Response to reviewers' comments

We thank the reviewers for the constructive comments and suggestions, which are very positive to improve scientific content of the manuscript. We have revised the manuscript appropriately and addressed all the reviewers' comments point-by-point for consideration as below. The remarks from the reviewers are shown in black, and our responses are shown in blue color. All the page and line numbers mentioned following are refer to the revised manuscript without change tracked.

Reviewer

The authors present measurements of a number of important atmospheric species, including O3, NOx, HONO, SO2, HCHO and VOCs, made in an urban environment in Shanghai during a five month period between May and September 2018. These measurements are used to constrain box model simulations, using the Master Chemical Mechanism (MCM), to study the atmospheric oxidising capacity (AOC, the sum of the rates of VOC oxidation reactions by OH, O3, and NO3), OH reactivity (the inverse of the OH lifetime), and the OH chain length (the ratio of OH recycling to OH termination). The authors focus on three short periods during the five month observation period, and determine that the main species contributing to ozone formation during these periods were formaldehyde, toluene, ethylene, and m/p-xylene, which have lower concentrations than other species but have greater contributions in terms of reactivity.

While the analysis and results reported in the paper will be of general interest to the atmospheric science community, the manuscript is somewhat limited in its scope. It is not entirely clear why the three short periods out of the full measurement period have been chosen for detailed study, or whether any of these three periods are representative of typical conditions. Some further discussion regarding the choice of these three periods is necessary, particularly since the authors comment several times on measurements made over five months but focus only on six days.

R: Thanks for the constructive comments. This study was aiming to explore the atmospheric oxidation capacity and photochemical reactivity during the summertime and their potential relationship with ozone pollution. Therefore, the main reason for three short periods out of the full five-months measurements for detailed study was that these three cases are selected to represent the typical similarities and differences of atmospheric photochemistry under different ambient O_3 levels, i.e. ozone pollution, moderate condition and non-pollution according to the Ambient Air Quality Standards of China (GB3095-2012).

As shown in Table 1, the ozone hourly mean values for the selected cases were 65.13±27.16 ppbv, 46.12±21.14 ppbv and 23.95±11.89 ppbv, respectively. Besides ozone pollution, other trace gases like NO_X, HONO, HCHO and the radiation were also showing different characteristics among these three cases. Figure R1 shows the mean diurnal profiles of O_3, other trace gases and J_{NO_2} for three selected cases. The overall trace gases were at low levels without significant diurnal variation in Case 3 under the low O_3 level, while their mixing ratios increased strongly and exhibited distinct diurnal profiles in Case 1 and Case 2 with relatively high O_3 levels. The differences in pollutant mixing ratios (Figure S1) and meteorological parameters (Figure S2) among the three cases manifest the three different atmospheric environments, which are helpful to explore the causes of changes in atmospheric oxidation capacity and photochemical reactivity.

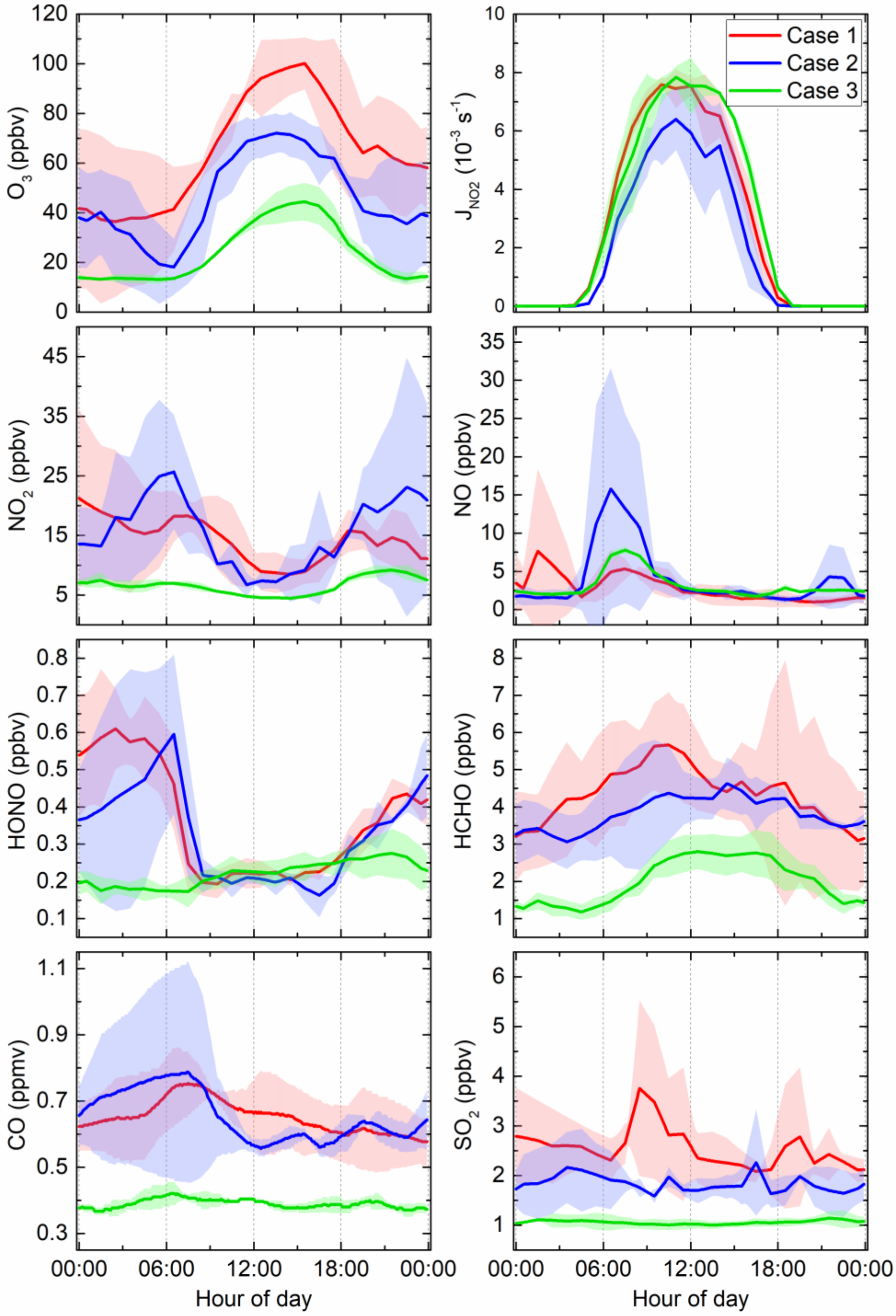

Figure R1. Mean diurnal profiles of measured trace gases mixing ratios for three cases. The shaded areas denote the standard deviation.

Details of the model simulations could also be expanded. How are model intermediates treated? Does the model include deposition terms to avoid build-up of high concentrations of model intermediates? If so, what were the deposition lifetimes and how do they impact the modelled AOC, OH reactivity and OH chain length? It would also be useful to include some discussion of the concentrations of modelled OH, HO2 and RO2 species.

R: Thanks for the suggestion. We have followed the comments to clearly describe the details of the model in the revised manuscript, such as whether to consider the deposition process and the boundary layer effect, and how they affect the model results. Please refer to Line 149-160.

Regarding to the deposition terms, it is regrettable that it was not taken into account previously, neither the accumulation of intermediates. Therefore, we have supplemented a simulation scenario considering the deposition process in order to discuss its impacts on intermediates. The loss of all unrestricted and model-generated species caused by the deposition is set as the accumulation of the deposition velocity of 0.01 m s^{-1} in the boundary layer (Santiago et al., 2016). Given that the boundary layer height (BLH) varied typically from 400 m at night to 1400 m in the afternoon during summer, which means that the lifetime of the model-generated species was ranged between ~11 h at night and ~40 h during the afternoon (Shi et al., 2015).

Afterwards, we have compared the simulated radical yields, AOC, OH reactivity, and OH chain length with or without considering the deposition process (see Table. R1). The simulated scenario without deposition is called Scenario N and the simulated scenario considering deposition is called Scenario Y. It can be clearly seen that the simulation results (OH, HO_2, RO_2, AOC, OH reactivity and OH chain length) without considering deposition term are enhanced to some extent compared with those with considering deposition term in three cases, especially for the intermediate (e.g. HO_2, RO_2), the results of Case 2 and Case 3 are increased by more than 50%. Therefore, it can be concluded that the deposition process has a great influence on the intermediates, which should be taken into account in the simulation.

Table R1. Summary of simulation results considering and not considering deposition process. All results are the average value of 06:00-18:00. N – Not considering deposition; Y – considering deposition.

Case 1	**OH** **10^6 mole cm^{-3}**	**HO_2** **10^8 mole cm^{-3}**	**RO_2** **10^8 mole cm^{-3}**	**AOC** **10^8 mole cm^{-3} s^{-1}**	**OH reactivity** **s^{-1}**	**OH chain length**
N	5.65±3.16	2.40±1.46	1.48±0.86	0.45±0.23	11.71±2.37	3.39±0.69
Y	5.27±3.13	1.99±1.29	1.09±0.70	0.42±0.22	11.48±2.16	3.17±0.63
(N-Y)/Y	7.21%	20.60%	35.78%	7.14%	2.00%	6.94%
Case 2	**OH** **10^6 mole cm^{-3}**	**HO_2** **10^8 mole cm^{-3}**	**RO_2** **10^8 mole cm^{-3}**	**AOC** **10^8 mole cm^{-3} s^{-1}**	**OH reactivity** **s^{-1}**	**OH chain length**
N	4.73±2.77	2.86±1.65	2.33±1.26	0.44±0.24	13.48±4.29	4.61±1.15
Y	4.05±2.68	1.87±1.18	1.34±0.82	0.37±0.22	12.86±3.80	3.75±0.90
(N-Y)/Y	16.79%	52.94%	73.88%	18.92%	4.82%	22.93%

Case 3	**OH** 10^6 mole cm^{-3}	**HO$_2$** 10^8 mole cm^{-3}	**RO$_2$** 10^8 mole cm^{-3}	**AOC** 10^8 mole cm^{-3} s^{-1}	**OH reactivity** s^{-1}	**OH chain length**
N	6.99±3.13	2.66±1.58	2.46±1.49	0.45±0.23	8.43±1.53	6.06±1.31
Y	6.12±3.37	1.76±1.22	1.51±1.08	0.40±0.23	8.41±1.21	4.96±1.08
(N-Y)/Y	14.22%	51.14%	62.91%	12.50%	0.24%	22.18%

Since the used deposition velocity and the BLH are empirical values from the previous literatures (Shi et al., 2015; Santiago et al., 2016), we have also carried out the sensitivity study on the deposition velocity and boundary layer height. The basic simulation scenario was set as deposition velocity of 0.01 m s^{-1} and the height of boundary layer varied from 400 m at night to 1400 m in the afternoon. Table R2 shows the settings of different simulation scenarios for the sensitivity study.

Table R2. Settings of simulation scenarios for sensitivity study.

Scenarios	deposition velocity (m s^{-1})	boundary layer-night (m)	boundary layer-noon (m)	Lifetime
Basic	0.01	400	1400	Night: 11 h; Day: 49 h
A	0.01	400	1000	Night: 11 h; Day: 28 h
B	0.01	400	2000	Night: 11 h; Day: 56 h
C	0.01	300	1400	Night: 8 h; Day: 39 h
D	0.01	500	1400	Night: 14 h; Day: 39 h
E	0.008	400	1400	Night: 14 h; Day: 49 h
F	0.012	400	1400	Night: 9 h; Day: 32 h

The sensitivity simulation results are summarized in Table R3, which demonstrated that the impacts of variations of deposition velocity and BLH on the modeling results could be negligible (i.e. < 3% in OH, HO$_2$, RO$_2$, AOC, OH reactivity and OH chain length).

Table R3. Summary of model sensitivity test results

Case 1	**OH** 10^6 mole cm^{-3}	**HO$_2$** 10^8 mole cm^{-3}	**RO$_2$** 10^8 mole cm^{-3}	**AOC** 10^8 mole cm^{-3} s^{-1}	**OH reactivity** s^{-1}	**OH chain length**
Basic	5.27±3.13	1.99±1.29	1.09±0.70	0.42±0.22	11.48±2.16	3.17±0.63
A	5.26±3.12	1.97±1.27	1.07±0.68	0.42±0.22	11.46±2.16	3.16±0.62
B	5.28±3.13	2.01±1.29	1.11±0.71	0.42±0.22	11.49±2.16	3.17±0.63
C	5.25±3.13	1.97±1.28	1.07±0.69	0.42±0.22	11.44±2.13	3.16±0.63
D	5.29±3.12	2.01±1.29	1.11±0.70	0.42±0.22	11.50±2.18	3.17±0.62
E	5.30±3.12	2.02±1.29	1.12±0.71	0.42±0.22	11.51±2.18	3.18±0.62
F	5.25±3.12	1.97±1.28	1.07±0.69	0.42±0.22	11.45±2.14	3.16±0.63
(A-Basic)/Basic	-0.23%	-0.90%	-1.87%	-0.48%	-0.17%	-0.22%
(B-Basic)/Basic	0.21%	0.79%	1.64%	0.43%	0.15%	0.20%
(C-Basic)/Basic	-0.42%	-0.92%	-1.78%	-0.84%	-0.29%	-0.30%
(D-Basic)/Basic	0.33%	0.74%	1.45%	0.67%	0.23%	0.24%

(E-Basic)/Basic	0.46%	1.26%	2.54%	0.95%	0.33%	0.37%
(F-Basic)/Basic	-0.39%	-1.05%	-2.10%	-0.79%	-0.27%	-0.31%
Case 2	**OH 10^6 mole cm^{-3}**	**HO$_2$ 10^8 mole cm^{-3}**	**RO$_2$ 10^8 mole cm^{-3}**	**AOC 10^8 mole cm^{-3} s^{-1}**	**OH reactivity s^{-1}**	**OH chain length**
basic	4.05±2.68	1.87±1.18	1.34±0.82	0.37±0.22	12.86±3.80	3.75±0.90
A	4.04±2.68	1.84±1.16	1.31±0.80	0.37±0.22	12.83±3.80	3.73±0.90
B	4.07±2.69	1.89±1.19	1.37±0.83	0.37±0.22	12.89±3.80	3.75±0.90
C	4.02±2.68	1.84±1.17	1.31±0.81	0.36±0.22	12.80±3.76	3.73±0.90
D	4.08±2.68	1.89±1.19	1.37±0.83	0.37±0.22	12.92±3.83	3.76±0.90
E	4.09±2.69	1.91±1.20	1.38±0.84	0.37±0.22	12.94±3.83	3.77±0.90
F	4.03±2.68	1.84±1.16	1.31±0.80	0.36±0.22	12.81±3.77	3.73±0.90
(A-Basic)/Basic	-0.38%	-1.30%	-2.06%	-0.67%	-0.23%	-0.28%
(B-Basic)/Basic	0.35%	1.17%	1.85%	0.63%	0.21%	0.26%
(C-Basic)/Basic	-0.76%	-1.52%	-2.22%	-1.38%	-0.50%	-0.49%
(D-Basic)/Basic	0.62%	1.26%	1.84%	1.12%	0.40%	0.40%
(E-Basic)/Basic	0.86%	2.08%	3.13%	1.57%	0.55%	0.57%
(F-Basic)/Basic	-0.68%	-1.63%	-2.47%	-1.22%	-0.44%	-0.46%
Case 3	**OH 10^6 mole cm^{-3}**	**HO$_2$ 10^8 mole cm^{-3}**	**RO$_2$ 10^8 mole cm^{-3}**	**AOC 10^8 mole cm^{-3} s^{-1}**	**OH reactivity s^{-1}**	**OH chain length**
basic	6.12±3.37	1.76±1.22	1.51±1.08	0.40±0.23	8.41±1.21	4.96±1.08
A	6.10±3.37	1.74±1.21	1.48±1.06	0.40±0.23	8.39±1.22	4.95±1.08
B	6.14±3.37	1.78±1.23	1.54±1.10	0.41±0.23	8.42±1.21	4.97±1.08
C	6.09±3.39	1.74±1.22	1.49±1.08	0.40±0.23	8.38±1.20	4.94±1.08
D	6.14±3.35	1.77±1.22	1.53±1.08	0.41±0.23	8.43±1.23	4.97±1.08
E	6.16±3.35	1.79±1.23	1.55±1.10	0.41±0.23	8.44±1.22	4.97±1.08
F	6.09±3.38	1.74±1.21	1.48±1.07	0.40±0.23	8.38±1.20	4.94±1.08
(A-Basic)/Basic	-0.30%	-1.44%	-2.08%	-0.59%	-0.25%	-0.20%
(B-Basic)/Basic	0.26%	1.22%	1.76%	0.52%	0.20%	0.18%
(C-Basic)/Basic	-0.47%	-0.93%	-1.30%	-0.85%	-0.37%	-0.28%
(D-Basic)/Basic	0.38%	0.79%	1.10%	0.70%	0.28%	0.23%
(E-Basic)/Basic	0.56%	1.60%	2.28%	1.05%	0.43%	0.35%
(F-Basic)/Basic	-0.46%	-1.33%	-1.90%	-0.85%	-0.36%	-0.28%

Finally, the basic simulation scenario of deposition velocity of 0.01 m s^{-1} and the height of boundary layer varied from 400 m at night to 1400 m in the afternoon were used in the simulation for the three cases study. And the relevant simulated results and discussion were replaced in the manuscript.

Minor comments are given below.
Page 1, line 19: ‘Five months of observation’ to ‘Five months of observations’.
R: The ‘observation’ has been corrected to ‘observations’. Please refer to Line 19.

Page 1, line 21: State clearly what the 92.2 % refers to, presumably of the observation

period?
R: Ambient Air Quality Index (AQI) was less than 100 for 141 days during the whole observation period, accounting for 92.2% of the total observational period. We have rewritten this sentence as 'Five months of observations from 1 May to 30 September 2018 showed that the air quality level is in lightly polluted and even worse (Ambient Air Quality Index, AQI>100) for 12 days, of which ozone is the primary pollutant for 10 days, indicating ozone pollution is the main challenge of air quality in Shanghai during summer of 2018.'. The detailed statement can be found on Line 19-22.

Page 1, line 28: '... of the OH lifetime'.
R: We have added 'the' before 'OH lifetime'. Please refer to Line 29.

Page 1, line 29: 'condition' to 'conditions'.
R: We have corrected it. Please refer to Line 30.

Page 1, line 31: 'the HONO photolysis' to 'HONO photolysis' and 'the O3 photolysis' to 'O3 photolysis'.
R: We have followed the comments and deleted both 'the'. Please refer to Line 32.

Page 1, line 32: The statement regarding the reaction with NO2 completely dominating seems over-exaggerated, there are surely some other contributions. 'radicals termination' to 'radical termination', and 'reactions of radical-radical' to 'radical-radical reactions'.
R: Thanks for the suggestion. According to the results in this study, the reaction with NO_2 accounts for 98% of the HO_x sinks during 05:30-11:00 in Case 1, and the contribution of reaction with NO_2 to the HO_x sinks reaches 98.9% and 99.7% during 05:30-09:00 in Case 2 and 3, respectively, suggesting that the cross-reactions between radicals contribute only nearly 1% in three cases at rush hour. Therefore, it can be concluded that the reaction with NO_2 are the most important sink of radicals during the morning rush hour. We have revised the over-exaggerated expression. Please refer to Line 32-33.

Page 2, line 56: Hydroperoxy is preferred over hydroperoxyl.
R: Thanks for the suggestion. The 'hydroperoxy' has been replaced with 'hydroperoxyl'. Please refer to Line 57.

Page 3, line 76: There are more recent measurements in London than those referenced.
R: Thanks for the information. We have reviewed the related literatures, e.g. Whalley et al. (2016; 2018). In these recent measurements in London, it is reported that OH reactivity was 15~27 s^{-1} and HONO photolysis dominated OH source in central London in the summer of 2012. We have also cited in the revised manuscript, please refer to Line 76.

Page 3, line 85: 'a emissions' to 'an emissions'.
R: We have corrected 'a' to 'an'. Please refer to Line 91.

Page 3, line 98: 'suburban' to 'suburban areas'.
R: The 'suburban' has been corrected to 'suburban areas'. Please refer to Line 104.

Page 4, line 111: ‘vehicle’ to ‘vehicles’.
R: We have made the revision. Please refer to Line 117.

Page 4, line 113: Please expand on what you mean by a clean environment. Clean air? Free of rubbish waste?
R: Thanks for the suggestion. We have rewritten this sentence as ‘The campus itself is relatively clean air condition without significant sources of air pollutants, mainly is affected by traffic emissions from viaducts and residential areas nearby.’. Please refer to Line 119-120.

Page 4, line 117: Please clarify what is analyzed further? How is the initial analysis performed? Why is further analysis necessary and what does it achieve?
R: We are apologized for the improper statements leading misunderstanding. Here we restructured this sentence like “O_3 and NO were measured by the short-path DOAS (Differential Optical Absorption Spectroscopy) instrument with a light path of 0.15 km and time resolution of 1 min. The fitting windows of them are 250-266 nm and 212-230 nm, respectively.” Please refer to line 122-124.

Page 4, line 122: ‘Photolysis frequency of...’ to ‘The photolysis frequency of...’.
R: We have added ‘the’ before ‘photolysis frequency of...’. Please refer to Line 128.

Page 5, line 135: How were deposition rates implemented in the model, if at all? What was the impact of these?
R: We have supplemented the discussion on the impacts of the deposition process on the simulation results and related sensitivity study. As shown in Tables R1 and R3, the results indicated that neglecting the deposition process can cause build-up of high concentrations of model intermediates. So we have re-simulated these three cases with consideration of the deposition process and further discussed atmospheric photochemistry for different ozone levels in Shanghai in the revised manuscript. Therefore, the corresponding figures and contents in the manuscript have been replaced. Please also refer to the Supplement.

Page 5, line 137: ‘last’ to ‘latest’.
R: We have corrected it and please refer to Line 143.

Page 5, line 144: How reliable is the use of measured JNO2 to scale calculated JO1D? They are known to be affected differently by cloud cover.
R: Thanks for the suggestion. The impacts of cloud cover on J_{NO2} and J_{O1D} are considerably complex. Crawford et al. (2003) reported that the observed UV actinic flux under cloudy conditions that unoccluded the sun disk is 40% higher than the clear sky value. When the solar disk is occluded, reductions in actinic flux appear to vary inversely with cloud fraction in some instances. In the broken cloud field, the fluctuation ranges of J_{O1D} and J_{NO2} are different, and the change of J_{NO2} is larger than that of J_{O1D}. Monks et al. (2004) research also revealed that the photolysis frequencies in the UVB and UVA do not vary linearly under different atmospheric conditions in a cloudy field. Cloud cover and its quantitative effects on UVA and UVB are important for the correction of J_{O1D} from the measured J_{NO2} scaling. Whalley et al. (2018) used the ratio of the model calculated J_{O1D} in the clear sky to the observed J_{O1D} to account

for clouds and to determine photolysis rates of other photolabile species.

Since we have not measured J_{O1D} but only for J_{NO_2}, we are not able to use this method to determine cloud cover. However, we try to seek an approximate quantitative relationship between the fluctuation magnitude of J_{NO_2} and J_{O1D} in cloudy days compared to clear sky:

$$\%\ \text{reduction or enhancement}\ in\ j(X) = \left(\frac{j(X)_{clear} - j(X)_{cloudy}}{j(X)_{clear}}\right) \times 100 \qquad \text{(E1)}$$

$$\%j(O^1D) \approx 1.08\%j(NO_2) - 0.12 \qquad \text{(E2)}$$

Where $\%j(O^1D)$ and $j(NO_2)$ is calculated by the equation (E1). Please note that the equation (E2) here is an approximate relationship between $\%j(O^1D)$ and $\%j(NO_2)$ on a certain summer day in the study by Monks et al. (2004).

In addition, it is also necessary to correct the cloudy day values of J_{O1D} considering the changes in overhead ozone column between the cloudy and clear day. The ratio of the overhead ozone column of clear sky day to that of cloudy day is used as the calibration coefficient *k*. The J_{O1D} of cloudy day can be calculated by equation (E3):

$$j(O^1D)_{cloud} = kj(O^1D)_{clear}\left(1 - \%j(O^1D)\right) \qquad \text{(E3)}$$

Table R4 lists the overhead total ozone column and calibration coefficient *k* for three cases, in which total ozone column data taken from OMI (download from https://disc.gsfc.nasa.gov/datasets/OMDOAO3_003/summary) and taken for 121.51°E, 31.34°N with a radius of 20 km at 13:45 local overpass time. The OMI data from September 2nd to 4th are missing due to no data available after the filtering (filtering conditions: solar zenith angles < 70°, cloud cover < 0.5, pixels were not affected by the row anomaly are used), and we took the mean value of available total ozone column from May to October as the reference data (294.262±18.240 DU). Considering that the total column concentration was relatively low in September, the final total ozone column of 290.000 DU was used.

Table R4. Daily ozone total column for three cases in Shanghai. Data taken from OMI. NOTE: Missing data on September 2, 3 and 4.

	Date	O_3 total column/DU	k
Case 1	11-Jun	341.955	0.874
	12-Jun	319.755	0.935
	13-Jun	321.510	0.929
Case 2	2-Sep	*290.000*	*1.030*
	3-Sep	*290.000*	*1.030*
	4-Sep	*290.000*	*1.030*
Case 3	12-Jul	277.529	1.077
	13-Jul	299.974	0.996
	14-Jul (clear sky)	298.841	1.000

In this study, we have used the observed J_{NO_2} data and the J_{O1D} data scaled by J_{NO_2}. As shown in Figure R2, it is a clear sky on July 14, 2018 in Case 3. The J_{NO_2} on this day and the J_{O1D} obtained by scaling J_{NO_2} can be considered as real or 'measured' $j(X)_{clear}$. The images of sky conditions for the remaining days of these three cases are shown in

Figure R3 (the images on July 12 are missing).

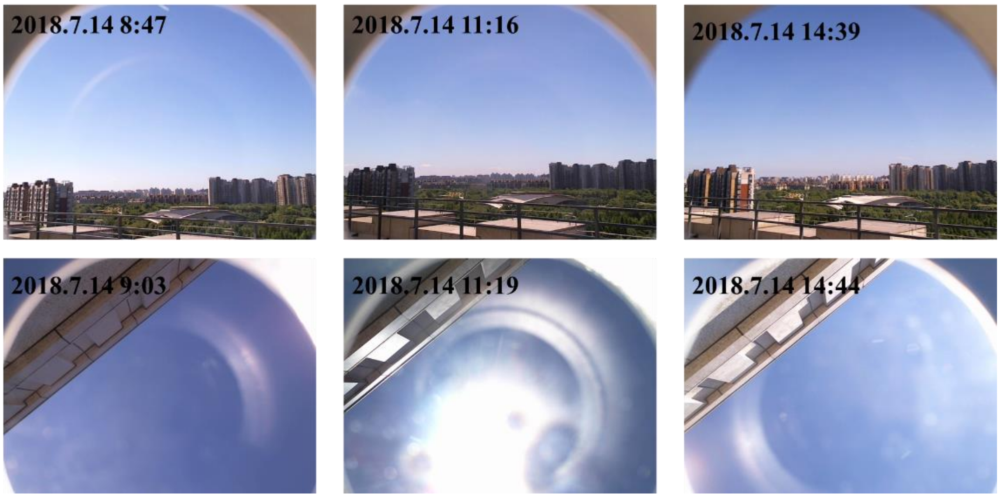

Figure R2. Sky images on July 14, 2018

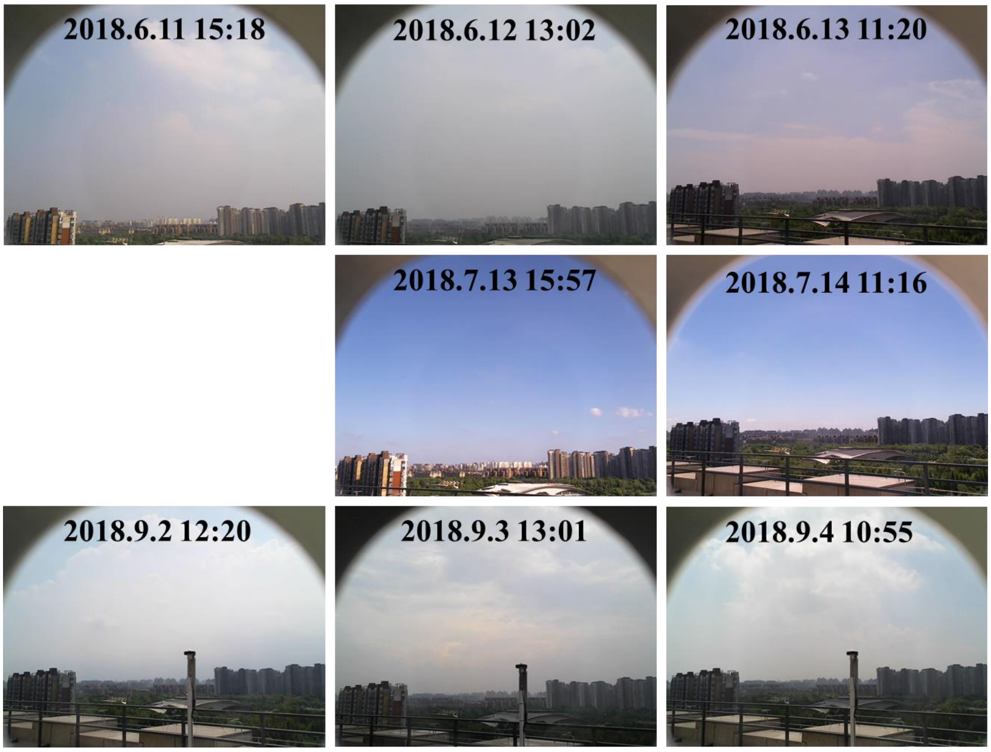

Figure R3. Representative sky images in three cases

Therefore, we can determine $\%j(NO_2)$ by the difference between J_{NO_2} on clear sky and cloudy days, and then calculate the $J_{O1Dcloudy}$ via equation (E3). Figure R4 shows the difference of calibrated J_{O1D} and J_{O1D} without calibration for clouds in three cases. Compared with the J_{O1D} scaled by the measured J_{NO_2} directly, the calibrated J_{O1D} of the three cases changed by -0.75%, 32.22%, and 7.97%, respectively.

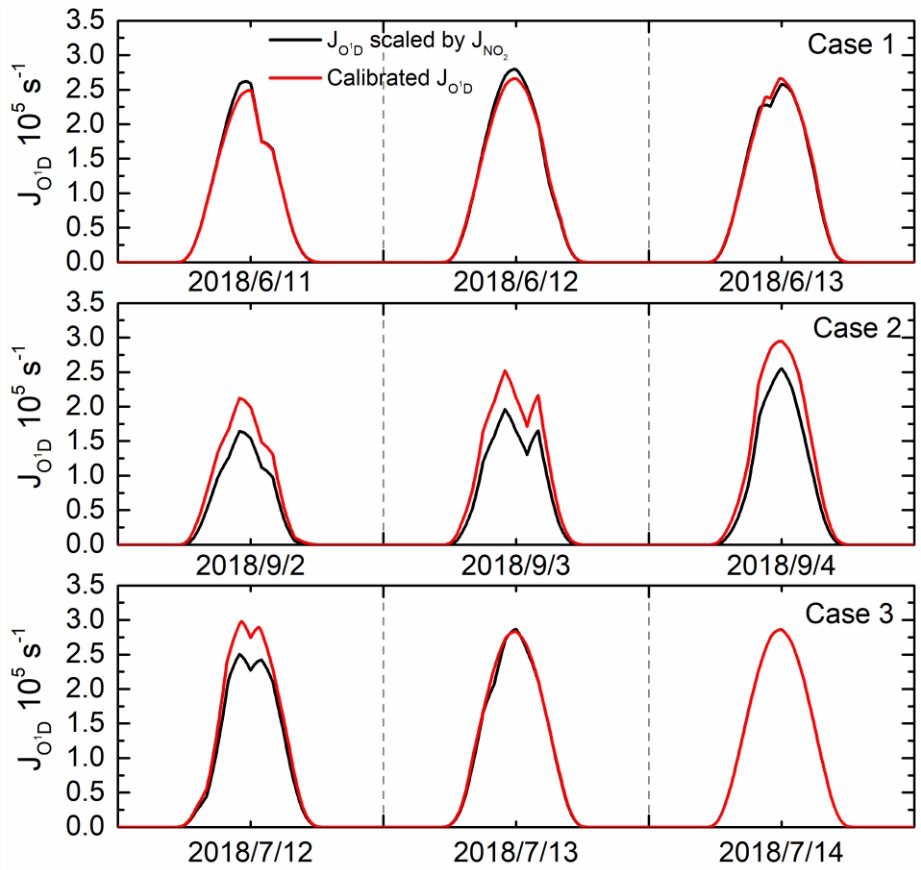

Figure R4. Comparison of calibrated J_{O1D} for cloud covers and J_{O1D} without calibration scaled directly by J_{NO2} in three cases

Then, we have ran the simulation scenarios G with the calibrated J_{O1D} and compared the results with simulation scenarios Basic, as listed in Table R5. The impact of J_{O1D} on the simulation results of Case 1 was negligible, and the impact on the simulation results of Case 3 was less than 3%. In Case 2 with the largest change in J_{O1D}, the effects on radicals and AOC were less than 10%, and the effects on OH reactivity and OH chain length could be ignored.

Table R5. Summary of simulation results with or without J_{O1D} calibration

Case 1 Scenarios	**J_{O1D}** **10^{-5} s^{-1}**	**OH** **10^6 mole cm^{-3}**	**HO_2** **10^8 mole cm^{-3}**	**RO_2** **10^8 mole cm^{-3}**	**AOC** **10^8 mole cm^{-3} s^{-1}**	**OH reactivity** **s^{-1}**	**OH chain** **length**
Basic	1.32±0.93	5.28±3.12	1.99±1.28	1.09±0.70	0.42±0.22	11.48±2.16	3.17±0.63
G	1.31±0.90	5.26±3.10	1.99±1.29	1.09±0.70	0.42±0.22	11.48±2.16	3.17±0.63
Discrepancy	-0.75%	-0.40%	0	0	0	0	0
Case 2 Scenarios	**J_{O1D}** **10^{-5} s^{-1}**	**OH** **10^6 mole cm^{-3}**	**HO_2** **10^8 mole cm^{-3}**	**RO_2** **10^8 mole cm^{-3}**	**AOC** **10^8 mole cm^{-3} s^{-1}**	**OH reactivity** **s^{-1}**	**OH chain** **length**
Basic	0.90±0.72	4.06±2.68	1.88±1.18	1.35±0.82	0.37±0.22	12.96±3.89	3.77±0.89
G	1.19±0.89	4.41±2.94	2.03±1.29	1.46±0.89	0.40±0.24	12.84±3.80	3.74±0.89
Discrepancy	32.22%	8.62%	7.98%	8.15%	8.11%	-0.93%	-0.80%
Case 3 Scenarios	**J_{O1D}** **10^{-5} s^{-1}**	**OH** **10^6 mole cm^{-3}**	**HO_2** **10^8 mole cm^{-3}**	**RO_2** **10^8 mole cm^{-3}**	**AOC** **10^8 mole cm^{-3} s^{-1}**	**OH reactivity** **s^{-1}**	**OH chain** **length**

Basic	1.40±0.97	6.13±3.36	1.76±1.22	1.51±1.08	0.40±0.23	8.41±1.21	4.96±1.08
G	1.49±0.97	6.22±3.44	1.78±1.23	1.53±1.09	0.41±0.24	8.41±1.21	4.95±1.08
Discrepancy	7.98%	1.47%	1.14%	1.32%	2.50%	0	-2.02%

Based on the discussion above, it is found that the calibrated J_{O1D} considering clouds condition deviated from the J_{O1D} directly scaled by the measured J_{NO_2} for -0.75%, 32.22%, and 7.97% during these three cases. Additionally, the modelling results shows the limited impacts of J_{O1D} calibration for clouds on the results and has not changed the main conclusions for the three cases in this study.

Due to the particularity in the approximation method of equation (E2) and uncertainty on ozone column data, we think this calibration method is not an accurate way to calibrate J_{O1D} for this study. Therefore, we decided to use the J_{O1D} scaled by the measured J_{NO_2} as the O_3 photolysis frequency in three cases. We have also mentioned this impacts in the manuscript. Please refer to Line 152-153 and the Supplement.

Page 5, line 155: There are better references to provide for the definition of OH reactivity (similarly for OH chain length). The equation given could be generalized more widely instead of showing several species explicitly and ‘other’.

R: We have found a better equation of OH reactivity from previous study (Whalley et al., 2016) and have cited it as $k_{OH} = \sum_i k_{OH+X_i}[X_i]$, where $[X_i]$ represents the concentration of species (VOC, NO_2, CO etc.) which react with OH and k_{OH+X_i} is the corresponding reaction rate coefficients. Please refer to Line 170-174.

Page 6, line 170: ‘pollutants’ to ‘pollutant’.

R: Thanks for the suggestion. The ‘pollutants’ has been corrected to ‘pollutant’. Please refer to Line 187.

Page 6, line 173: ‘concentrations’ to ‘mean concentrations’. It would be helpful to include the standard deviation and median (and elsewhere where mean concentrations are referred to).

R: We have followed the suggestion and replaced ‘concentrations’ with ‘mean mixing ratios’ (also pointed by Reviewer #2 to change the concentration to mixing ratio), as well as added standard deviation and elsewhere in the manuscript. Please refer to Line 190 and elsewhere.

Page 7, Figure 1 caption: ‘of Shanghai’ to ‘in Shanghai’.

R: Thanks for the suggestion. The ‘of Shanghai’ has been replaced with ‘in Shanghai’. Please refer to Line 199.

Page 7: Are any of the cases chosen for detailed study representative of typical behavior?

R: Please also refer to the responses to the main comments #1. As shown in Table 1, the ozone hourly mean values for the selected cases were 65.13±27.16 ppbv, 46.12±21.14 ppbv and 23.95±11.89 ppbv, respectively, representing ozone pollution, moderate condition and non-pollution. Meanwhile, the five month observations shows that ozone is the primary air pollutant for the air quality degraded during summer of 2018 in Shanghai. So we have selected these three cases to explore the atmospheric oxidation capacity and photochemical reactivity during the summertime and their potential relationship with ozone pollution. In addition, the comparison of other trace gases is shown in Figure R1, showing the different characteristics of the three cases.

Page 7, line 189/Figure 1: The differences in wind speed are difficult to see in the figure. ‘the unfavourable diffusion condition is’ to ‘unfavourable diffusion conditions are’.
R: Thanks for the suggestion. We have redrawn the Figure 1 to ensure a clear view of the wind speed. And the ‘the unfavourable diffusion condition is’ has been corrected to ‘unfavourable diffusion conditions are’. Please refer to Line 208.

Page 7, line 192: ‘lead’ to ‘leads’. ‘the JNO2’ to ‘when the JNO2’.
R: The ‘the J_{NO_2}’ have been corrected to ‘when the J_{NO_2}’. The ‘lead’ does not need to be modified in the revised manuscript. Please refer to Line 212.

Page 8, line 204: ‘an average total VOCs’ to ‘average total VOC’.
R: Thanks for the suggestion. We have corrected the ‘an average total VOCs’ to ‘average total VOC’. Please refer to Line 223-224.

Page 9, line 213: ‘highest concentrations in alkanes’ to ‘highest concentration alkanes’ and ‘the main species in alkenes’ to ‘the main alkene species’.
R: Thanks for the suggestion. The ‘highest concentration in alkanes’ and the ‘the main species in alkenes’ have been corrected to ‘highest mixing ratio alkanes’ and ‘the main alkene species’ (also pointed by Reviewer #2 to change the concentration to mixing ratio), respectively. Please refer to Line 230-231.

Page 9, line 215: Define the meaning of ‘maximum incremental reactivity’.
R: Thanks for the suggestion. We have defined the MIR in the calculation formula of the OFP in Line 433. And we have followed the suggestion and added the definition of maximum incremental reactivity in the table caption here. Please refer to Line 234-236.

Page 10, line 220: ‘due to acetylene is’ to ‘since acetylene is’ or ‘due to acetylene being’. Would it be more sensible to group as saturated aliphatic hydrocarbons and unsaturated aliphatic hydrocarbons?
R: Thanks for the suggestion. The ‘due to acetylene is’ has been corrected to ‘due to acetylene being’. Considering that both acetylene and alkenes are unsaturated aliphatic hydrocarbons, which have unsaturated bonds, acetylene and other species with carbon-carbon double bonds are classified as alkenes category for the convenience of statistics. As pointed by the Reviewer #2, it should be clarified that the reactivity of acetylene with OH is far less than that of alkenes with OH, and be noted in the footnote of the table.
We have rewritten this sentence into ‘Due to acetylene being similar in nature to alkenes, acetylene is classified into the alkenes category. It should be noted that the reactivity of acetylene with OH is far less than that of alkenes with OH’. Please refer to Line 238-239.

Page 10, section 3.2: What was the AOC in Berlin?
R: Geyer et al. (2001) reported that the maximum AOC value reached 1.4×10^{7} molecules cm^{-3} s^{-1} in Berlin and much lower than that of this study. And we have added relevant data in the revised manuscript. Please refer to Line 245.

Page 11, Figure 2: It would be interesting to be able to see the nighttime data as well,

perhaps a log scale for the y-axis or a separate plot?
R: We have followed the suggestion and drew a separate plot to show the nighttime data series clearly in the Supplement (see Figure S3).

Page 11, line 251: ‘lower than that of Case 2 and Case 3’ should be ‘lower than that of Case 1 and Case 2’? Do the calculated losses of OH include reactions of OH with model generated oxidation intermediates or are the values reported given for observed concentrations only? If model generated oxidation intermediates are included, what are the impacts of deposition rates on the calculated reactivity? On page 12 it is stated that measured species are used to calculate OH reactivity, but intermediates from the model simulations could be included. If they haven’t been, why not?
R: We are really sorry for the mistakes, which have been corrected. Please refer to Line 271. The calculated losses of OH just include reactions of OH with the species observed previously.
The influence of the deposition process on the simulation results was discussed in the response to main comments #1. After comparing the simulation results with or without consideration of the deposition process, it is definitely necessary to consider the deposition process in the simulation and re-discuss the corresponding results, which are updated in the revised manuscript. In the revised manuscript, the intermediates from the model simulations were included in the discussion on OH reactivity. Please refer to Line 265-287.

Page 12, line 258: There are also measurements of OH reactivity in urban regions in London.
R: Thanks for the information. We have reviewed the related reference presented by Whalley et al. (2018), in which the OH reactivity has been measured to be 15~27 s^{-1} in central London in the summer of 2012 during the Clean air for London project (ClearfLo). We have also cited it in Line 280.

Page 12, Figure 3: The y scale chosen is not ideal, the plots would be clearer if a smaller scale were used.
R: Thanks for the suggestion. We have chosen a smaller y-scale to redraw Figure 3.

Page 13, line 277: ‘Case 1 about’ to ‘Case 1 was about’. The statement ‘may be caused’ could be strengthened – the data are there to show this either way without conjecture.
R: Thanks for the suggestion. The ‘Case 1 about’ has been corrected to ‘Case 1 was about’. Please refer to Line 297-298. Data for trace gases and VOCs are shown in Table 1. We have rewritten this sentence into ‘This is caused by the higher VOCs levels of 29.73±12.10 ppbv during Case 2 as compared to Case 1 of about 15% lower’. Please refer to Line 299-300.

Page 13, line 284: Do the authors mean to say that OVOCs are the main contribution or the second highest contribution? The use of ‘predominant’ indicates they are the main contributions, but the following discussion states alkenes represent the largest contribution.
R: As we have recalculated the OH reactivity including model-generated intermediate species, OVOCs were the highest contribution to OH reactivity for total NMVOCs. We still use this predominant to describe the important contribution of OVOC to OH reactivity, but to modify the description of the contribution of alkenes to OH reactivity.

Please refer to Line 303-309.

Line 13, line 290: Please quantify the statements ‘similar’ and ‘negligible’.
R: Thanks for the suggestion. In three periods, the contributions of aromatics and alkanes to OH reactivity were comparable, both in the range of 0.3~0.6 s^{-1}, accounting for 10%~20%. And the contribution of other VOCs to OH reactivity was negligible, and the contribution ratio was only 0.4% or less. We have quantified the statement ‘similar’ and ‘negligible’ in Line 309-312.

Line 13, line 291: Are there any alcohol concentrations in similar locations? Do the authors expect significant contributions from these species?
R: The observed alcohol data are rarely reported in Shanghai and we have only found few useful data for reference. The data observed by Cai et al. (2010) showed that the mean mixing ratio of isopropyl alcohol is 0.27±1.08 ppbv and the fluctuation range is 0 ~ 14.32 ppbv from July 2006 to February 2010 in Shanghai. The mean mixing ratio of isopropyl alcohol measured by Zhang et al. (2018) reached 2.3 pbbv in Nantong, Jiangsu Province, situated to north of Shanghai, ranking third among the 105 VOCs measured. And the paper reported that the OFP of alcohols reached about 3.5 $\mu g\ m^{-3}$, which indicated that alcohols have high activity and contribute to OH reactivity.
We have re-calculated the OH reactivity including the simulated intermediate species. The contribution of OVOCs to OH reactivity was 1.77 s^{-1}, 2.05 s^{-1} and 1.26 s^{-1}, while the OH reactivity of OVOCs calculated by considering only the measured species was 1.28 s^{-1}, 1.43 s^{-1}, and 0.82 s^{-1} in three cases, respectively. So we expect that unmeasured species (e.g. alcohols) may cause underestimation the contribution of OVOCs to OH reactivity. In the revised manuscript, the model-calculated OH reactivity include the contribution of the simulated intermediate species to OH reactivity.

Page 14, line 305: ‘evaluating the HOx’ to ‘evaluating HOx’.
R: We have deleted ‘the’ before ‘HOx’. Please refer to Line 324.

Page 14, line 310: ‘within’ to ‘less than’?
R: The ‘within’ has been replaced with ‘less than’. Please refer to Line 329.

Page 15, line 322: Why were contributions from peroxides excluded?
R: The contribution of peroxides to HO_X is limited. For example, the rates of H_2O_2 to HO_x in three cases were 7.65×10^4 molecules $cm^{-3}\ s^{-1}$, 6.98×10^4 molecules $cm^{-3}\ s^{-1}$ and 4.28×10^4 molecules $cm^{-3}\ s^{-1}$, which are two orders of magnitude smaller compared to O_3, HONO, HCHO photolysis, and alkenes ozonolysis. So there's no discussion here.

Page 15, line 324: ‘sinks of HOx was’ to ‘sinks of HOx were’.
R: Thanks for the suggestion. The ‘sinks of HO_x was’ has been corrected to ‘sinks of HO_x were’. Please refer to Line 345.

Page 15, line 331: ‘generation rate of HOx was’ to ‘generation rates of HOx were’.
R: Thanks for the suggestion. The ‘generation rate of HO_x was’ has been corrected to ‘generation rates of HO_x were’. Please refer to Line 352.

Page 15, line 332: ‘loss rate was’ to ‘loss rates were’. Please include ‘and’ before the final value.

R: Thanks for the suggestion. The ‘loss rate was’ has been corrected to ‘loss rates were’. And we have rewritten this sentence into ‘while the average loss rates were 1.34±0.7×10^7 molecules cm^{-3} s^{-1}, 1.00±0.55×10^7 molecules cm^{-3} s^{-1} and 0.8±0.52×10^7 molecules cm^{-3} s^{-1}’. Please refer to Line 353-354.

Page 15, line 336: What were the concentrations of HONO and O3? Did the HONO concentration change significantly between cases?

R: As listed in Table 1, the mean mixing ratios of O_3 were 65.13±27.16 ppbv, 46.12±21.14 ppbv and 23.95±11.89 ppbv in three cases, respectively, while the mean mixing ratios of HONO were 0.36±0.16 ppbv, 0.32±0.17 ppbv and 0.22±0.05 ppbv, respectively. In addition, the mean diurnal profiles of O_3 and HONO are shown in figure R1. HONO were at low levels without significant diurnal variation in Case 3 under the low O_3 level, however, its mixing ratios increased strongly and exhibited distinct diurnal profiles in Case 1 and Case 2 of relatively high O_3 levels.

Page 16: It would be helpful to include some discussion of the concentrations of OH, HO2 and RO2, and any details of the main RO2 species in the model, with comparison to measured values in similar locations. Some discussion of the nighttime chemistry would also be of interest.

R: We have discussed the simulation results with deposition process in the revised manuscript instead of the previous simulation results without deposition process. Since the Sect 3.3 focuses on the discussion about sources and sinks of HO_x radicals, we have followed the suggestion and supplemented a discussion of the concentration of HO_x and their comparison with measured values from other sites in the revised manuscript, and won’t discuss here for RO_2. Please refer to Line 387-398.

Since this article mainly discusses daytime photochemistry and there is no observation of NO_3 and N_2O_5 related to nighttime photochemistry, we have not discussed nighttime chemistry so much here. But we also mentioned the important contribution of NO_3 to AOC during nighttime in this study. Please refer to Line 254-256. In the future, we can strengthen the observations at night to better discussion on nighttime chemistry.

Page 17, line 373: ‘VOCs concentrations’ to ‘VOC concentrations’.

R: The ‘VOCs concentrations’ has been corrected to ‘VOC mixing ratios’ (also pointed by Reviewer #2 to change the concentration to mixing ratio). Please refer to Line 410.

Page 18, line 386: ‘VOC groups’ to ‘VOC group’.

R: The ‘VOC groups’ has been corrected to ‘VOC group’. Please refer to Line 412.

Page 18, line 390: ‘OVOCs shows its significant contribution’ to ‘OVOCs show significant contributions’.

R: Thanks for the suggestion. The ‘OVOCs shows its significant contribution’ has been corrected to ‘OVOCs show significant contributions’. Please refer to Line 428.

Page 18, line 401: Is this 14.6 % of the total NMVOC concentration?

R: Yes, during Case 1, the mean mixing ratio of NMVOC was 25.31±6.16 ppbv, and the average mixing ratio of acetone was 3.69±0.78 ppbv, accounting for 14.6%. We have clarified, and please refer to Line 439-440.

Page 20, line 430: ‘increase of radicals level’ to ‘increase of radical levels’.

R: The ‘increase of radicals level’ has been corrected to ‘increase of radical levels’. Please refer to Line 468.

Page 20, line 433: If each radical could generate more O3, why is the O3 level lower?
R: After in-depth relevant literature review, we try to explain the relationship between higher O_3 concentration and shorter chain length as following.
The ratio of the rate of HO_x cycling reactions to HO_x termination is called the chain length, as in equation (E4) (Martinez et al., 2003). When the termination reaction of HO_x is dominated by the reaction of NO_2 and OH, the definition can be simplified as equation (E6).

$$\text{Chain Length} = \frac{[OH]k_{OH} - L(HO_x)}{L(HO_x)} \qquad \text{(E4)}$$

$$L(HO_x) = k_{OH+NO_2}[OH][NO_2] + 2k_{HO_2+HO_2}[HO_2]^2 + 2k_{OH+HO_2}[OH][HO_2] + 2k_{HO_2+RO_2}[HO_2][RO_2] + 2k_{RO_2+RO_2}[RO_2][RO_2] \qquad \text{(E5)}$$

$$OH\ Chain\ Length = \frac{k_{OH}[OH] - k_{OH+NO_2+M}[OH][NO_2]}{k_{OH+NO_2+M}[OH][NO_2]} \qquad \text{(E6)}$$

During daytime, the greater the chain length, the greater the amount of O_3 produced per NO_X molecule converted to HNO_3, rather than the more ozone produced per OH radical. In the profile of OH chain length in Figure 5, the OH chain length in Case 3 with the lowest ozone mixing ratio is the largest, meaning that per NO_X converted into HNO_3 produces more O_3, but the daytime NO_X mixing ratio in Case 3 is almost half that of Case 1 and 2 (see Figure R1), causing ozone mixing ratios to be lower than Case 1 and 2. In addition, we found that the OH chain length was opposite to the ozone level, and the explanation given was also due to the lower NO_X mixing ratios in previous studies (Mao et al., 2010; Ling et al., 2014).

Data availability: It would be preferable to host the data at a secure and available site/database rather than needing to contact the corresponding author.
R: Since the measured VOC data were provided by another group, it is not suitable to be published by us. We are very willing to provide the data of DOAS measurements and modelling simulation for scientific aims with contacts from others, and the communication for the VOCs data availability.

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