Supplement of Atmos. Chem. Phys., 25, 7087–7109, 2025
https://doi.org/10.5194/acp-25-7087-2025-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Comparative ozone production sensitivity to NO_x and VOCs in Quito, Ecuador, and Santiago, Chile

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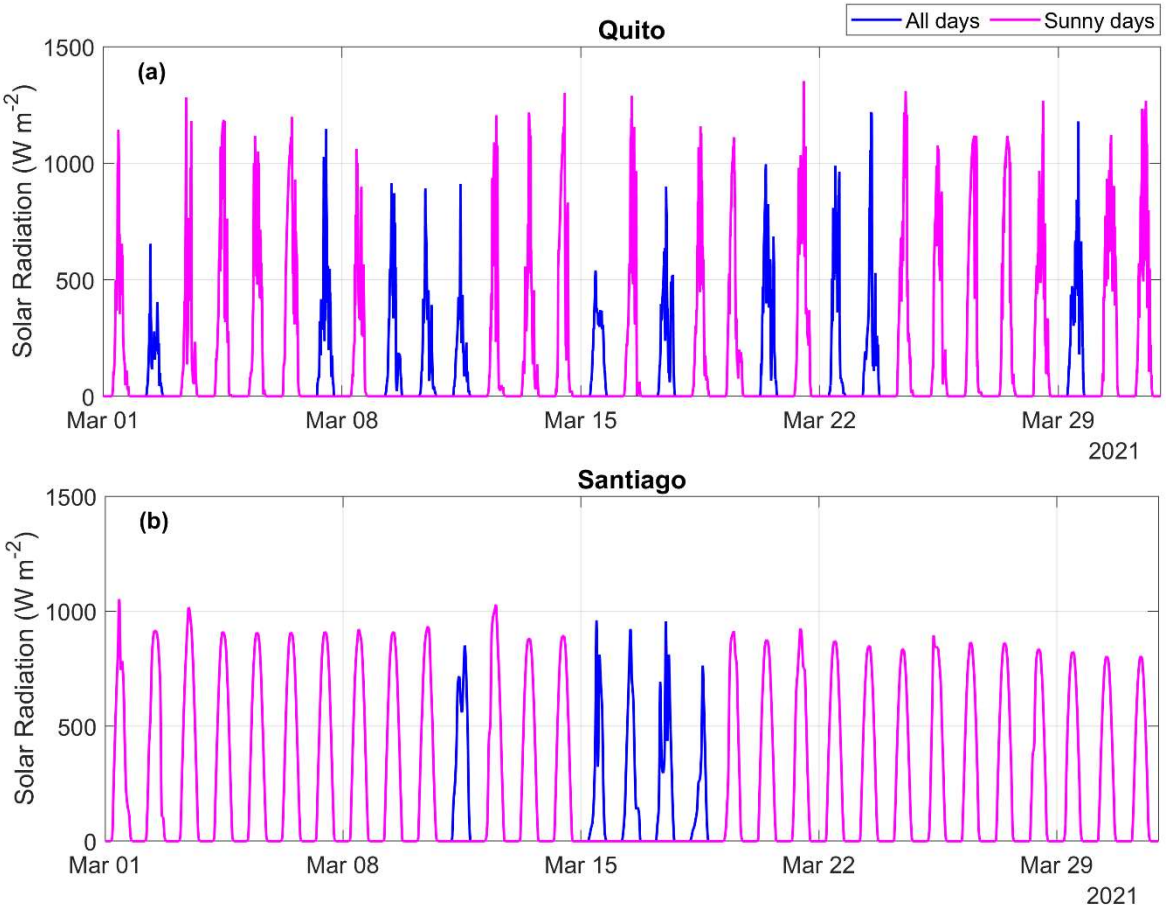

Figure S1. 10-minute time series of solar radiation in Quito and Santiago overlapping sunny days to all days.

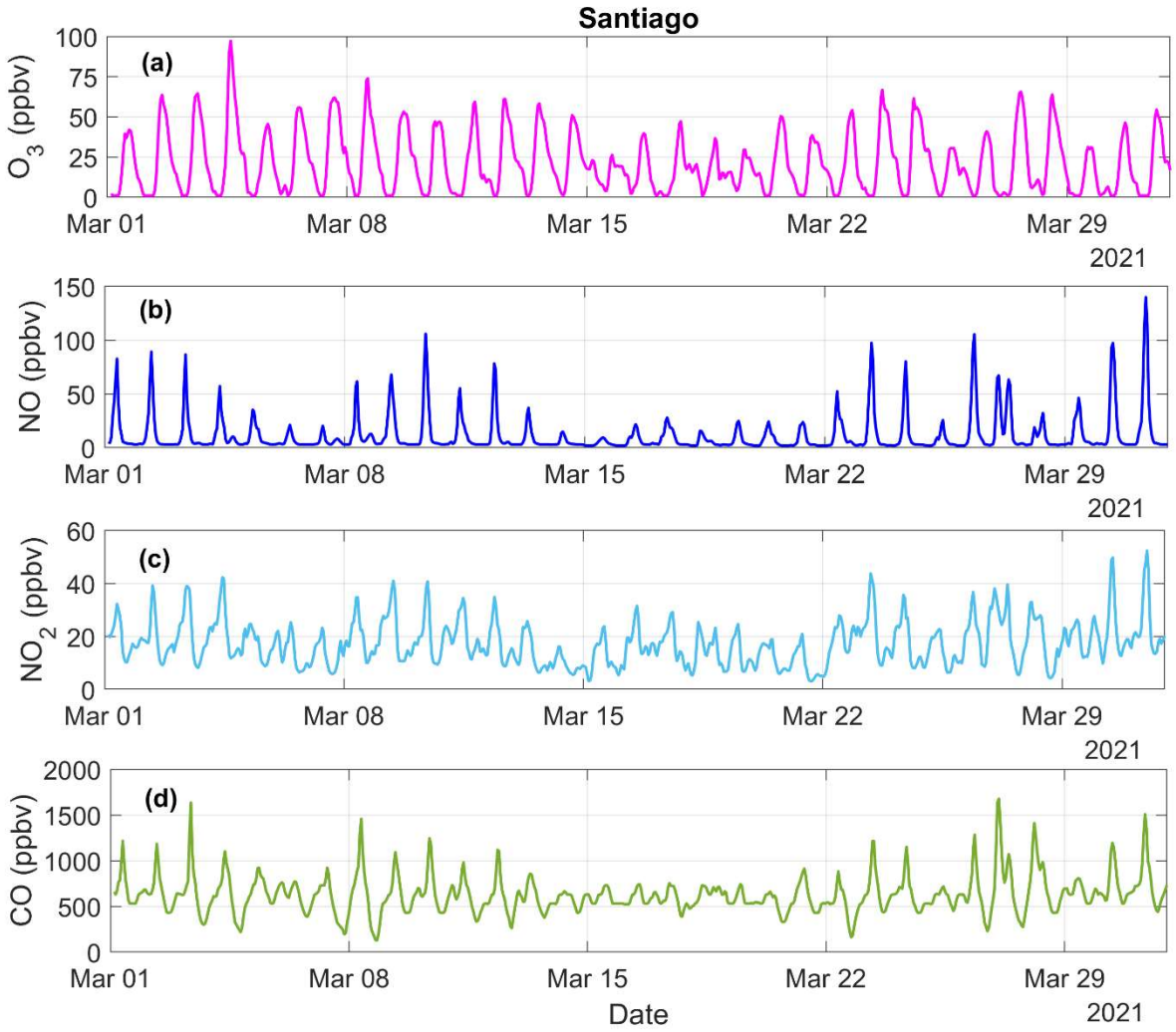

Figure S2. 1-hour air quality time series for Santiago (O'Higgins Station).

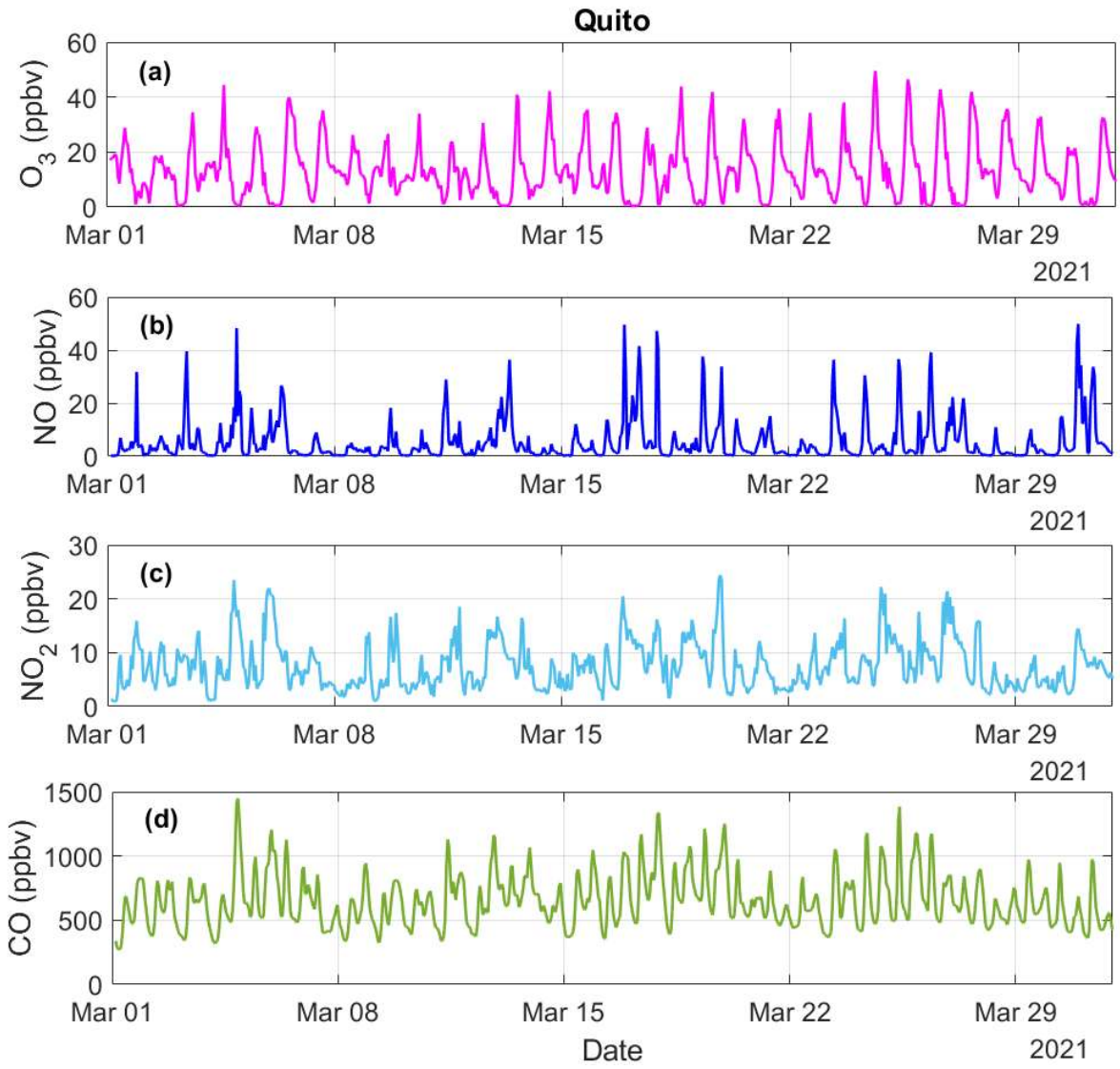

Figure S3. 1-hour air quality time series for Quito. Ozone, NO, and NO_2 are from EMA USFQ station. CO was obtained by averaging data from Belisario, Centro and Tumbaco stations from the Quito Air Quality Network (Secretariat of the Environment, Quito, Ecuador, https://aireambiente.quito.gob.ec/).

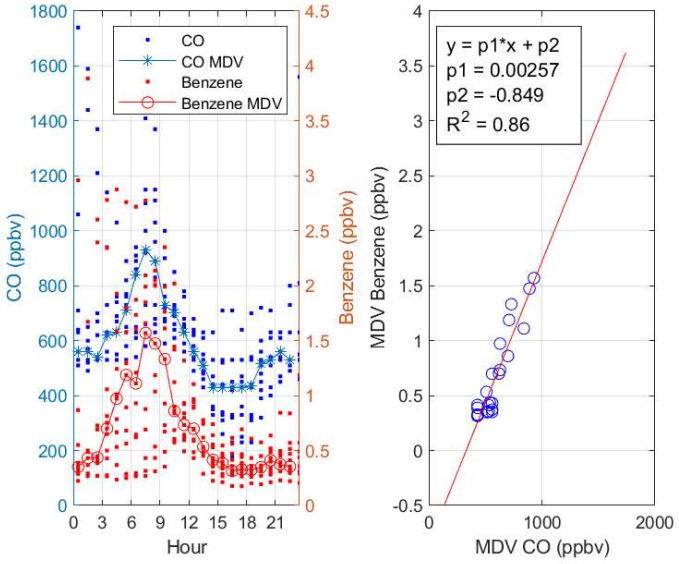

Figure S4. Left panel: Santiago 1-hour measurements and mean diurnal variation of CO (blue dots and blue line with stars) and benzene (red dots and red line with circles). Right panel: linear regression of the mean diurnal variations of benzene vs. CO.

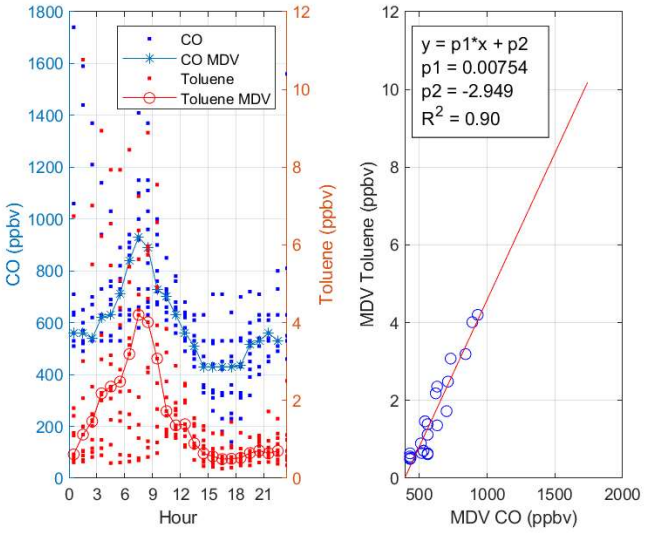

Figure S5. Left panel: Santiago 1-hour measurements and mean diurnal variation of CO (blue dots and blue line with stars) and toluene (red dots and red line with circles). Right panel: linear regression of the mean diurnal variations of toluene vs. CO.

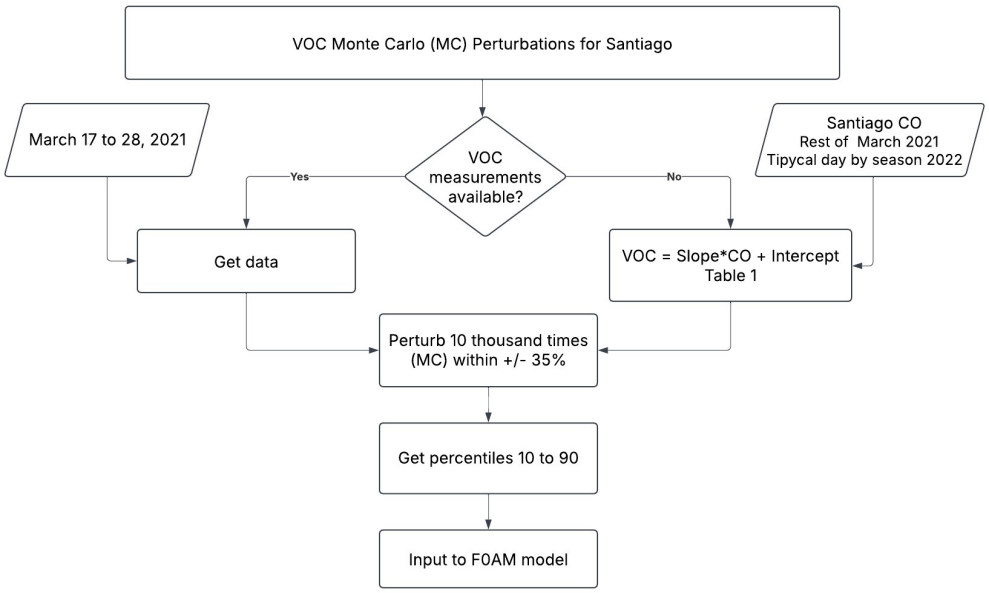

Figure S6. Flow diagram followed to perturb VOCs in Santiago.

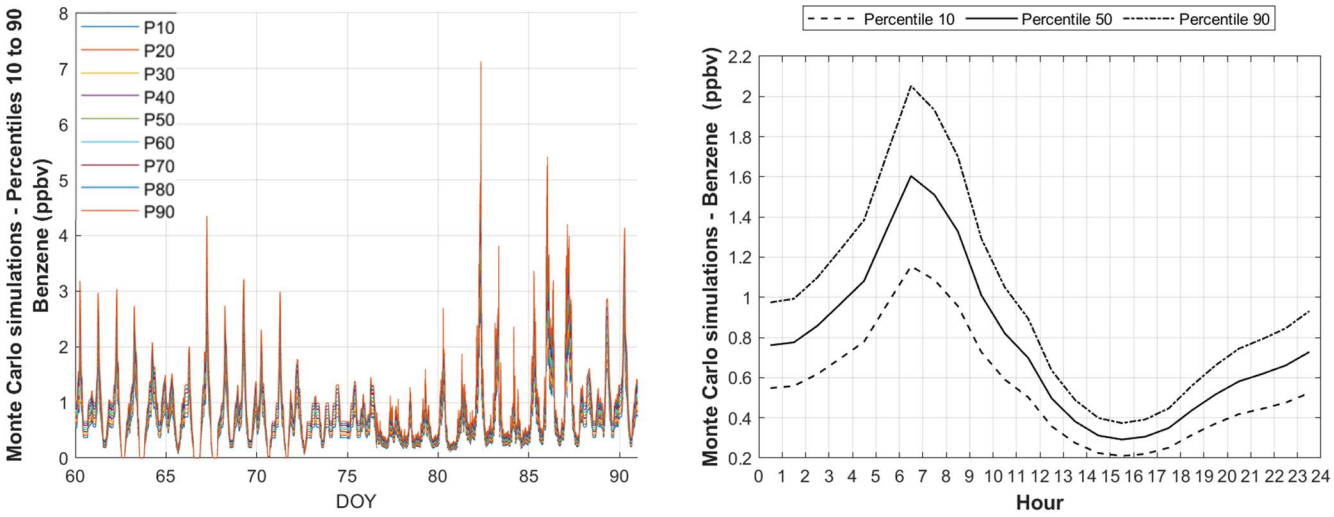

Figure S7. Monte Carlo simulations for benzene for Santiago. Left panel: 10-minute time series for percentiles 10 to 90. Right panel: mean diurnal variation for percentiles 10, 50 and 90.

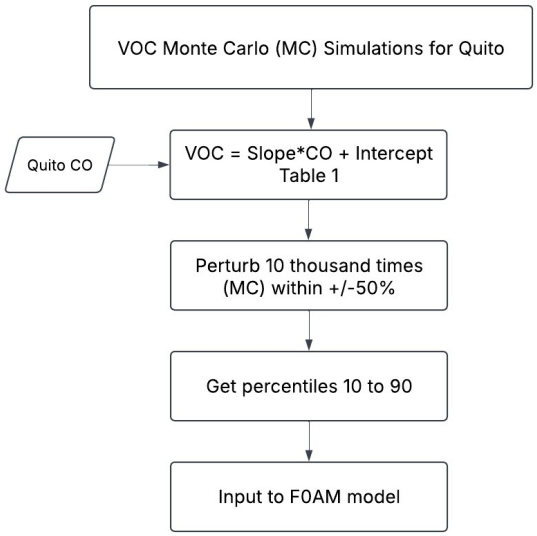

Figure S8. Flowchart synthesizing the method applied to simulate VOCs for Quito.

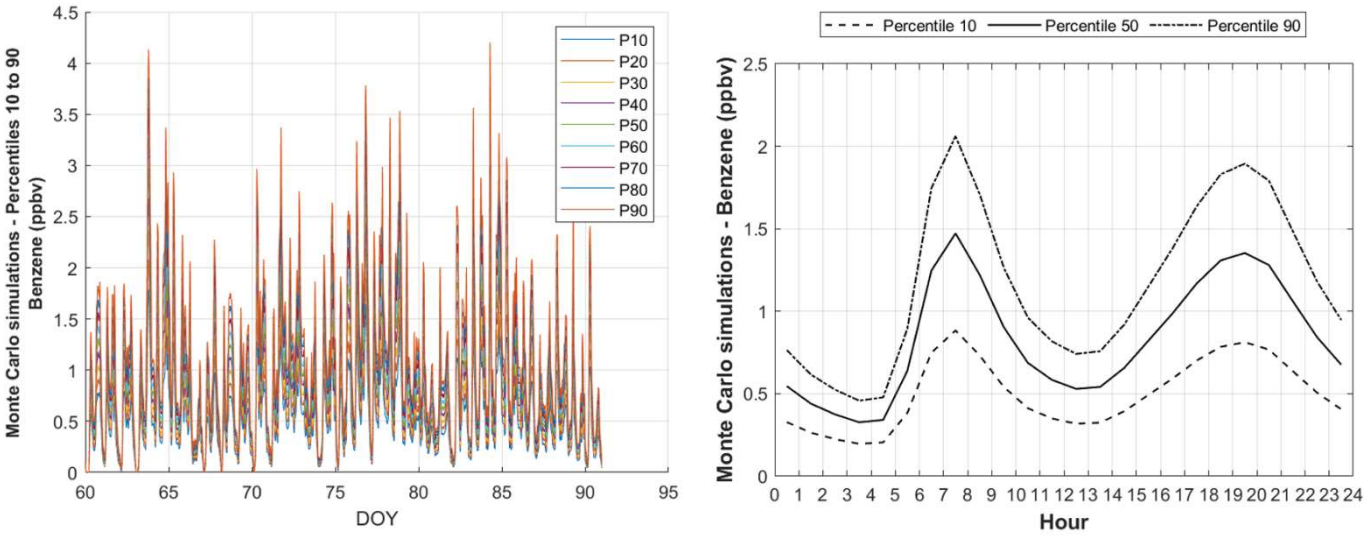

Figure S9. Monte Carlo simulations for benzene for Quito. Left panel: 10-minute time series for percentiles 10 to 90. Right panel: mean diurnal variation for percentiles 10, 50 and 90.

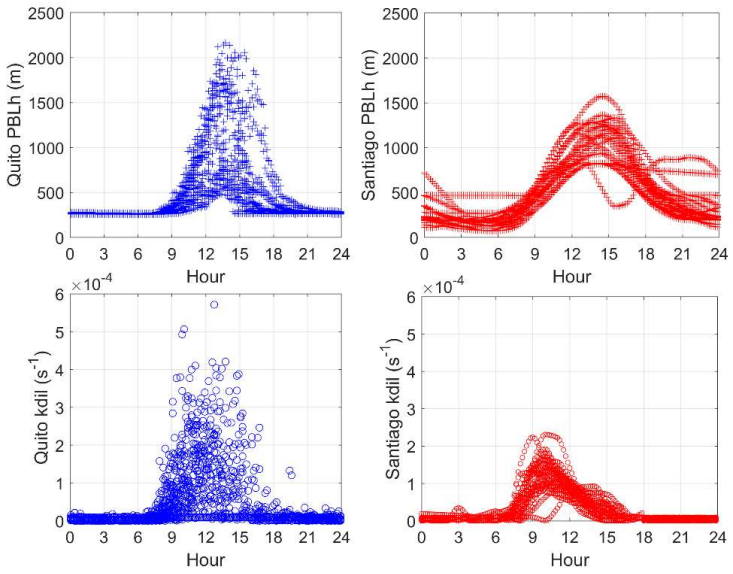

Figure S10. Boundary layer depth (PBLh) for Quito and Santiago (top panels) and first order dilution constant for the F0AM model (kdil) for both cities (bottom panels).

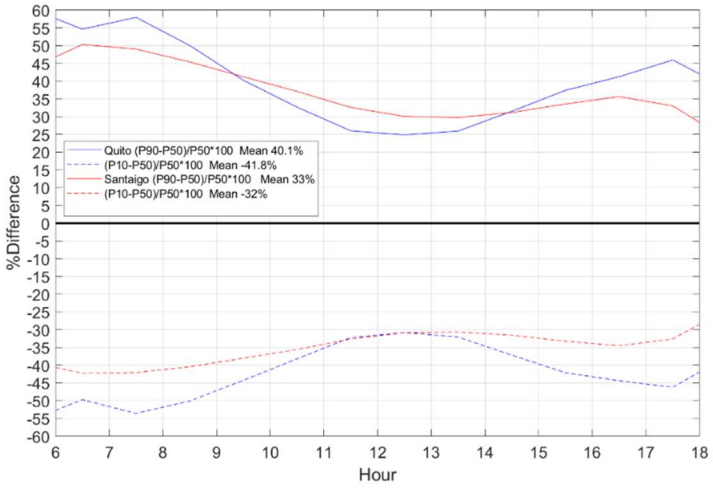

Figure S11. Ozone production P(O_3) percentage differences from Figure 7a.

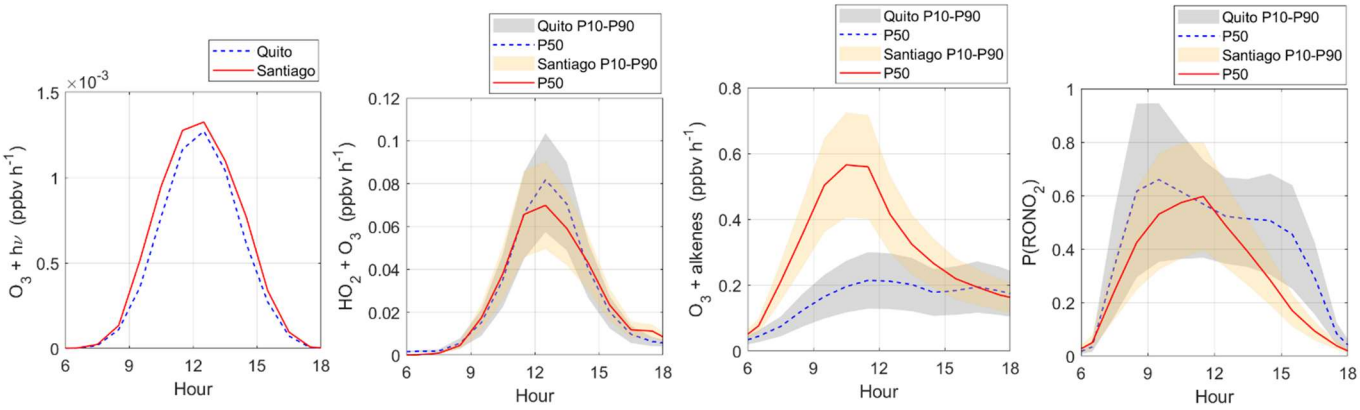

Figure S12. Left to right: ozone losses due to ozone photolysis, ozone reaction with HO_2, ozone reaction with alkenes, and losses to $P(RONO_2)$ for Quito and Santiago.

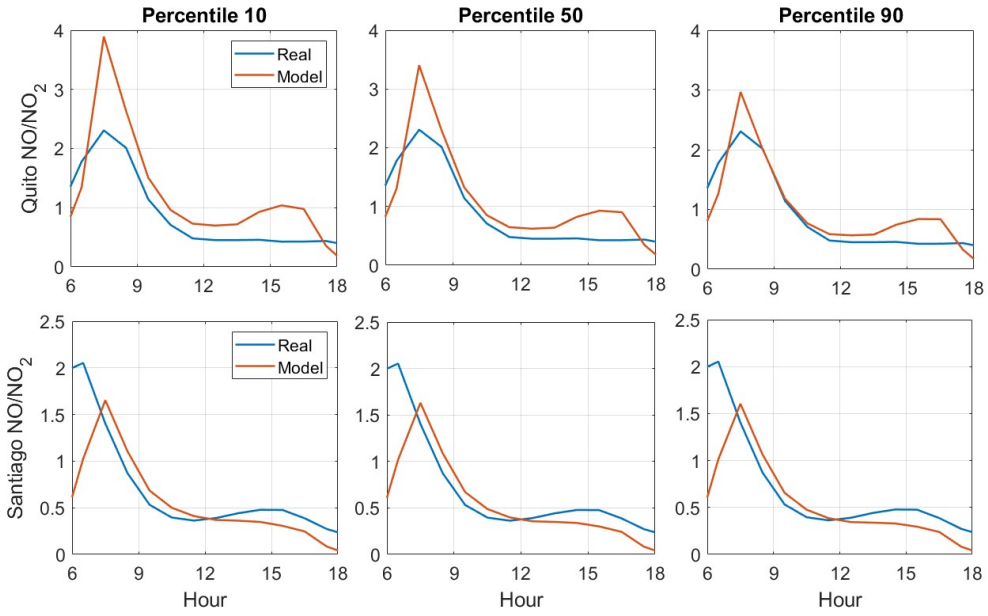

Figure S13. NO/NO_2 ratio for Quito and Santiago comparing the real data (blue) versus the unconstrained scenario from the model (orange).

Table S1. Linear regressions obtained for measured VOCs in Santiago using both methods

		VOC regressions for Santiago (ppbv)					
Group	Compound	Method 1: Original regression using mean diurnal cycles			Method 2: Regression with nighttime data and w/o background CO		
		Slope	Intercept	R^2	Slope	Intercept	R^2
ALK	Propene	0.00746	-2.467	0.87	0.00467	0.738	0.58
	Butene	0.00966	-3.066	0.84	0.00608	0.826	0.62
ARO	Benzene	0.00257	-0.849	0.86	0.00215	0.096	0.74
	Toluene	0.00754	-2.949	0.90	0.00543	0.138	0.60
	Ethylbenzene (C8)	0.01573	-6.437	0.83	0.01026	-0.104	0.66
	Styrene (C8)	0.00096	-0.243	0.87	0.00062	0.151	0.73
	C8 (sum)	0.01664	-6.646	0.84	0.01089	0.047	0.66
	C9 Aromatics	0.00364	-1.466	0.90	0.00222	0.059	0.73
OXY	Methanol	0.01959	-5.099	0.87	0.01597	2.365	0.65
	Ethanol	0.00487	-2.227	0.87	0.00313	-0.222	0.67
	Phenol	0.00098	-0.016	0.84	0.00066	0.406	0.68
	Cresol	0.00019	0.229	0.25	0.00029	0.266	0.45
ALD	Acetaldehyde	0.01222	-1.008	0.58	0.08050	3.349	0.62
	Acetic acid	0.01470	-2.062	0.59	0.00678	4.155	0.28
	Acetone	0.00506	2.623	0.32	0.00857	3.333	0.61
	Butanone	0.00467	-1.300	0.73	0.00298	0.599	0.61
	Methacrolein	0.00088	0.211	0.74	0.00090	0.556	0.60
ISO	Isoprene	0.00079	0.325	0.49	0.00088	0.575	0.56
	Monoterpenes	0.00066	-0.143	0.82	0.00041	0.164	0.57

Table S2: VOC compounds used in the model with the measurement nomenclature and the attributed weighing factors

Group	Measured Compounds	MCM Nomenclature	Name	Attributed Factor
ALK	Propene/Cyclopropane	C3H6	Propene	1
	1- Butene/2-Butene	BUT1ENE	1-butene	0.288
		CBUT2ENE	Cis-2-butene	0.356
		TBUT2ENE	Trans-2-butene	0.356
ARO	Benzene	BENZENE	Benzene	1
	Toluene	TOLUENE	Toluene	1
	Styrene	STYRENE	Styrene	1
	Ethyl benzene/Xylenes	EBENZ	Ethylbenzene	0.195
		OXYL	O-xylene	0.241
		MXYL	M-xylene	0.282
		PXYL	P-xylene	0.282
	C9-Aromatics	PBENZ	Propylbenzene	0.077
		IPBENZ	Isopropylbenzene	0.026
		TM123B	1,2,3-trimethylbenzene	0.109
		TM124B	1,2,4-trimethylbenzene	0.202
		TM135B	1,3,5-trimethylbenzene	0.099
		OETHTOL	2-ethyltoluene	0.090
		METHTOL	3-ethyltoluene	0.251
		PETHTOL	4-ethyltoluene	0.104
ALD	Acetaldehyde	CH3CHO	Acetaldehyde	1
	Methacrolein/MVK	MACR	Methacrolein	1
		MVK	Methyl Vinyl Ketone	1
	Butanone / Butanal	MEK	Butanone	1
		C3H7CHO	Butanal	1
	Acetone / Propanal	CH3COCH3	Acetone	1
		C2H5CHO	Propanal	1
OXY	Acetic Acid / Glycolaldehyde	CH3CO2H	Acetic acid	1
		HOCH2CHO	Glycolaldehyde	1
	Methanol	CH3OH	Methanol	1
	Ethanol	C2H5OH	Ethanol	1
	Phenol	PHENOL	Phenol	1

	Cresol	CRESOL	Cresol	1
ISO	Isoprene	C5H8	Isoprene	1
	Monoterpenes	APINENE	Alpha-pinene	0.33
		BPINENE	Beta-pinene	0.33
		LIMONENE	Limonene	0.33

Table S3: F0AM input options chosen for model runs

Parameter	Variables	Name in model	Units	Input
Meteorology	Pressure	P	mbar	Meteorological dataset
	Temperature	T	K	
	Relative humidity	RH	%	
Dilution	Dilution constant	kdil	s^{-1}	From PBL evolution and height
Photolysis options	J-value function	MCMv331_J(Met, Jmethod)	s^{-1}	MCMv331_J(Met,0)
Emissions/Deposition	Boundary layer depth	BLH	m	Quito: https://doi.org/10.1002/asl.829, 2018 Santiago: https://doi.org/10.5194/gmd-17-7467-2024
Radiation-Related	Solar zenith angle	SZA	degree	Calculated and checked MCMv331
	Ozone column	O3col	DU	Merra-2 1 hour dataset of Area-Averaged of total ozone column
	Albedo	Albedo	-	Merra-2 1 hour dataset of Area-Averaged of surface albedo
	Altitude	ALT	m	538.4 (S), 2414(Q)
Chemical Concentrations	O_3, CO and VOC's	InitConc	ppb	Dataset of air quality variables and 36 VOC´s
	NO, NO_2, NO_x	InitConc	ppb	Unconstrained NO, NO_2 NO_x family conservation
	Background concentration	BkgdConc	ppb	0 (default)
Chemistry	MCM scheme	ChemFiles	-	Subset of chemical species
Model options	Verbose	Verbose	-	3 (flag for verbose command window output)
	End points	EndPointsOnly	-	1 (flag for concentration and rate outputs)
	Link step	LinkSteps	-	0 (flag for using end-points of one run to initialize next run)

Table S4: Ozone and NO statistics for 2022 data at Quito and Santiago

Month 2022	Days	Quito		Santiago	
		Days with O_3 higher than 60 ppbv	Days with NO higher than 100 ppbv	Days with O_3 higher than 60 ppbv	Days with NO higher than 100 ppbv
January	31	0	5	2	1
February	28	1	1	6	0
March	31	0	0	7	12
April	30	0	0	5	17
May	31	0	0	1	27
June	30	0	1	0	25
July	31	0	0	0	24
August	31	0	0	2	22
September	30	0	0	2	13
October	31	0	4	4	6
November	30	0	10	6	1
December	31	0	10	13	0
Sum	365	1	31	48	148