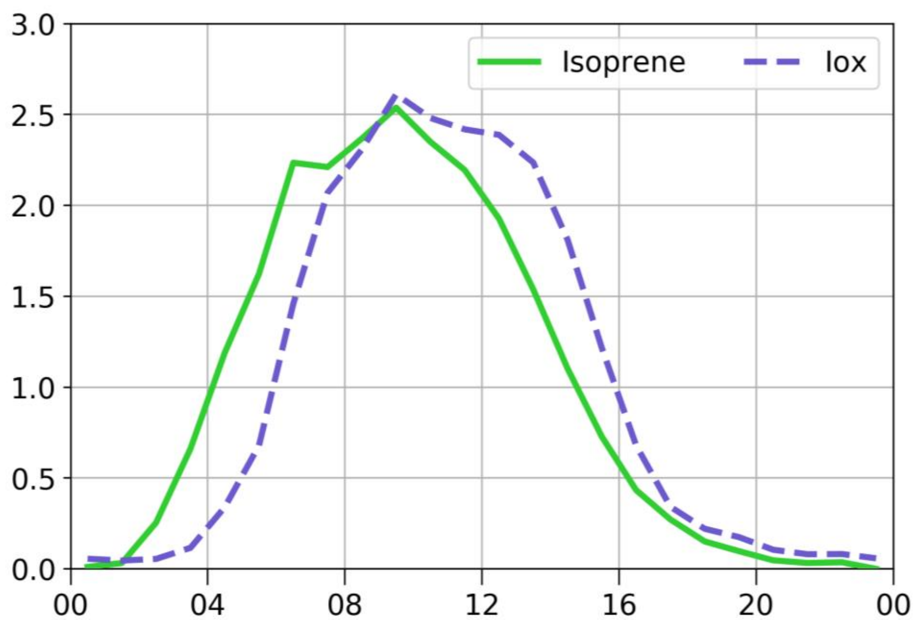


Figure S4. Average diurnal cycle of observed isoprene (green) and Iox mixing ratios (purple), normalized by their respective means, for the month of January.

Table S5: 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 S6. 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_2H_6 + OH	27.2	10.7
C_3H_8 + OH	1.2	0.6
C_3H_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_2H_5OH + OH	23.0	13.3

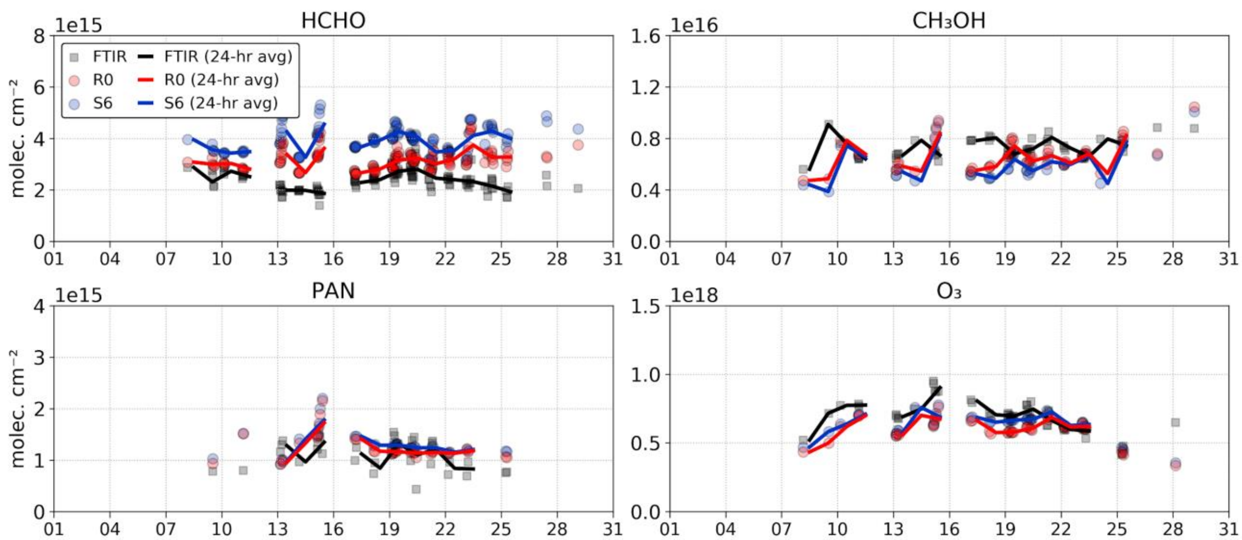


Figure S5. Time series of FTIR-measured and modelled HCHO, CH_3OH, PAN and O_3 tropospheric columns in January 2019. S6 includes NOx emissions from lightning, which has a moderate influence on these four species, while the others shown in Fig. 15 are essentially unchanged (CO and C_2H_6).

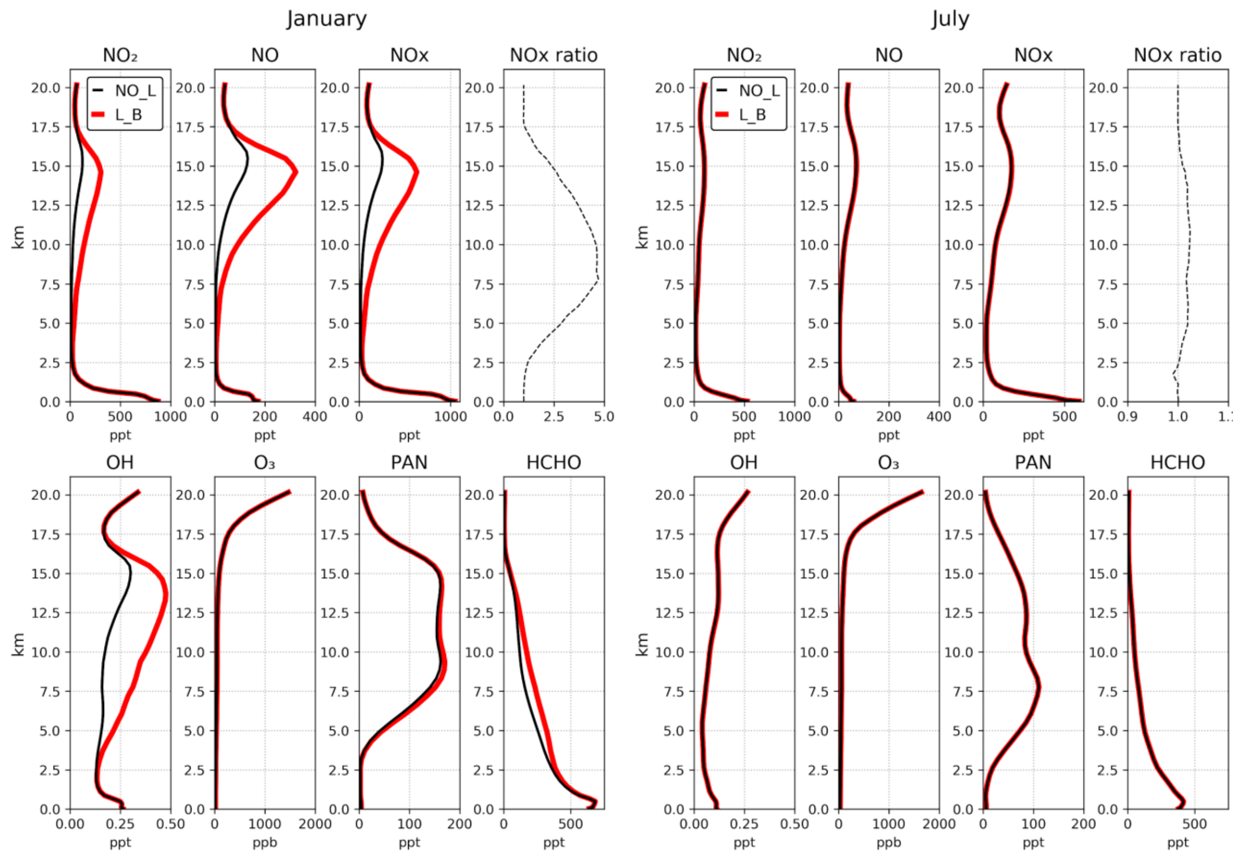


Figure S6. Monthly-averaged vertical profiles for NO_2, NO, NOx, OH, O_3 and PAN from WRF-Chem simulations using the R0 settings, with lightning turned off (black line, NO_L) and lightning turned on with the Barten et al. (2020) settings (red line, L_B). The NOx ratio is obtained by dividing L_B NOx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

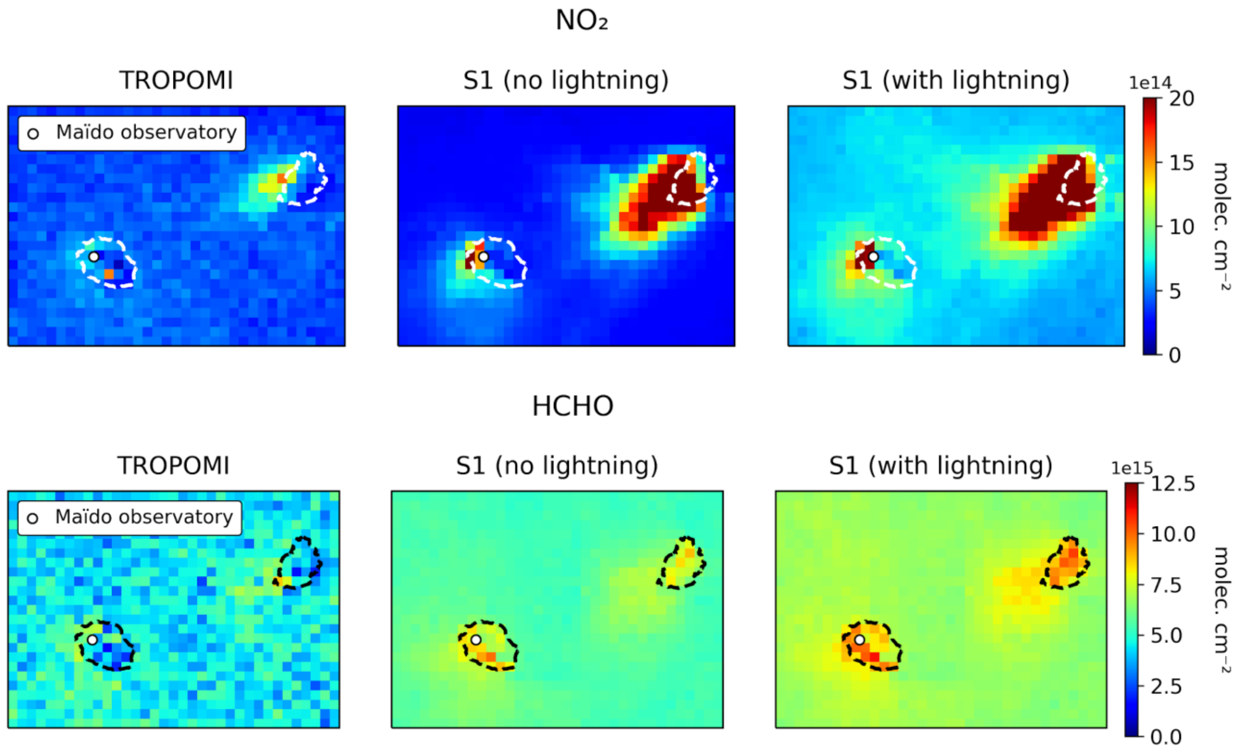


Figure S7. Monthly-averaged NO_2 and HCHO columns from TROPOMI and WRF-Chem simulation S1 for January, regridded to 0.1° resolution. S1 simulation was conducted without lightning (middle panel) and with lightning (right panel).

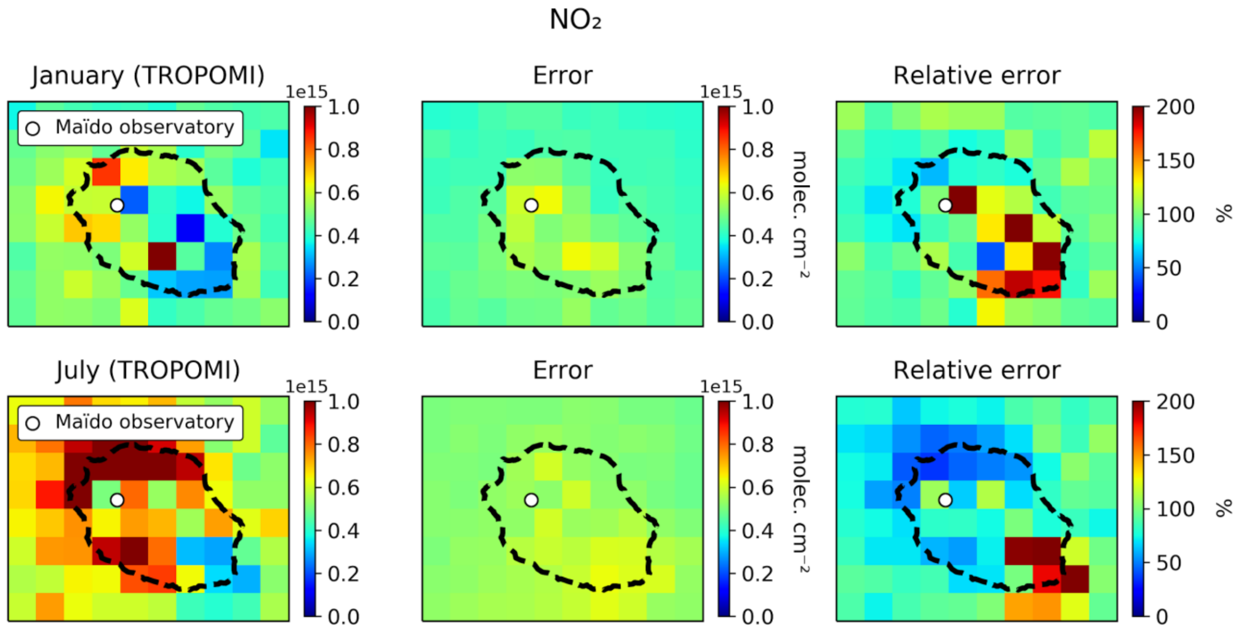


Figure S8. Monthly-averaged TROPOMI NO_2 column (left) and uncertainty (middle) in January and July, regridded to 0.1° resolution, in molec. cm^{-2}. The relative error is also shown (%, right panel). The NO_2 error excludes the component due to the vertical profile assumption in the retrieval, given that averaging kernels are used in the model comparisons with TROPOMI data.

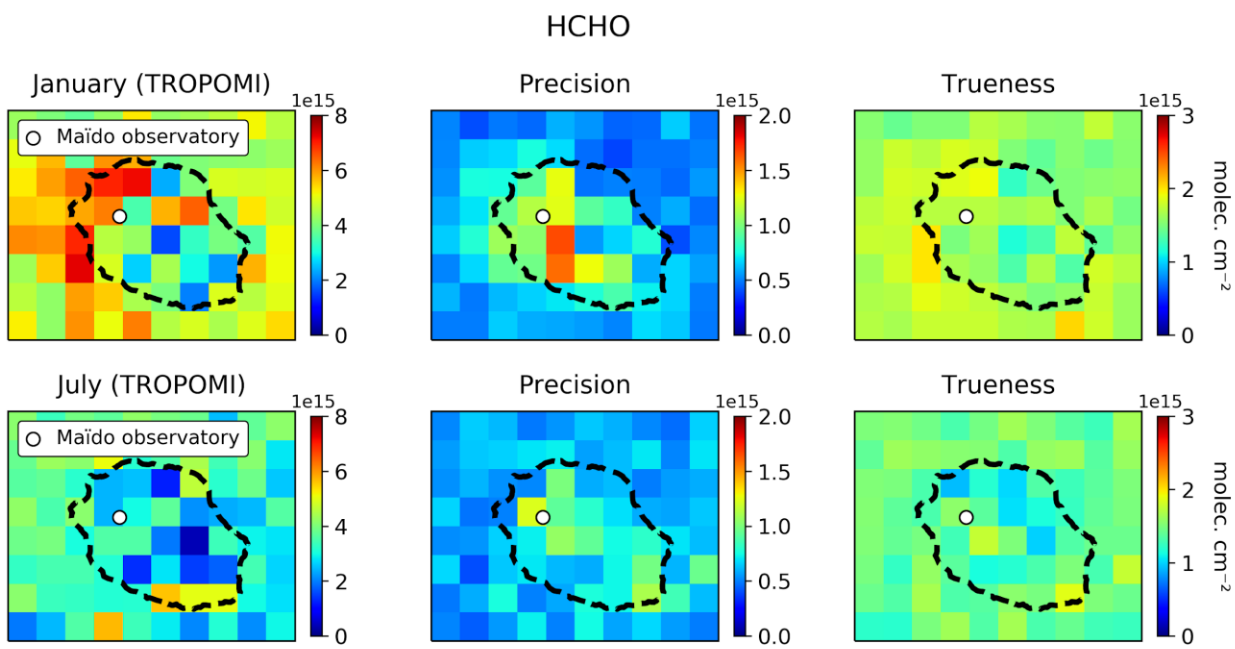


Figure S9. Monthly-averaged TROPOMI HCHO columns at 0.1° resolution (left), precision (mean pixel-level precision from TROPOMI divided by the square root of the number of data) and trueness, for January and July (molec. cm^{-2}). The HCHO trueness excludes the component due to the vertical profile assumed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