Supporting Information for

Causes of a continuous summertime O_3 pollution event in Ji'nan, a central city in the North China Plain

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Contents of this file

Additional Supporting Information (Files uploaded separately)

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Introduction

The supporting information mainly include twelve figures and four tables. All the supplementary information is helpful for the reviewers and readers to better understand this study. The dataset used in this study is comprised of hourly mixing ratios of inorganic trace gases and mass concentration of $PM_{2.5}$, meteorological parameters on hourly basis, hourly average mixing ratios of VOCs and OVOCs, the emission inventories and some open source data accessible online. Trace gases, $PM_{2.5}$ and meteorological parameters were measured continuously, while VOCs and OVOCs samples were collected and analyzed off-line. The data can be accessible at

https://drive.google.com/open?id=1_KeOxOuVsLY83xL74RtcRORsiiyIR8FZ. Overall, we used the data to do basic statistical analyses and to construct the photochemical box model and chemical transport model. The completeness and quality of the data are high enough to support us to do analyses and draw important conclusions in this study.

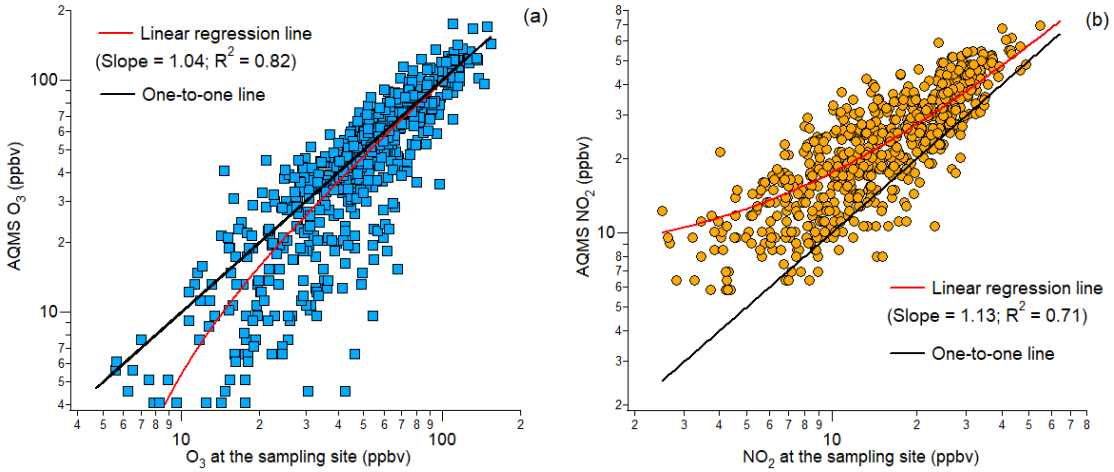
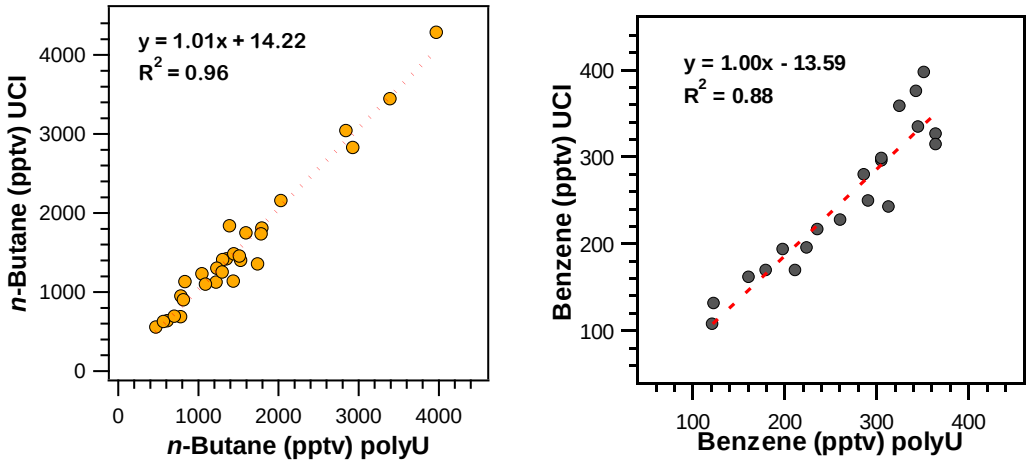


Figure S1. Agreement of the hourly (a) O_3 and (b) NO_2 between our observations on the campus of Shandong University and those monitored at the nearest AQMS by CNEMC.



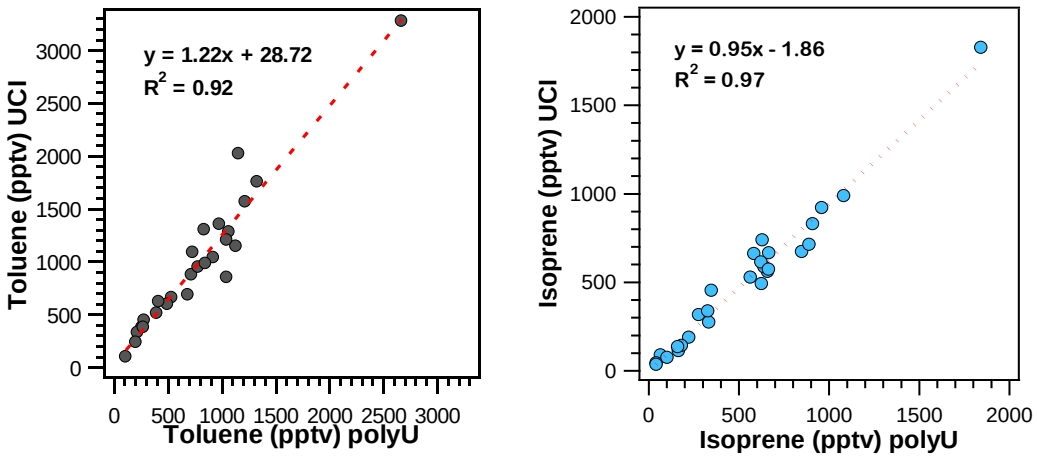


Figure S2. Inter-comparison of VOC analysis results between our laboratory (x axis) and Prof. Donald Blake's group (y axis). *n*-butane, benzene, toluene and isoprene are selected as examples. The red dashed line represents the linear regression between VOCs analyzed in two laboratories.

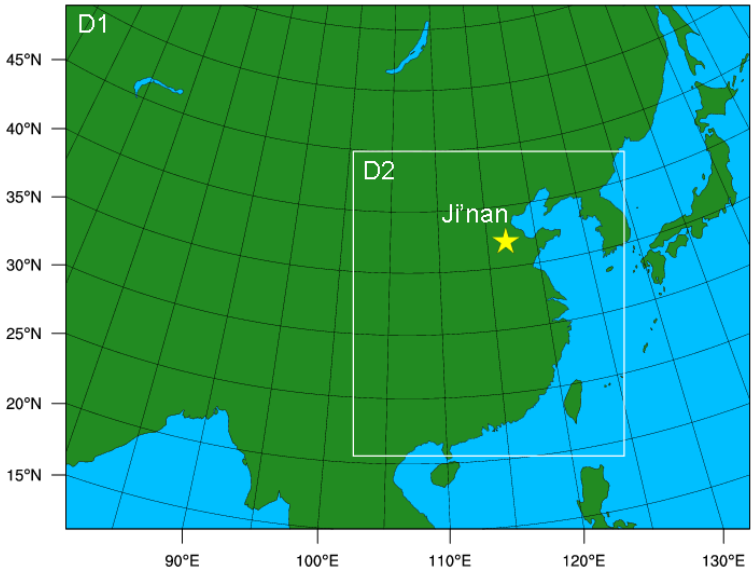


Figure S3. Settings of the two-nested domains for the WRF-CMAQ model. D1 and D2 are the outer and inner domain, covering the entire continental area of China and eastern China, respectively. The yellow star represents Ji'nan.

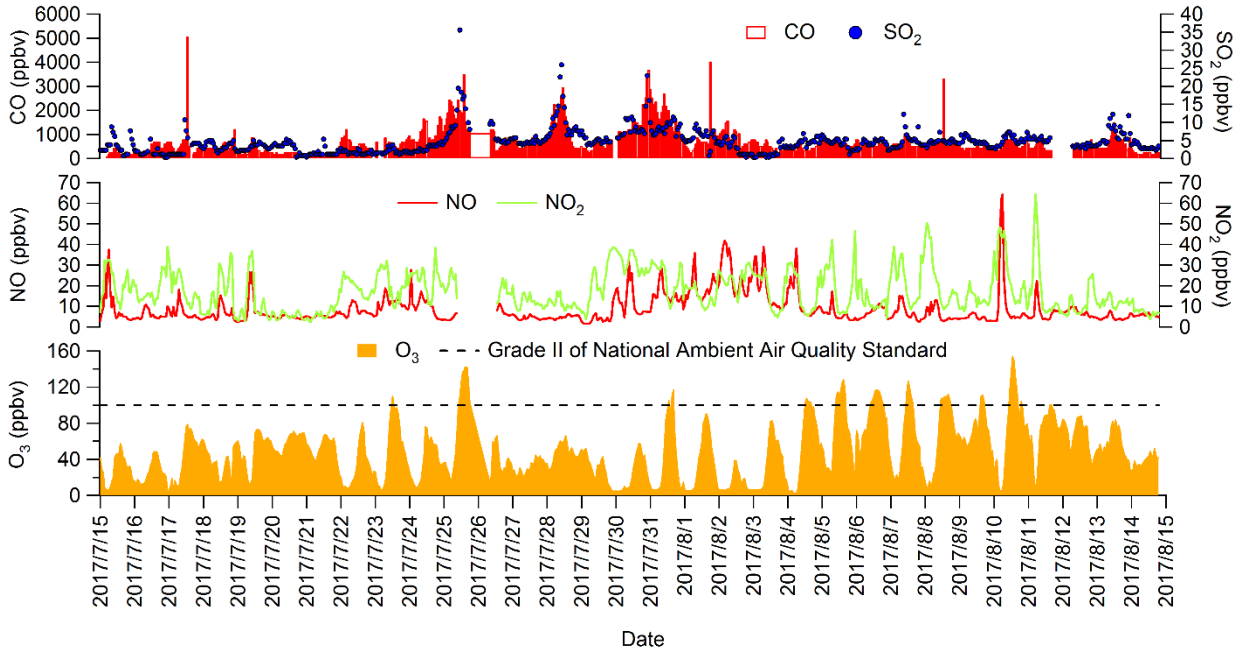
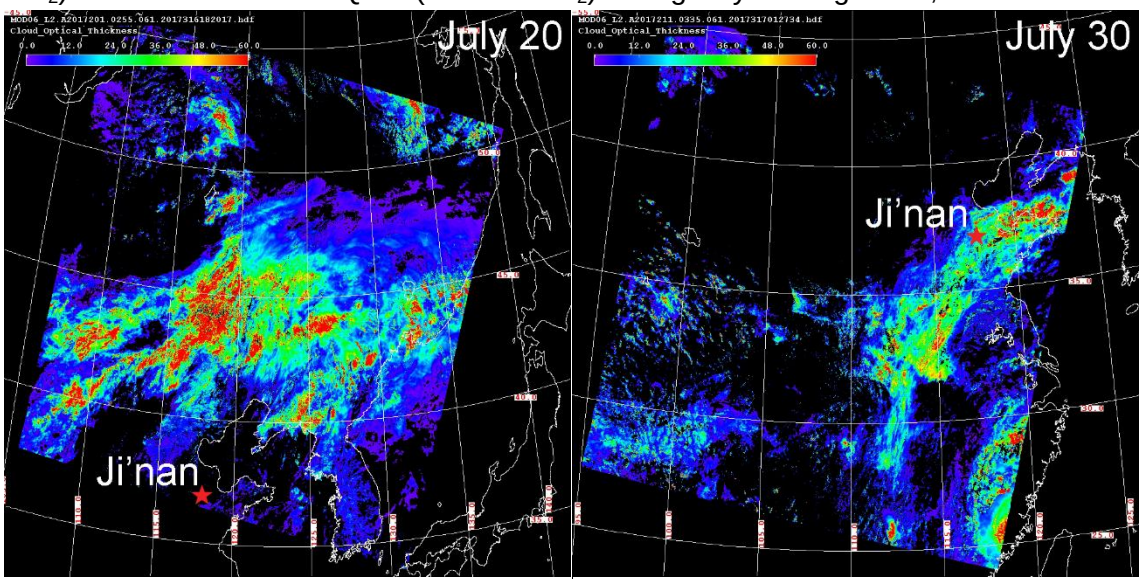
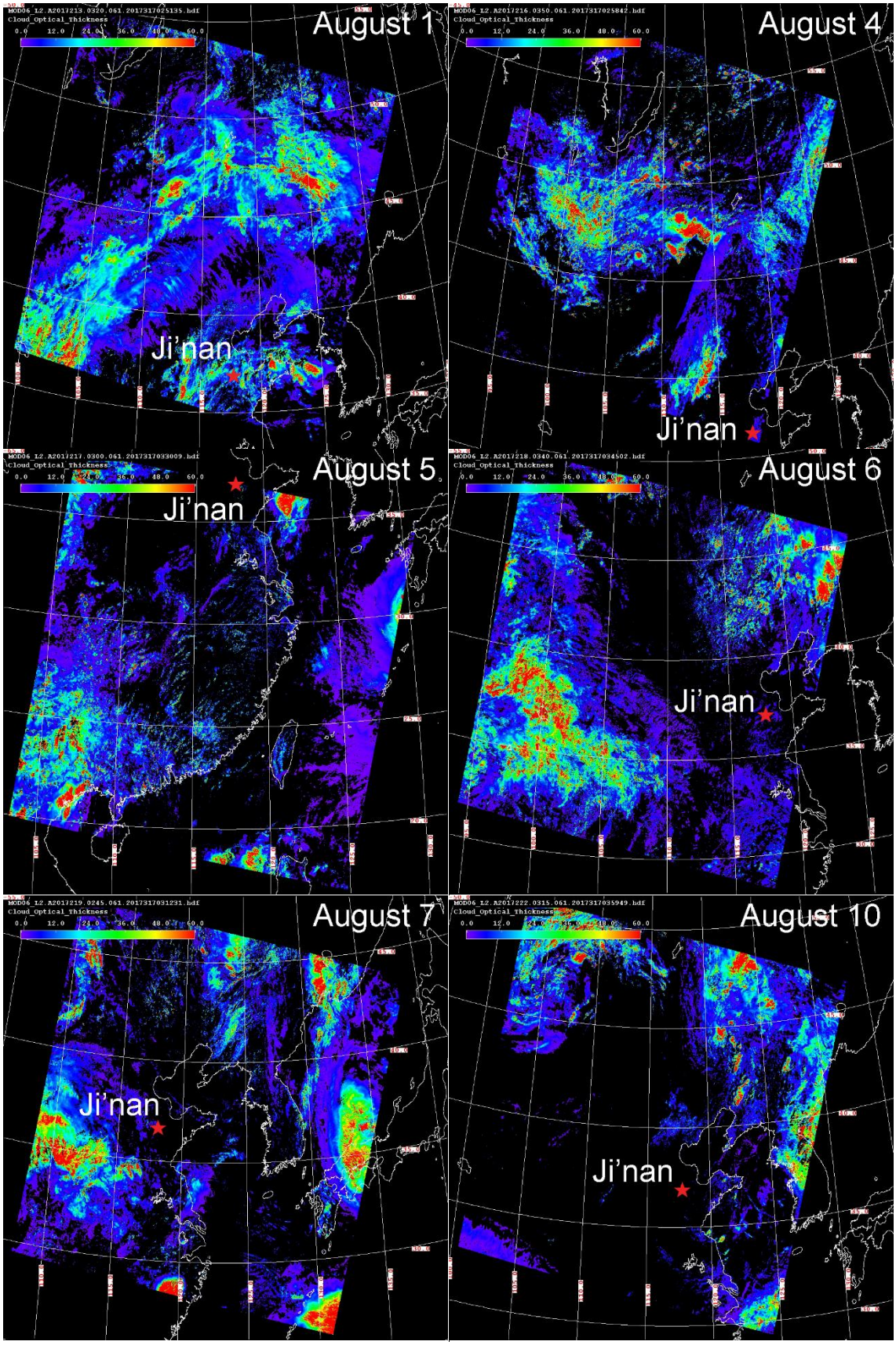


Figure S4. Hourly variations of trace gases monitored at the sampling site (O_3, NO and NO_2) and at the nearest AQMS (CO and SO_2) during July 15-August 14, 2017.




August 1
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August 7
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August 10
Ji'nan

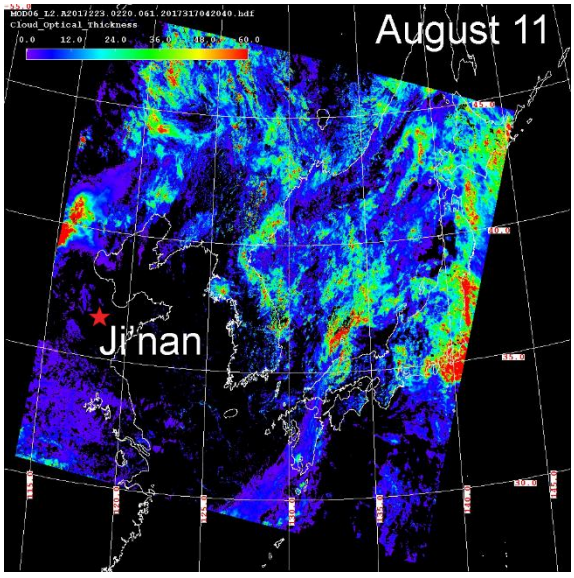
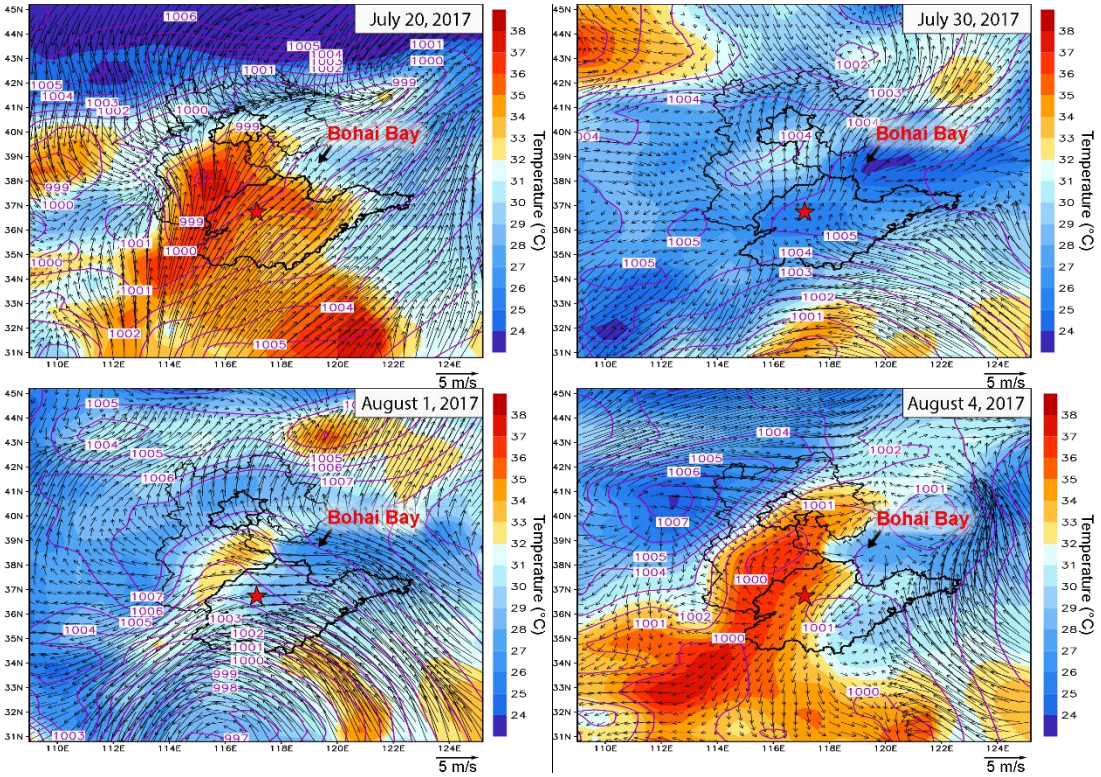


Figure S5. Cloud optical depth (COD) retrieved from terra/MODIS at noon (10:30 – 12:00 LT) of the canister sampling days. The color scale denotes for the COD within the range of 0 (purple) to 60 (red). The red star denotes Ji'nan.



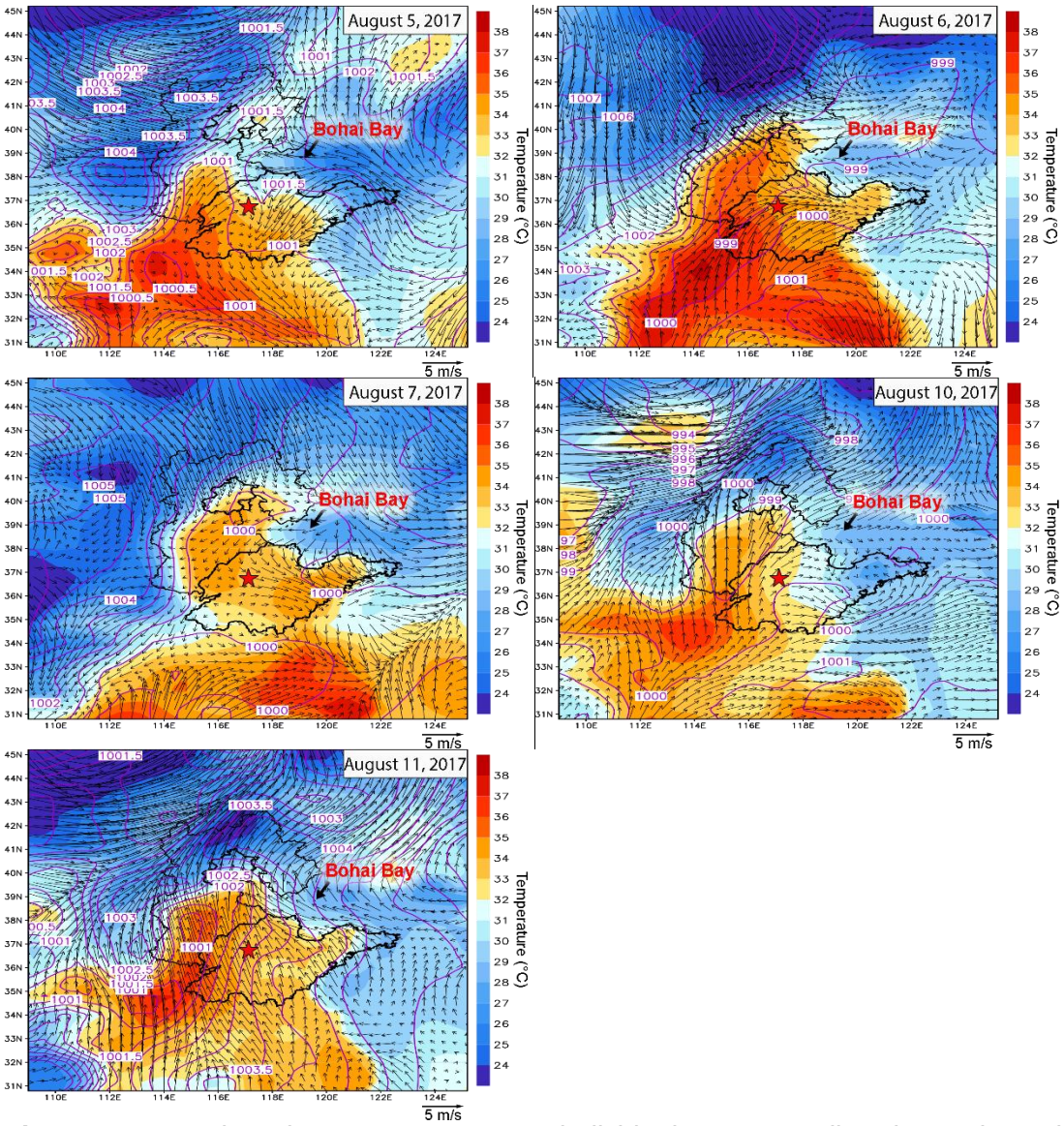
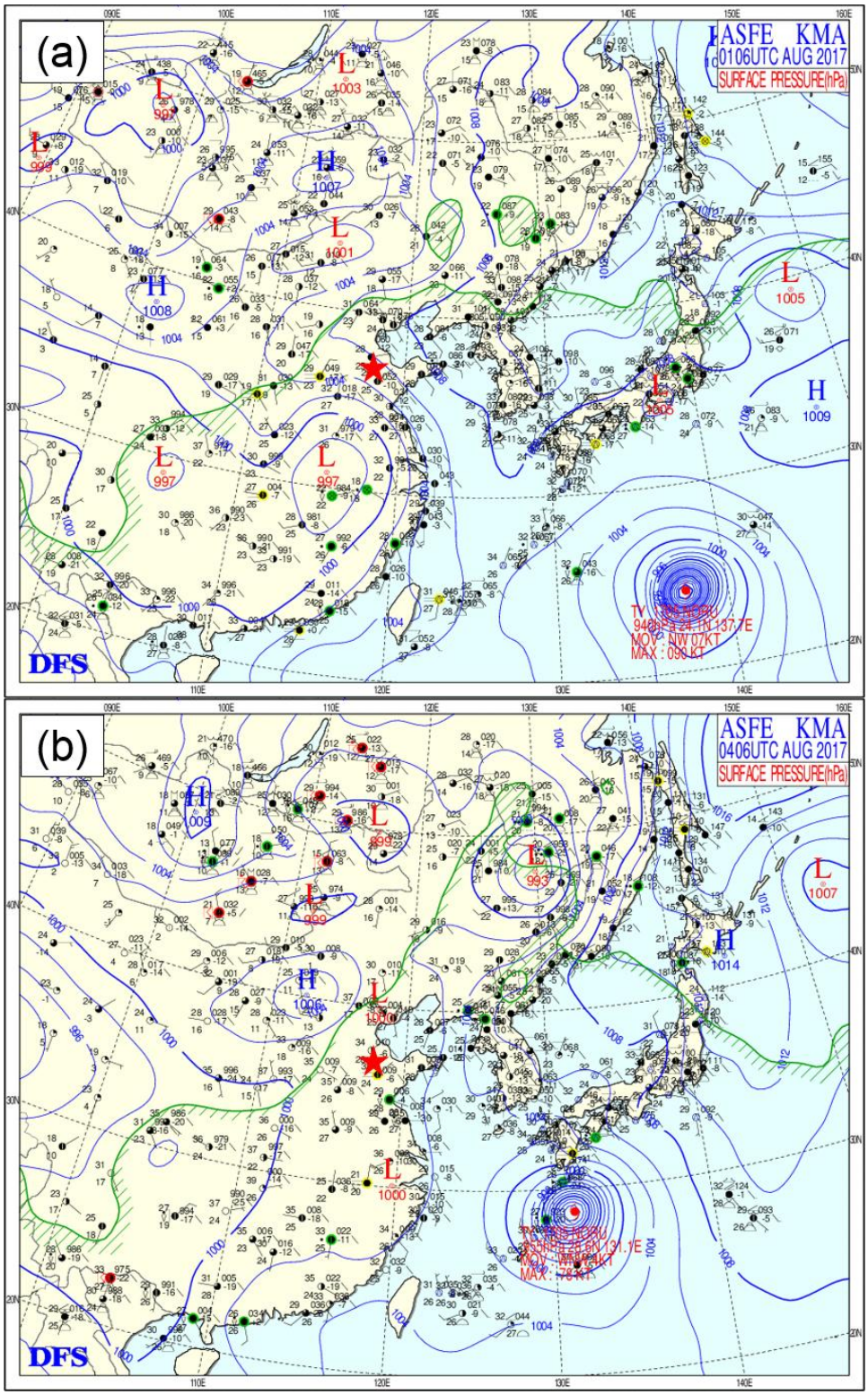


Figure S6. Weather charts at 14:00 LT on individual VOC sampling days. The red star denotes for Ji'nan.


(a)
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(b)
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SURFACE PRESSURE(hPa)
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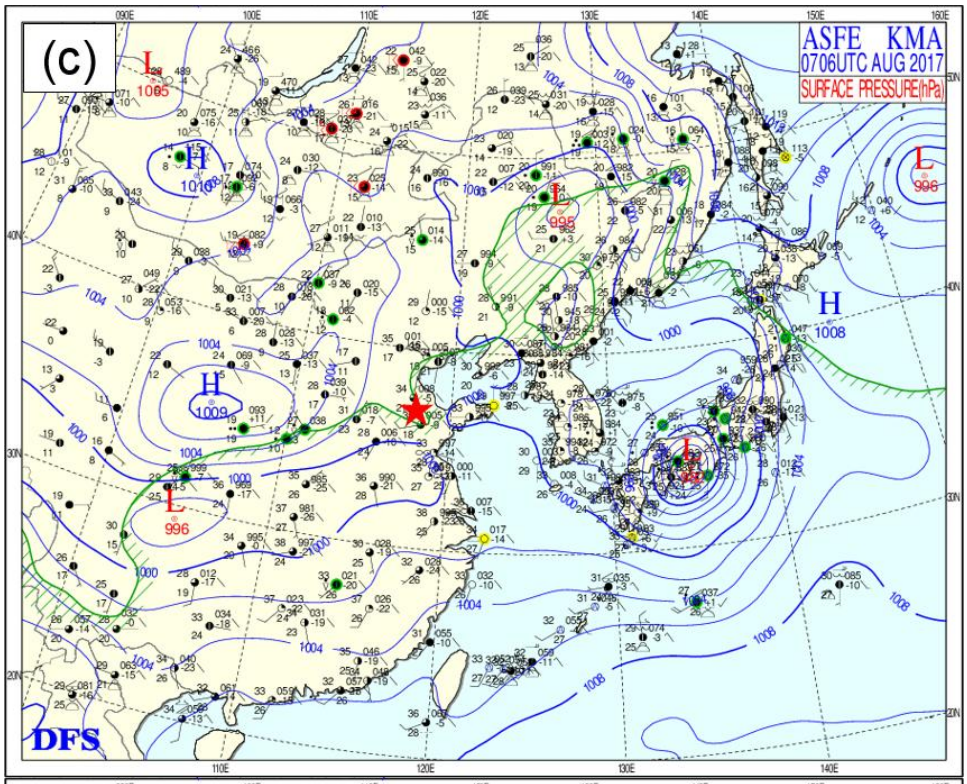
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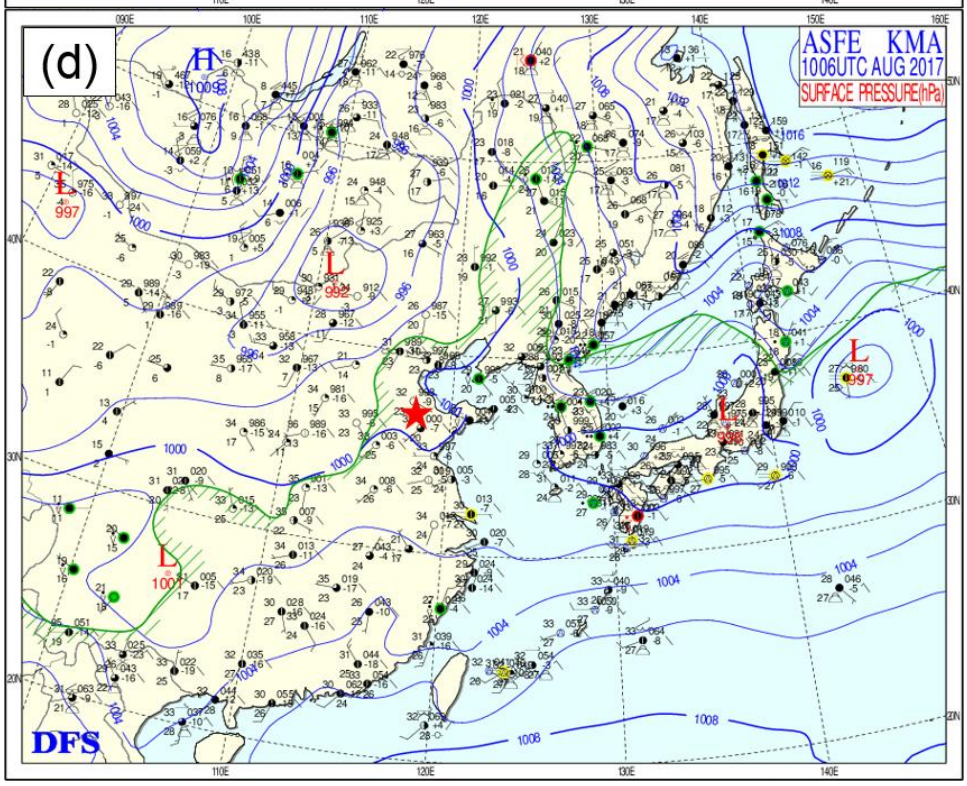
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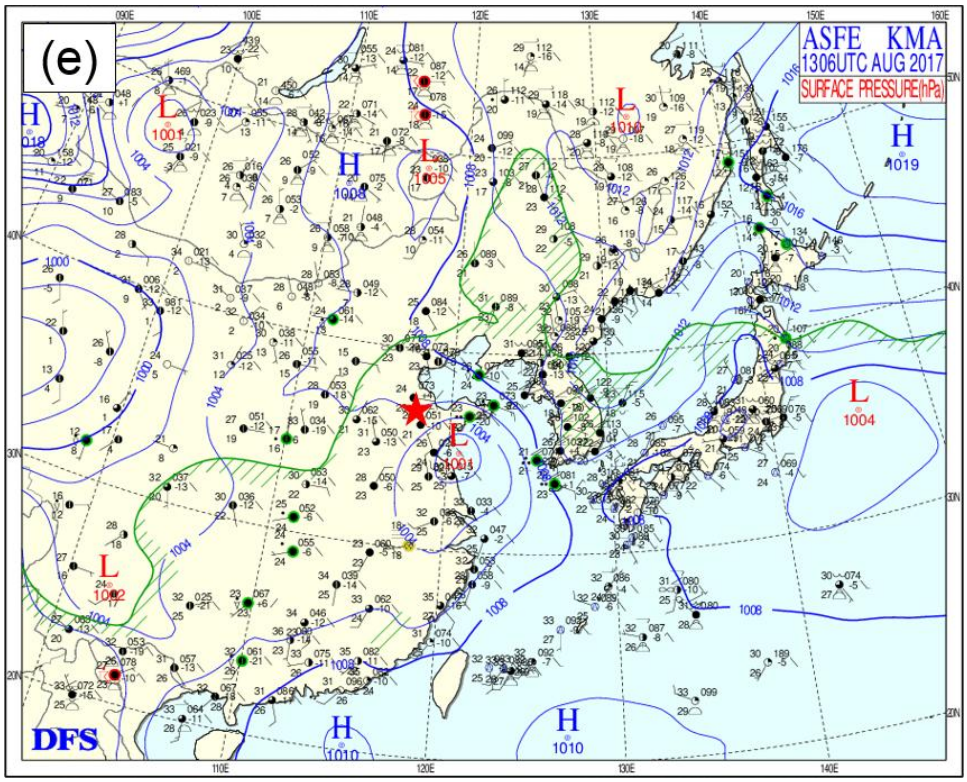
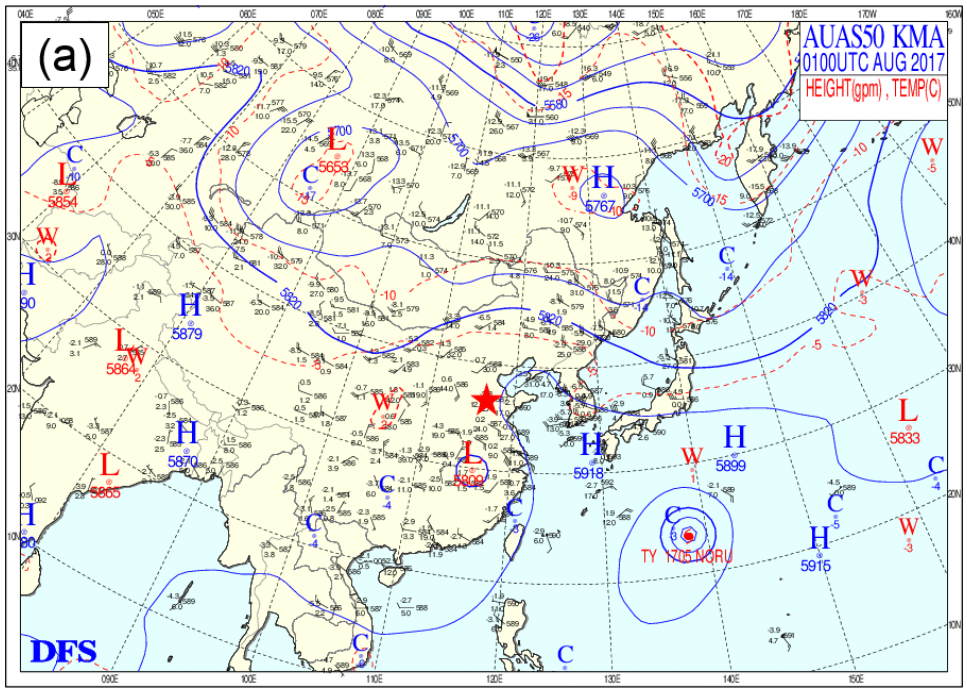
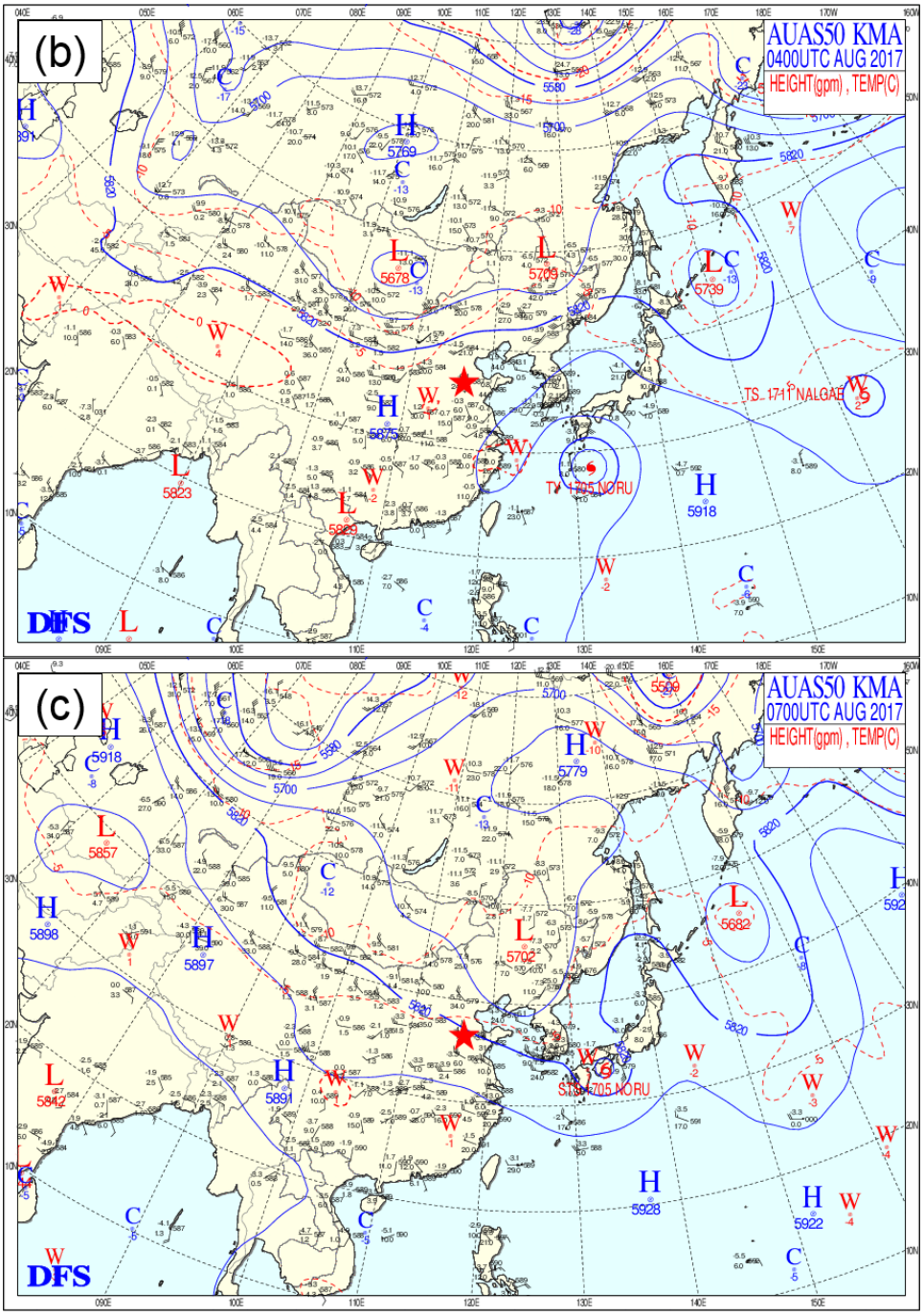


Figure S7. Weather chart over the Northeast Asia on (a) August 01, (b) August 04, (c) August 07, (d) August 10 and (e) August 13 at 06:00 UTC (14:00 LT) at surface level. The red star denotes Ji'nan city. The capital letter "H" and "L" represents high pressure center and low pressure center, respectively. Blue lines are the sea level isobars. Green line is the isometric humidity line with the specific humidity of ≥15g/kg on the grid side. All the charts can be accessed through the link: http://222.195.136.24/forecast.html.




(b)
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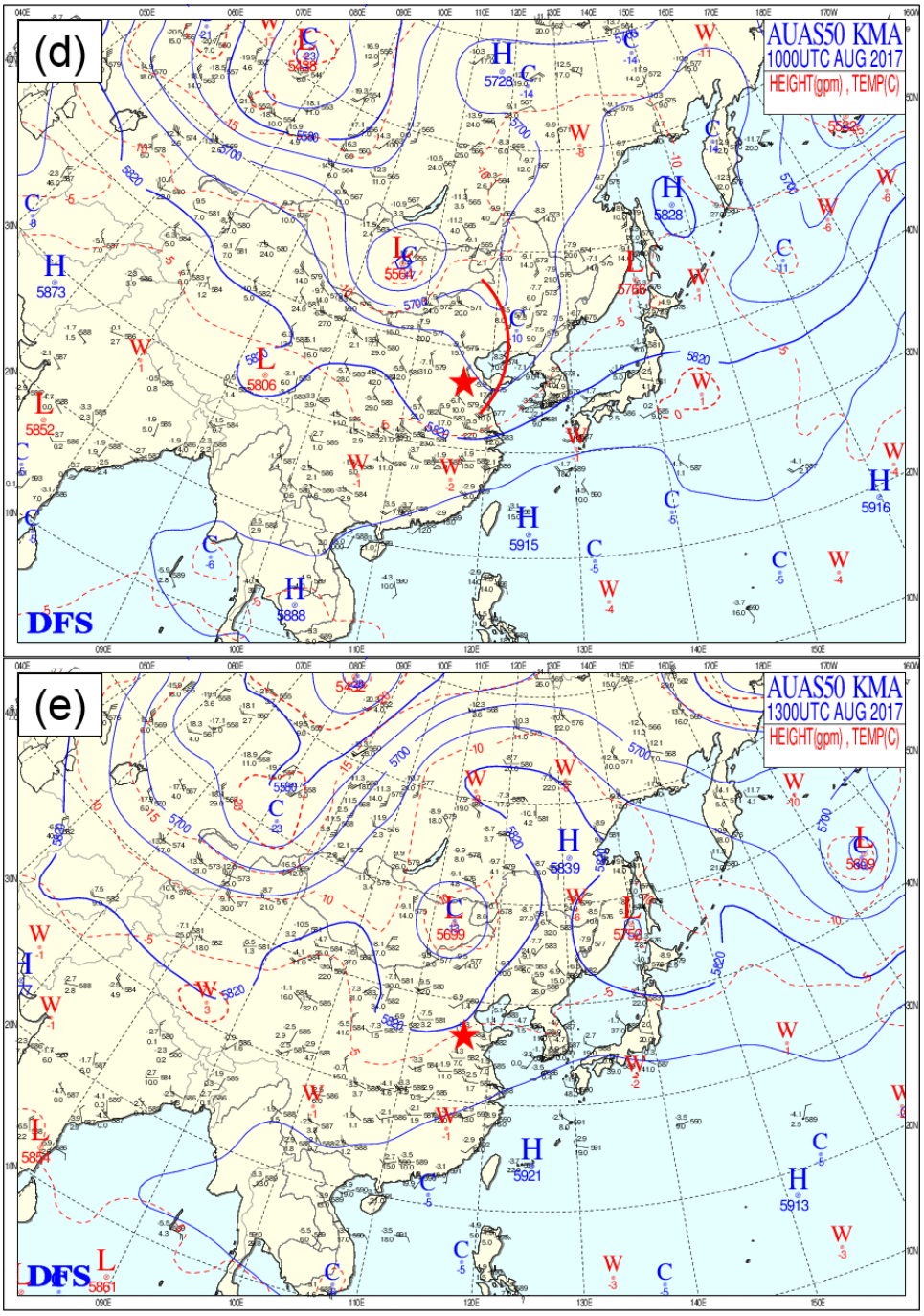

Figure S8. Weather chart over the Northeast Asia on (a) August 01, (b) August 04, (c) August 07, (d) August 10 and (e) August 13 at 00:00 UTC (08:00 LT) at altitude of 500 hPa. The red star denotes Ji'nan city. The capital letter "H" and "L" represents high pressure center and low pressure center, respectively. Blue lines are the 500 hPa geopotential height (gpm) lines. The red curve in panel (d) demonstrates the low pressure trough. All the charts can be accessed through the link: http://222.195.136.24/forecast.html.

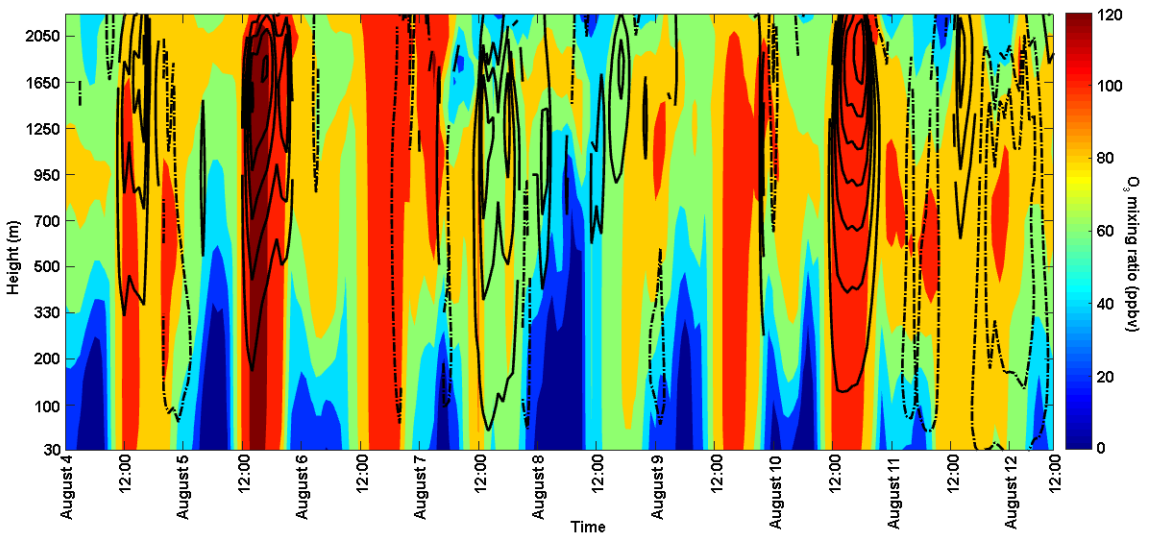

Figure S9. Vertical profile of the simulated O_3 over Ji'nan during August 4-11. The black solid and dotted lines represent the updraft and downdraft simulated by WRF-CMAQ, respectively. The areas with no line indicate that there were no simulated winds in vertical direction.

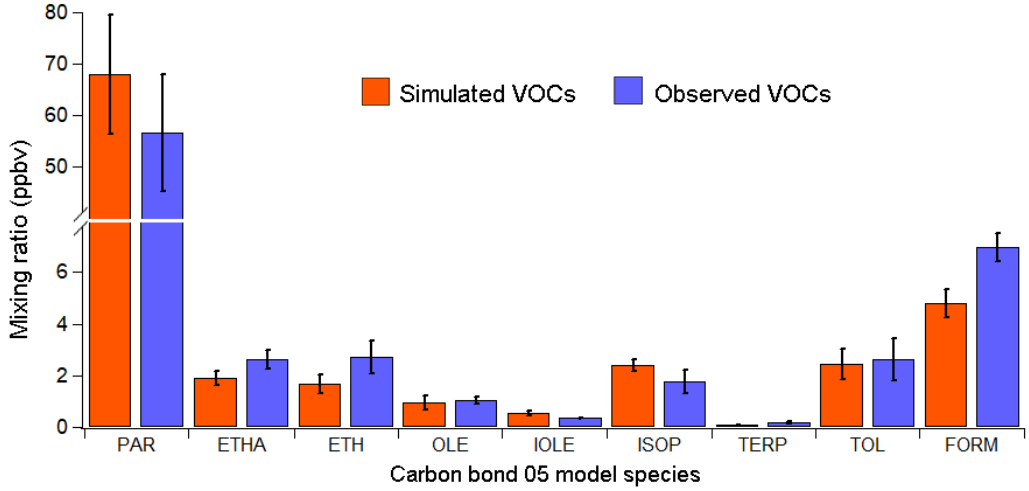

Figure S10. Comparison between the averages of the hourly observed and WRF-CMAQ simulated VOCs. PAR: paraffin carbon bond; ETHA: ethane; ETH: ethene; OLE: terminal olefin carbon bond; IOLE: internal olefin carbon bond; ISOP: isoprene; TERP: terpene; TOL: toluene and other monoalkyl aromatics; FORM: formaldehyde. The matrix of assignments from real compounds to carbon bond 05 model species can be found in Yarwood et al. (2005).

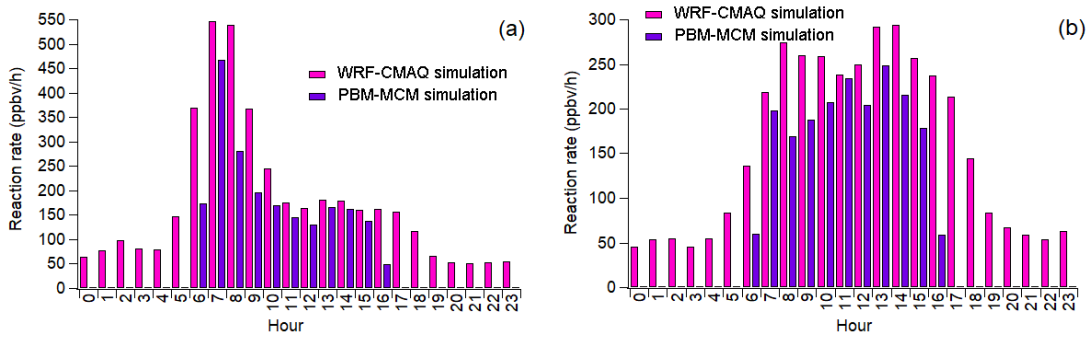

Figure S11. Average diurnal cycle of "NO+O_3" reaction rates simulated by WRF-CMAQ and PBM-MCM during (a) O_3 episodes and (b) non-episodes.

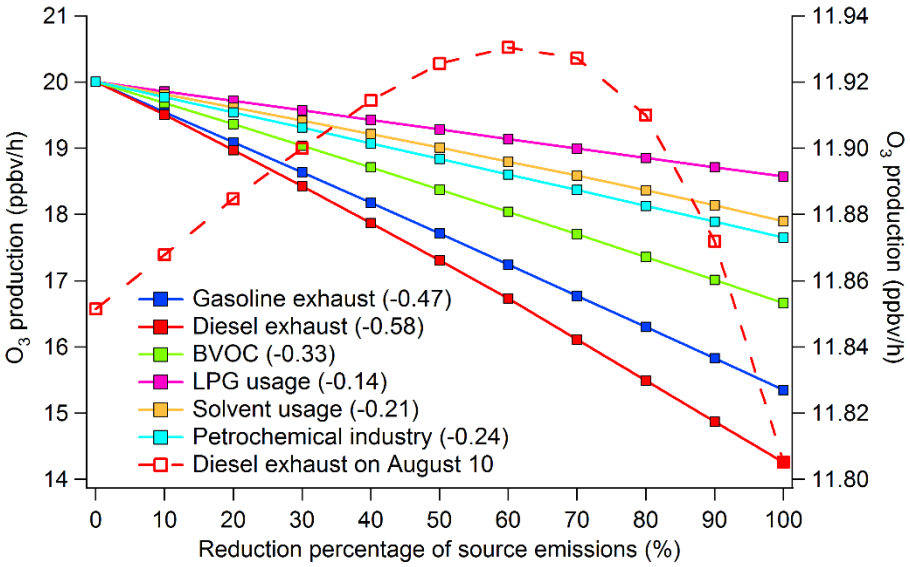

Figure S12. Relationship between O_3 production at 12:00 LT averaged over the O_3 episodes and the reduction percentage of source emissions (left Y-axis). Effect of the diesel exhaust reduction on O_3 production on August 10 is shown separately to illustrate the change of O_3 formation mechanism (right Y-axis). Numbers in the brackets are the average variations of O_3 production with 10% reduction of source emissions.

Species	Site	Instrument	Resolution	Accuracy	Precision	Detection limit
SO_2	AQMS*	API, Model 100 E	20 sec	<20%	0.5% of reading above 50 ppbv	0.4 ppbv
CO	AQMS	API, Model 300 E	10 sec	<20%	0.5% of reading	40 ppbv
NO-NO_2-NO_x	AQMS	API, model 200E	20 sec	<20%	0.5% of reading	0.4 ppbv
	Campus site #	Thermo, Model 42C	1 min	<15%	0.4 ppbv	0.4 ppbv
O_3	AQMS	API, model	10 sec	<20%	<0.5% of	0.6 ppbv

	Campus site	400E Thermo, Model 49C	20 sec	<15%	reading 1.0 ppbv	1.0 ppbv

* An air quality monitoring station of China National Environmental Monitoring Center closest to our sampling site in the campus of Shandong University; # Our sampling site on the campus of Shandong University.

Table S1. Descriptions of the trace gas analyzers used in this study.

Date	Episode/Non-episode	$J(O^1D)$ (s^{-1})	JNO_2 (s^{-1})
July 20	Non-episode	3.40×10^{-5}	9.27×10^{-3}
July 30	Non-episode	1.02×10^{-5}	2.73×10^{-3}
August 1	Non-episode	2.71×10^{-5}	7.50×10^{-3}
August 4	Episode	2.85×10^{-5}	7.95×10^{-3}
August 5	Episode	2.69×10^{-5}	7.50×10^{-3}
August 6	Episode	2.75×10^{-5}	7.70×10^{-3}
August 7	Episode	2.34×10^{-5}	6.52×10^{-3}
August 10	Episode	3.07×10^{-5}	8.72×10^{-3}
August 11	Episode	2.90×10^{-5}	8.25×10^{-3}

Table S2. Daily maximum photolysis rates of O_3 and NO_2 on VOC sampling days in Ji'nan.

OH reactivity of species X	Full name of species/VOC groups	Species included
RNO	Nitric oxide	Nitric oxide
RNO2	Nitrogen dioxide	Nitrogen dioxide
RCO	Carbon monoxide	Carbon monoxide
RCarbonyls	Carbonyls	Formaldehyde, acetaldehyde, acetone, hexanal
RBVOCs	Biogenic VOCs	Isoprene, *α*-pinene, *β*-pinene
RAromatics	Aromatics	Benzene, toluene, ethylbenzene, *m*/*p*-xylenes, *o*-xylene
RAlkenes	Alkenes	Ethene, ethyne, propene, 1-/*i*-butene, 1,3-butadiene, *trans*-2-butene, *cis*-2-butene, 1-pentene
RAlkanes	Alkanes	Ethane, propane, *n*/*i*-butanes, *n*/*i*-pentanes

Table S3. Full name of inorganic trace gases and VOC species for the calculation of OH reactivity.

O_3 production pathway	O_3 destruction pathway
$HO_2 + NO$	$OH + NO_2$
$RO_2 + NO$	$O^1(D) + H_2O$

	O_3 + OH
	O_3 + HO_2
	O_3 + alkenes

Table S4. Production and destruction pathways of O_3.