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Ozone pollution around a coastal region of South China Sea: interaction between marine and continental air

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Table S1. Gradient separation of $C_1 - C_9$ aldehyde and ketone derivatives.

Column	Nava-Pak C18 3.9 ×150 mm
Mobile phase	A: Water/Acetonitrile/Tetrahydrofuran 60/30/10
Gradient	B: Water/Acetonitrile 40/60
Flow rate	100% A for 2 min then a linear gradient from 100% A to 100% B in 18 min, 100% B for 4min
Injection volume	20μL
Detection	Absorbance at 360 nm

Table S2. Description of parameters used in WRF-CMAQ simulation.

Model	**Parameters**	Value
WRF(v3.7.1)	**Microphysics**	WRF Single-Moment 3-class scheme
	Longwave Radiation	RRTM scheme
	Shortwave Radiation	Dudhia scheme
	Surface Layer	MM5 similarity
	Land Surface	Noah Land Surface Model
	Planetary Boundary layer	Yonsei University scheme
	Cumulus Parameterization	Kain-Fritsch scheme
	Diffusion Option	Simple diffusion
	K Option	2d Deformation
CMAQ(4.7.1)	**ModDriver**	**ctm_yamo**
	ModInit	**init_yamo**
	ModAdjc	**// yamo option does not need denrate**
	ModCpl	**gencoor**
	ModHadv	**hyamo**
	ModVadv	**vyamo**
	ModHdiff	**multiscale**
	ModVdiff	**acm2_inline**
	ModPhot	**phot**
	ModChem	**ebi_cb05cl_ae5**
	ModAero	**aero5**
	ModCloud	**cloud_acm_ae5**
	ModPa	**pa**
	ModUtil	**util**
	Mechanism	**cb05cl_ae5_aq**

Table S3. Index of agreement (IOA) between the simulated and observed meteorological parameters and air pollutants. IOA was calculated using the equation in Willmott (1982). Within the range of 0 – 1, higher IOA represents better agreement between the simulated and observed values.

	TC	WS
Temperature	0.81	0.84
Wind speed	0.56	0.54
Wind direction	0.60	0.51
Relative humidity	0.79	0.77
CO	0.88	0.87
NO_x	0.50	0.62
O_3	0.81	0.81

Table S4. Summary of O_3 episode days at WS and TC during the sampling period.

No.	Description	Date	SLB	WS	O_3_MAX.	TC	O_3_MAX.
0	Typhoon-related (Trami)	0820	Y	near-O_3 episode	92.6	near-O_3 episode	87.1
1		0821	N	episode	173.0	episode	159.9
2	Typhoon-related (Usagi)	0920	N	-	61.4	episode	126.8
3		0921	N	episode	116.0	-	69.3
4	Typhoon-related (Wutip)	0927	Y	near-O_3 episode	85.4	episode	102.4
5		0928	Y	episode	109.4	-	71.8
6	O_3 episode event I	1001	N	near-O_3 episode	89.8	episode	107.5
7		1002	Y	episode	126.9	near-O_3 episode	91.7
8		1003	Y	episode	119.1	episode	121.2
9		1004	Y	episode	121.3	episode	119.7
10		1005	Y	episode	163.2	episode	143.1
11		1006	N	episode	151.9	episode	119.7
12		1007	N	episode	118.7	near-O_3 episode	89.7
13		1008	N	episode	138.3	near-O_3 episode	84.1
14	typhoon-related (Nari)	1011	Y	episode	130.8	episode	130.4
15		1012	Y	near-O_3 episode	99.1	near-O_3 episode	90.2
16	O_3 episode event II	1019	Y	episode	155.0	episode	117.7
17		1020	Y	episode	122.1	episode	120.2
18		1021	Y	episode	124.0	episode	144.7
19		1022	N	episode	148.5	episode	104.4
20		1023	N	episode	152.3	episode	119.2
21		1024	N	episode	148.1	episode	116.1
22		1025	N	episode	135.8	near-O_3 episode	89.1
23		1026	N	episode	105.3	episode	117.2
24		1027	N	episode	106.2	near-O_3 episode	99.3
25	typhoon-related (Krosa)	1101	Y	near-O_3 episode	83.2	episode	106.5
26		1102	N	near-O_3 episode	95.6	-	35.1
27		1115	N	episode	109.8	-	66.2

Note: An O_3 episode day was defined when the peak one-hour averaged O_3 mixing ratio exceeded 100 ppbv (Level II of China National Ambient Air Quality Standard). A near-O_3 episode days was defined when the peak hourly average O_3 mixing ratio was lower than 100 ppbv but higher than 80 ppbv (Level I of China National Ambient Air Quality Standard).

Table S5. Statistics (Mean ± 95% C.I) of the top 10 NMHC and the top 3 carbonyl species observed at TC and WS during O_3 episodes and non- episodes.

Compound	**TC**		**WS**	
	Episode	*Non-episode*	*Episode*	*Non-episode*
Ethane	2179±222	1852±256	2077±182	1456±167
Propane	1966±277	1572±207	1523±126	866±126
Isobutane	1944±371	1433±166	1559±167	810±115
Acetylene	2083±165	1316±145	1805±133	1086±122
Toluene	1829±365	1357±254	1737±388	703±183
n-Butane	1437±163	1336±148	1160±145	480±113
n-Hexane	733±329	1351±443	980±299	447±121
Ethene	1140±167	1077±171	826±99	691±94
Isopentane	964±145	813±123	918±99	523±96
Benzene	614±49	428±51	587±47	381±44
Formaldehyde	5068±454	3522±286	4257±355	2471±180
Acetone	5064±831	3367±445	3984±287	2086±162
Acetaldehyde	1807±162	1241±115	1618±133	920±105

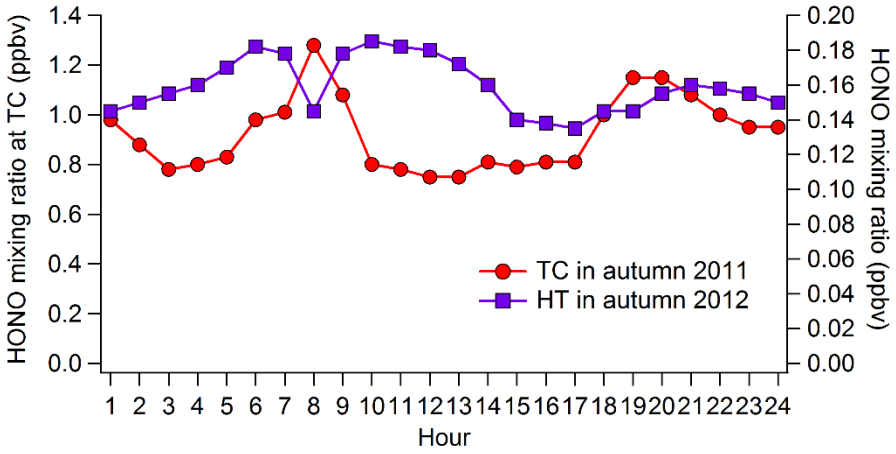

Figure S1 Average diurnal profiles of HONO observed at TC in autumn 2011 and at a coastal background site (Hok Tsui, HT) in southeast Hong Kong in autumn 2012.

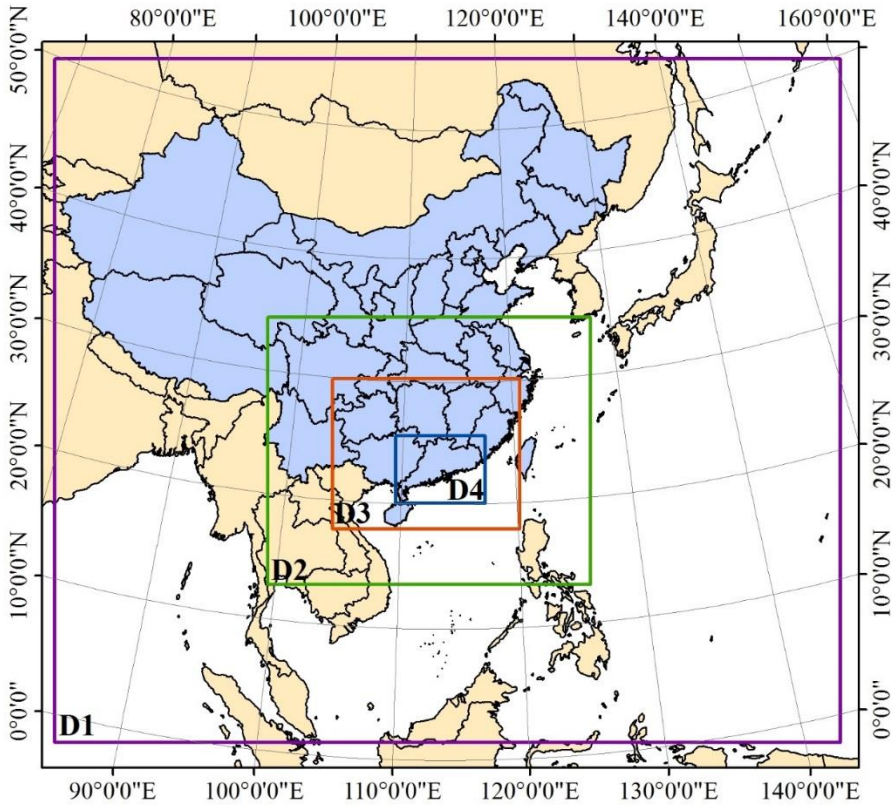

Figure S2 Nesting domain settings of the WRF model. D1, D2, D3 and D4 inside the figure denote domain 1, 2, 3 and 4, respectively. The outermost domain (D1) covers the entire China and East Asia with the resolution of 81 km × 81 km and 89 × 78 grids. D2 covers South China with the resolution of 27 km × 27 km and 109 × 91 grids. D3 covers Guangdong province and the surrounding areas with the resolution of 9 km × 9 km and 187 × 151 grids. The innermost domain (D4) covers Pearl River Delta region with the resolution of 3 km × 3 km and 186 × 150 grids.

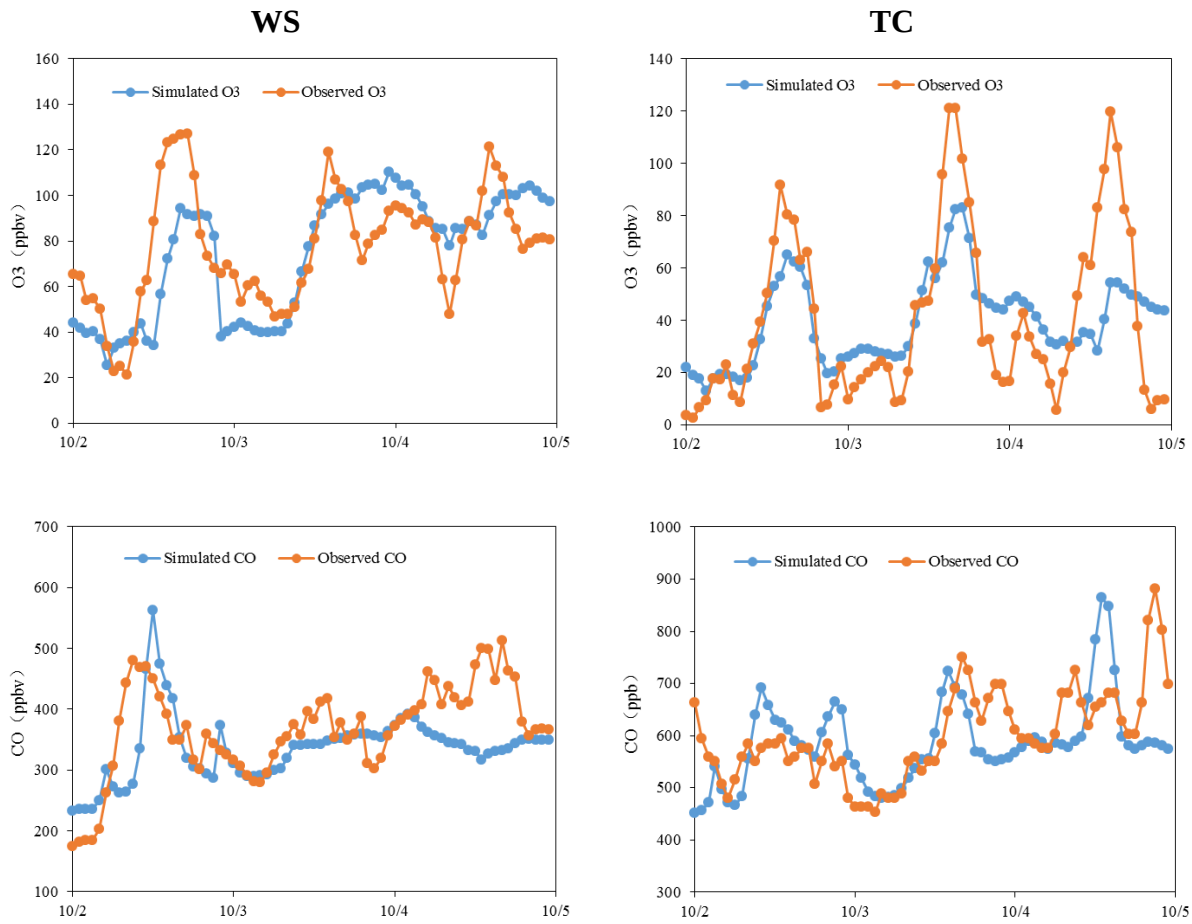

Figure S3. Time series of the WRF-CMAQ simulated and the observed CO and O_3 at WS (left panel) and TC (right panel) during a typical O_3 episode on Oct. 2-4, 2013.

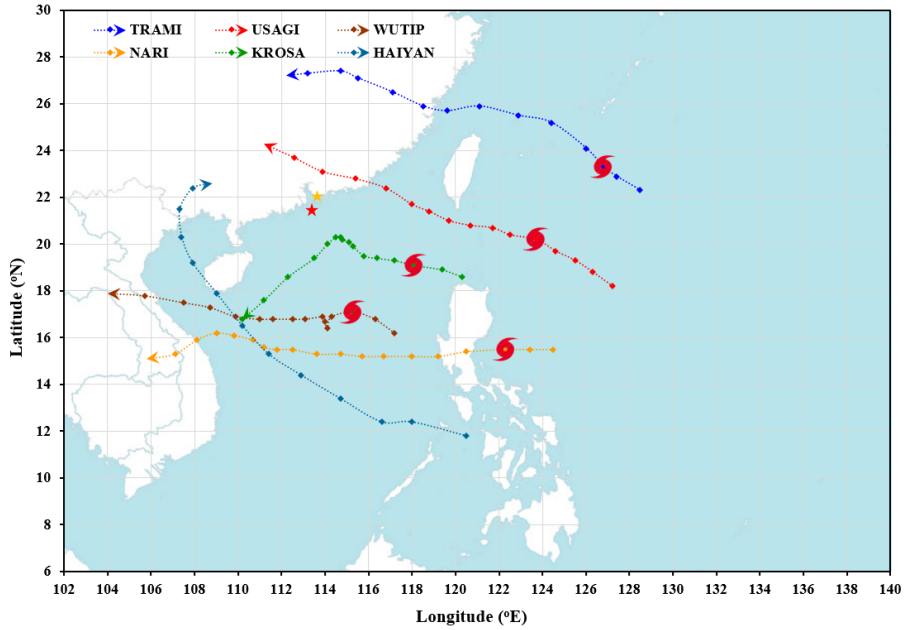

Figure S4. Track of typhoons during the sampling period. The typhoon labels mark the positions when O_3 episodes occur in Hong Kong. The dots represent intermediate 6-hourly positions.

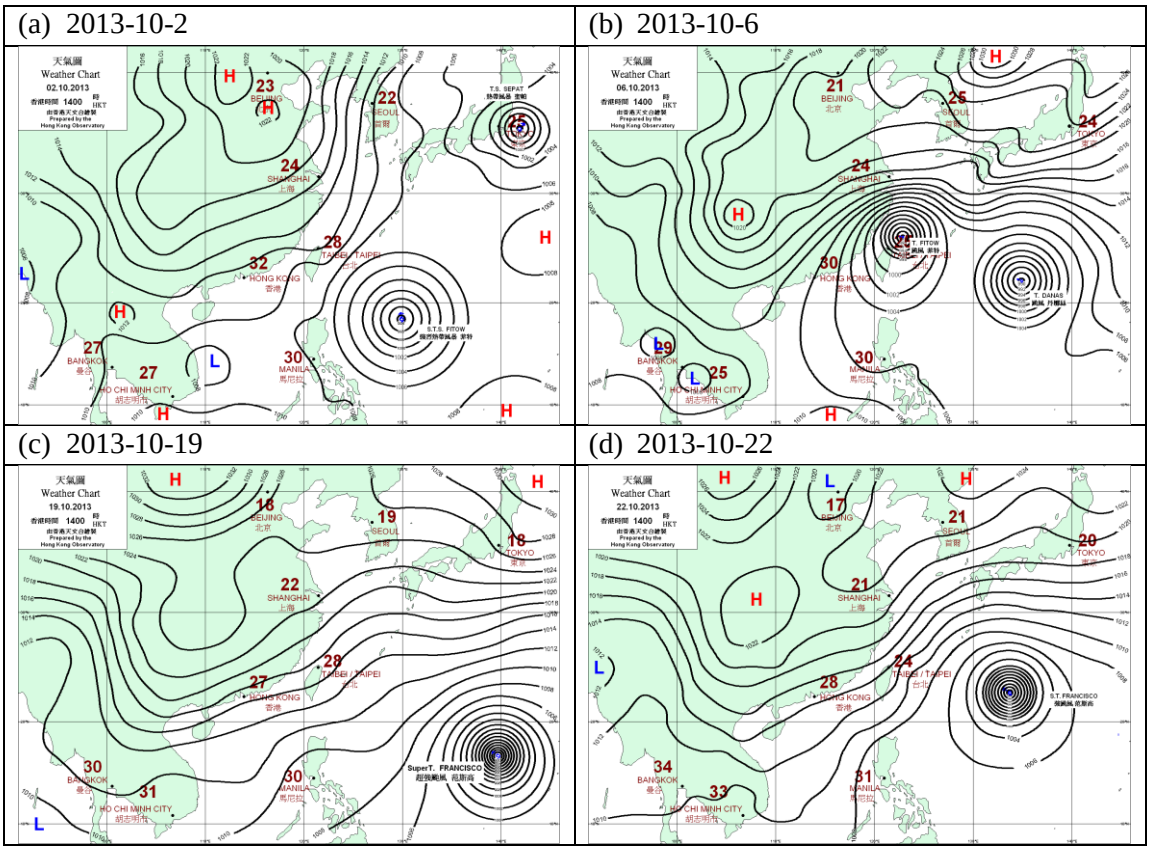

Figure S5. Selected examples of weather charts at 6 am during Continental High Pressure in October 2013. (a) & (c) Continental high pressure systems formed far away from the coastal areas and caused SLBs related O_3 episodes; (b) & (d) Continental high pressure systems approaching to the coastal areas and caused O_3 episodes not related to SLBs; The maps are courtesy provided by Hong Kong Observatory.

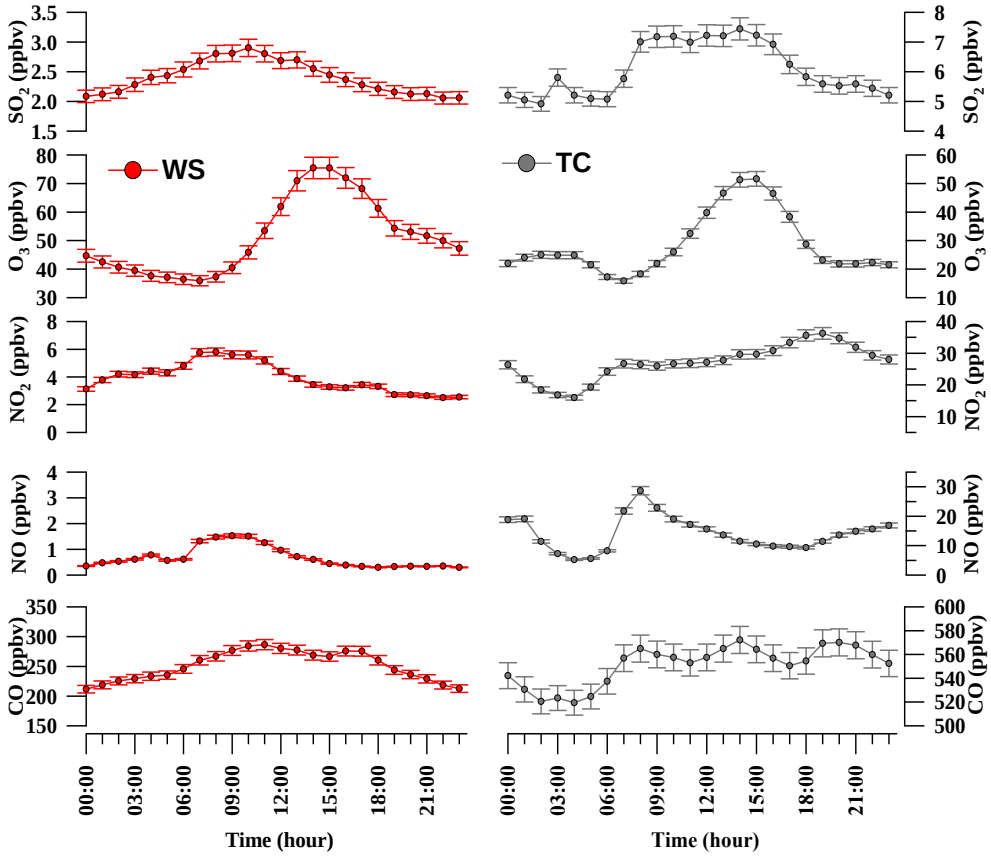

Figure S6. Diurnal variations of trace gases measured at WS and TC.

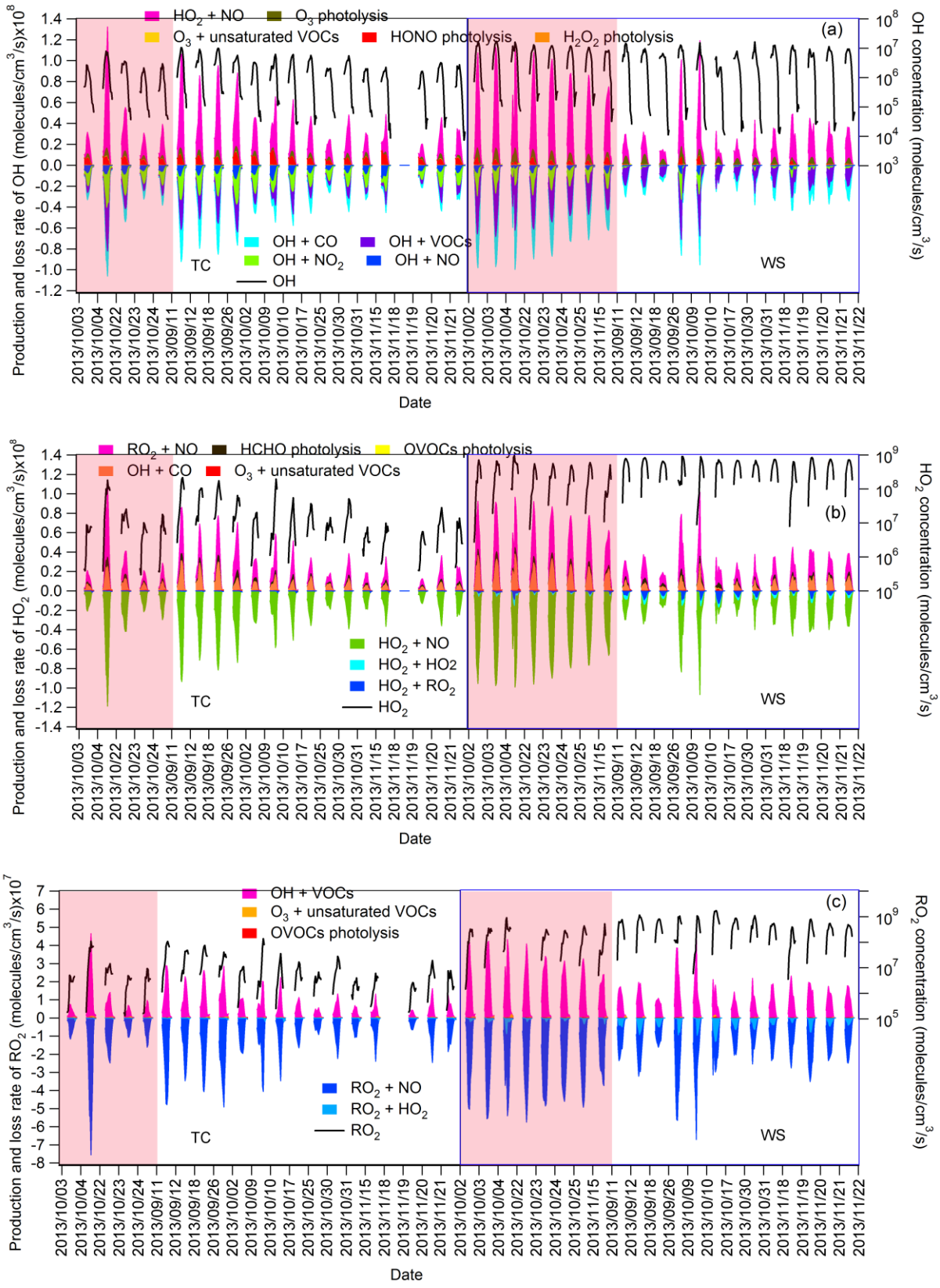

Figure S7. Daytime (7:00-19:00 LT) variations of the simulated production and loss rate of (a) OH, (b) HO_2 and (c) RO_2 at TC (left panel) and WS (right panel). O_3 episode days are highlighted in red background. The dates are not consecutive due to the discontinuous canister sampling of VOCs.

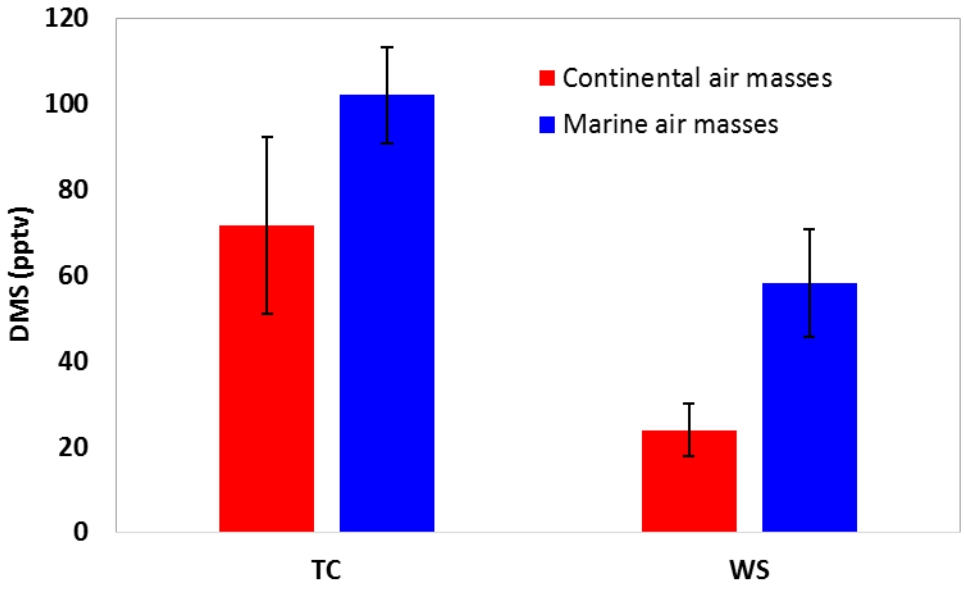

Figure S8 Average concentrations of dimethyl sulfide (DMS) observed at TC and WS when continental or marine air masses dominated.

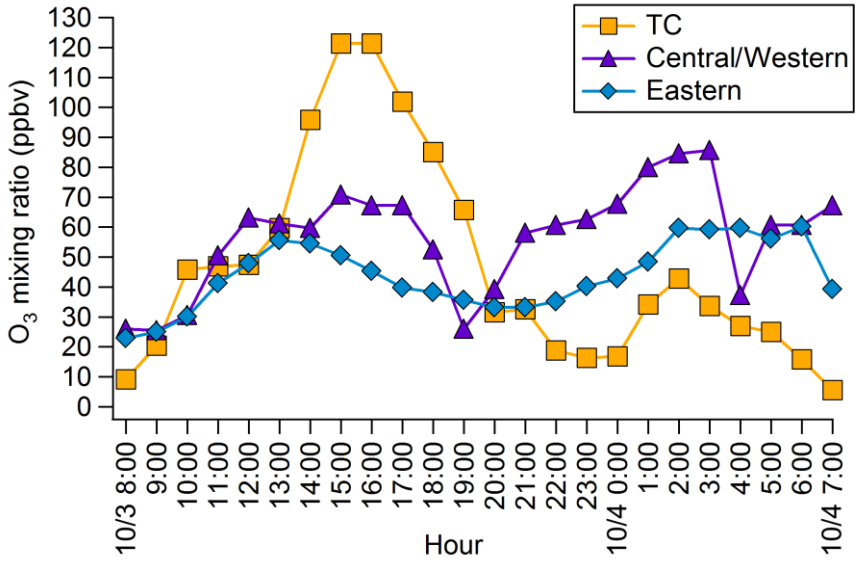

Figure S9. Hourly average O_3 observed at TC, Central/Western and Eastern from 08:00 on 3 October to 07:00 on 4 October. The three sites were located in southern Hong Kong, which were all non-roadside sites. Detailed information can be found on the website of HKEPD (http://www.aqhi.gov.hk/en/monitoring-network/air-quality-monitoring-stations9c57.html?stationid=81).