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Spatiotemporal source apportionment of ozone pollution over the Greater Bay Area

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Table S1. The WRF-CAMx model performance evaluation for temperature, wind speed and O_3 concentration

Variable	MB	NMB	IOA	RMSE	Mean Obs	Mean Mod
2-m Temp (℃)	0.33 (≤ ±0.50)	0.01	0.82(≥ 0.80)	1.79	28.77	29.11
10-m Wspd (m/s)	-0.45(≤ ±0.50)	0.05	0.70(≥ 0.60)	2.16(≤ 2.0)	3.21	2.76
O_3 (ppb)	3.09	0.13(≤ 0.15)	0.81	21.82	30.26	33.34

Temp is temperature. Wspd is wind speed. MB is mean bias. NMB is normalized mean bias. IOA is index of agreement. RMSE is root mean square error. Obs is observation. Mod is model.

Table S2. Contribution of pollutants from different source areas to the O_3 concentration over different sub-regions in different cases.

Sub-region	Case	Source Area									
		Local	GBAo	GDo	Neighbor	Other 1	EC	SWC	NCP	Other 2	Background
GF	Monthly	17%	15%	15%	16%	15%	3%	1%	1%	1%	17%
	Ep1	13%	8%	22%	36%	6%	3%	0%	0%	0%	11%
	Ep2	26%	33%	8%	6%	18%	0%	0%	0%	0%	9%
	Ep3	14%	8%	35%	23%	6%	3%	0%	1%	1%	8%
	Ep4	13%	13%	17%	18%	10%	8%	1%	5%	3%	13%
HK	Monthly	5%	10%	11%	17%	27%	3%	1%	1%	1%	23%
	Ep1	3%	18%	18%	32%	17%	1%	0%	0%	0%	11%
	Ep2	12%	8%	7%	10%	47%	0%	0%	0%	0%	14%
	Ep3	4%	23%	25%	22%	16%	3%	0%	0%	0%	7%
	Ep4	4%	11%	11%	18%	23%	9%	1%	4%	3%	15%
SD	Monthly	17%	12%	10%	15%	20%	3%	1%	1%	1%	19%
	Ep1	15%	14%	14%	32%	9%	2%	0%	0%	0%	12%
	Ep2	31%	16%	7%	7%	27%	0%	0%	0%	0%	10%
	Ep3	14%	15%	26%	22%	11%	3%	0%	1%	1%	7%
	Ep4	16%	11%	11%	16%	16%	9%	1%	4%	3%	13%
ZZJ	Monthly	10%	7%	14%	16%	24%	2%	1%	1%	1%	23%
	Ep1	11%	12%	27%	35%	20%	0%	0%	0%	0%	14%
	Ep2	23%	7%	7%	9%	39%	0%	0%	0%	0%	13%
	Ep3	9%	14%	38%	24%	11%	3%	0%	0%	1%	11%
	Ep4	12%	14%	19%	21%	24%	8%	1%	5%	3%	17%

* Here, GBAo represents the area outside the sub-region but within the GBA. GDo represents areas outside the GBA but within Guangdong province. Neighbor represents the provinces around Guangdong province. Other 1 represents ocean, other countries and regions. Other 2 represents other area within the mainland China in the simulation domain.

Table S3. Contribution of pollutants from different emitting periods to the average hourly O_3 concentration over the GBA and sub-regions in different cases.

Sub-region	Case	Day-0	Day-1	Day-2	Day-3	>=Day-4
GBA	Monthly	31%	25%	17%	10%	18%
	Ep1	28%	35%	21%	10%	7%
	Ep2	37%	30%	10%	4%	18%
	Ep3	24%	34%	19%	7%	16%
	Ep4	20%	25%	19%	12%	24%
GF	Monthly	37%	24%	15%	9%	15%
	Ep1	30%	33%	19%	10%	7%
	Ep2	43%	32%	9%	4%	12%
	Ep3	28%	31%	19%	7%	15%
	Ep4	24%	25%	18%	11%	22%
HK	Monthly	25%	24%	19%	12%	21%
	Ep1	32%	37%	18%	8%	5%
	Ep2	35%	14%	10%	5%	37%
	Ep3	28%	32%	17%	7%	16%
	Ep4	19%	22%	19%	13%	28%
SD	Monthly	36%	22%	15%	9%	18%
	Ep1	37%	33%	19%	8%	4%
	Ep2	48%	20%	8%	4%	19%
	Ep3	28%	30%	17%	7%	17%
	Ep4	25%	22%	18%	11%	24%
ZZJ	Monthly	27%	25%	19%	11%	19%
	Ep1	28%	34%	21%	11%	6%
	Ep2	40%	18%	9%	4%	29%
	Ep3	27%	35%	18%	7%	14%
	Ep4	22%	24%	18%	11%	25%

Table S4. The setting of the zero-out sensitivity experiment for typhoon case.

Sensitivity Experiment	Jul-04	Jul-05	Jul-06	Jul-07	Jul-08	Jul-09	Jul-10
Day-0				×	✓	☒	☑
Day-1 to Day-0			×	× ✓	✓ ☒	☒ ☑	☒ ☑
Day-2 to Day-0		×	× ✓	× ✓ ☒	✓ ☒ ☑	☒ ☑	☒ ☑
Day-3 to Day-0	×	× ✓	× ✓ ☒	× ✓ ☒ ☑	✓ ☒ ☑	☒ ☑	☒ ☑

Here, the symbols (×✓☒☑) represent a series of zero-out sensitivity experiments for the target date (7th,8th,9th, and 10th July, respectively). For each target date, four source time control simulations were conducted, including only control emission on the current day (Day-0), continuous emission control from 1day ago (Day-1 to Day0), continuous emission control from 2days ago (Day-2 to Day0), and continuous emission control from 3days ago (Day-3 to Day0).Three types of source area control were set, including only control emission within the GBA region, control emission within Guangdong province, and control emission from Guangdong and neighboring provinces. All source time control experiments were conducted for each type of source area control. In the zero-out simulations, the emission of NO_x and VOCs of the control time and area were set to 0.

Table S5. The setting of the zero-out sensitivity experiment for sub-tropical high case.

Sensitivity Experiment	Jul-21	Jul-22	Jul-23	Jul-24	Jul-25	Jul-26
Day-0				×	✓	☒
Day-1 to Day-0			×	× ✓	✓ ☒	☒
Day-2 to Day-0		×	× ✓	× ✓ ☒	✓ ☒	☒
Day-3 to Day-0	×	× ✓	× ✓ ☒	× ✓ ☒	✓ ☒	☒

Same as Table S4, but the symbols (×✓☒) represent a series of sensitivity experiments for the target date (24th,25th, and 26th July, respectively).

Table S6. The mathematical formula of statical metrices.

Statistic Metric	Formular
Mean bias (MB)	$\frac{1}{n}\sum_{i=1}^{n}(Mod_i - Obs_i)$
Normalized mean bias (NMB)	$\frac{\sum_{i=1}^{n}(Mod_i - Obs_i)}{\sum_{i=1}^{n} Obs_i}$
Index of agreement (IOA)	$1 - \frac{\sum_{i=1}^{n}(Mod_i - Obs_i)^2}{\sum_{i=1}^{n}(\lvert Mod_i - \overline{Obs}\rvert + \lvert Obs_i - \overline{Obs}\rvert)^2}$
Root mean square error (RMSE)	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Mod_i - Obs_i)^2}$

Here, n is the total numbers of observations. Obs is the observation. Mod is the model result. $\overline{Obs}$ is the average of observations. The MB, NMB, and RMSE are applied to evaluate how well models capture the magnitude of observations. The IOA is applied to evaluate how well models capture the variations in observations (Huang et al., 2021).

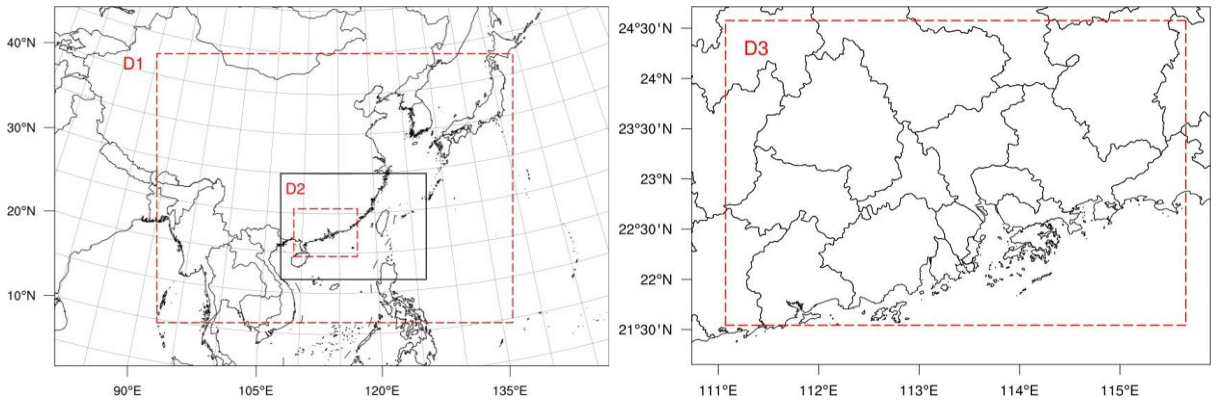


Figure S1. The three nested simulation domain setting of WRF (solid black line)-CAMx (red dash line) models

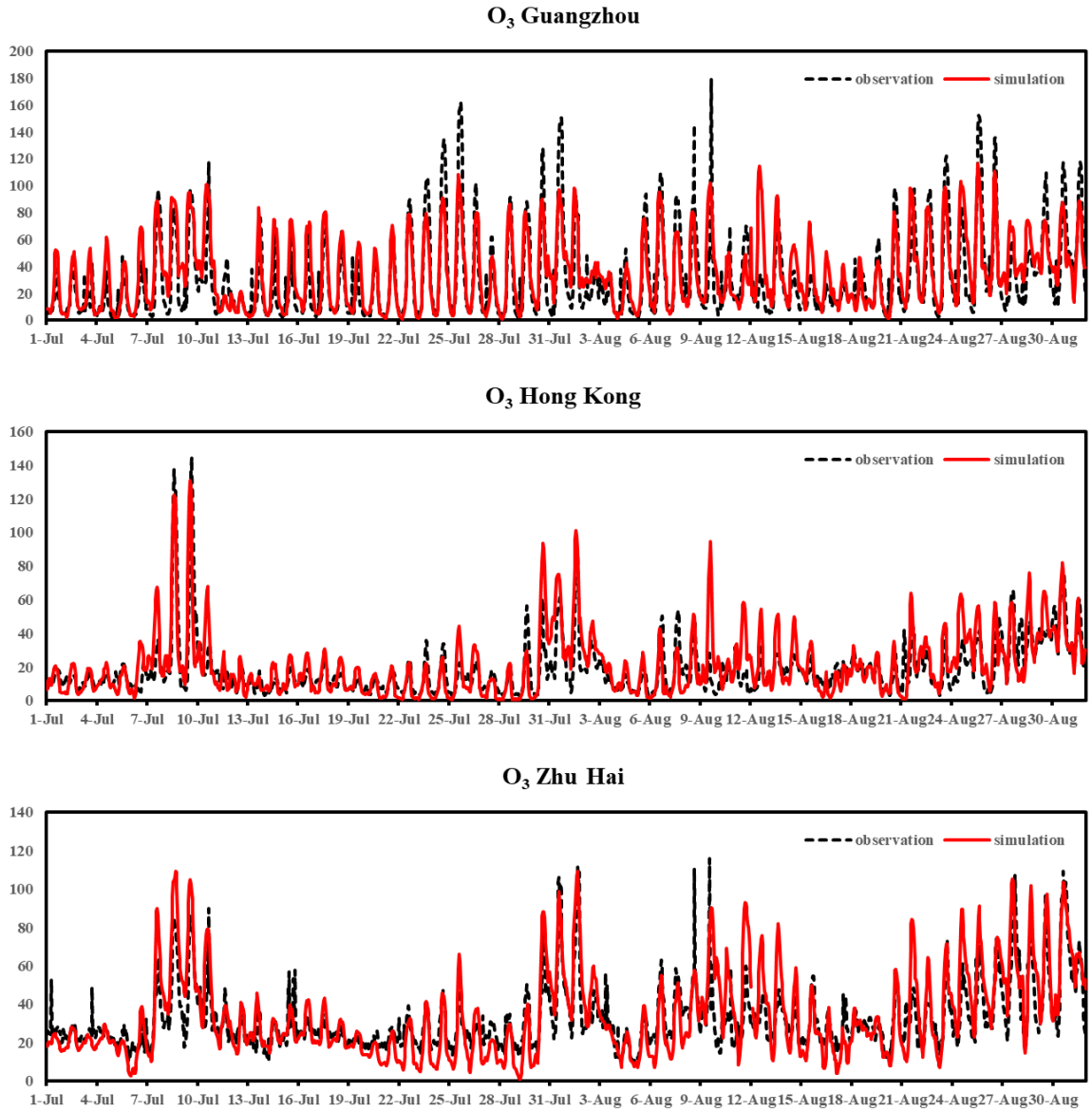


Figure S2. Time series comparison of observed and simulated average O_3 concentration in Guangzhou, Hong Kong, and Zhuhai cities.

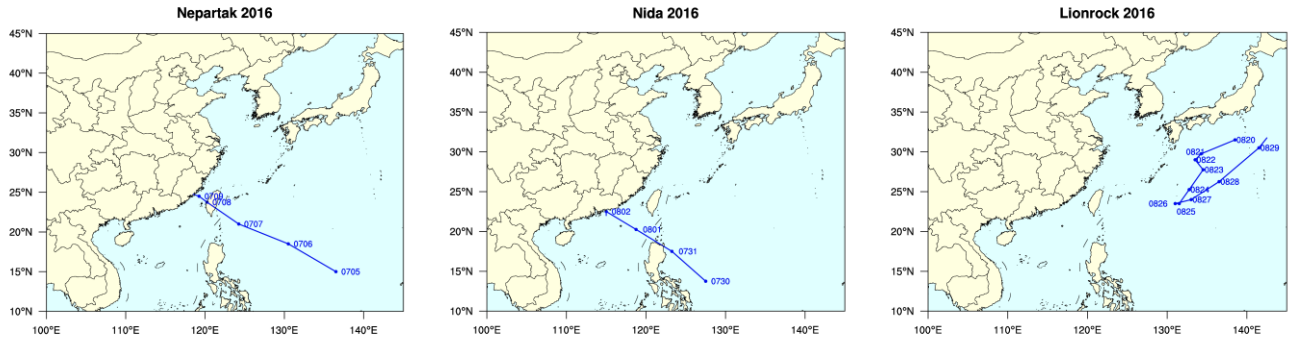


Figure S3. The moving paths of typhoons during the Ep1, Ep3 and Ep4 O_3 episodic cases. (The figures were plotted using the ERA5 reanalysis data. The data was download from https://www.ecmwf.int/en/forecasts/dataset/ecmwf-reanalysis-v5)

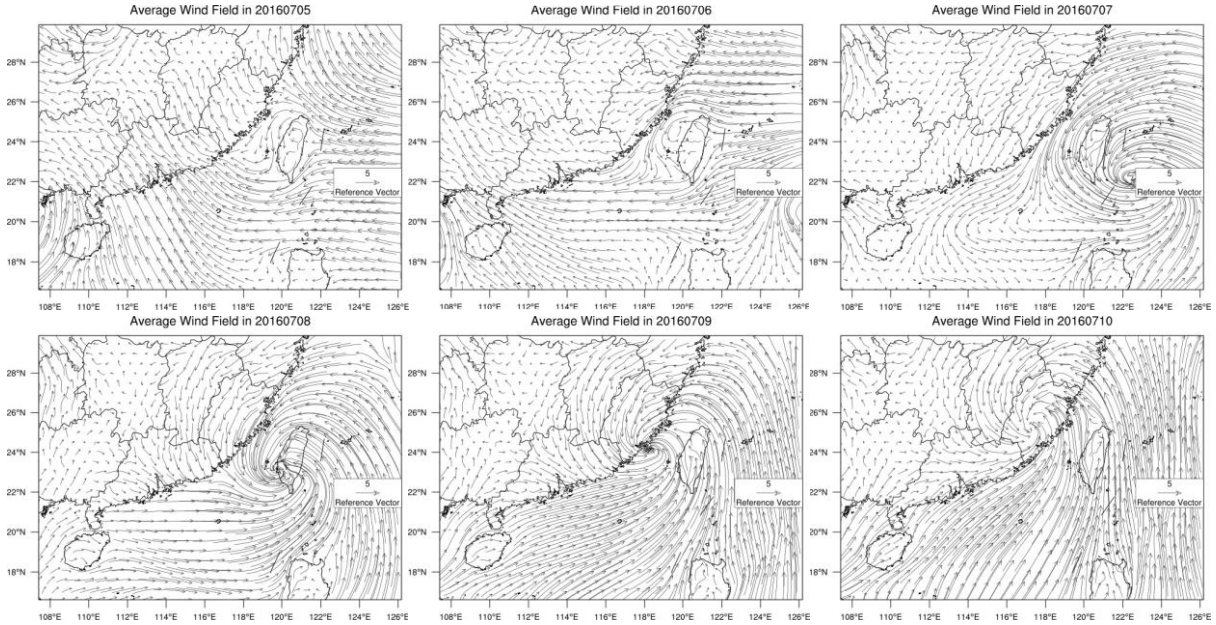


Figure S4. The daily average of 10-m wind field between 5th - 10th July.

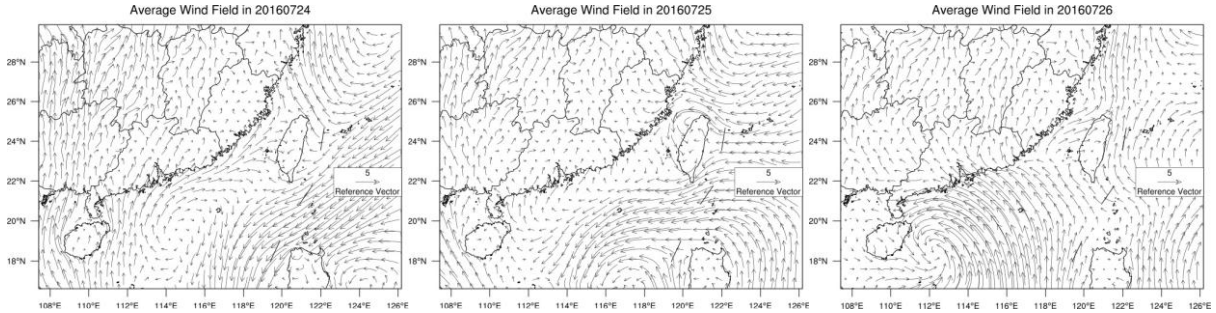


Figure S5. The daily average of 10-m wind field between 24th - 26th July.

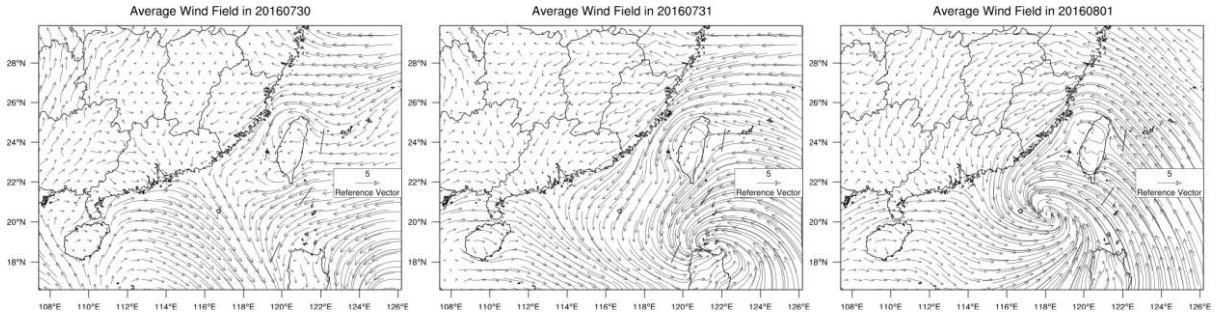


Figure S6. The daily average of 10-m wind field between 30th July – 1st August.

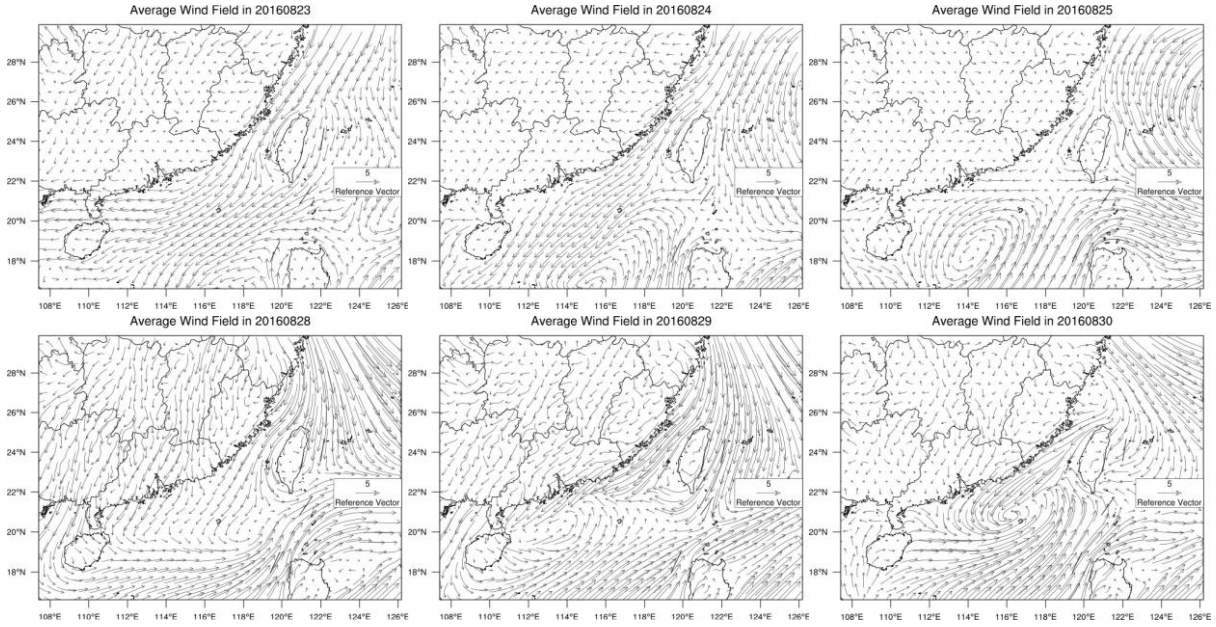
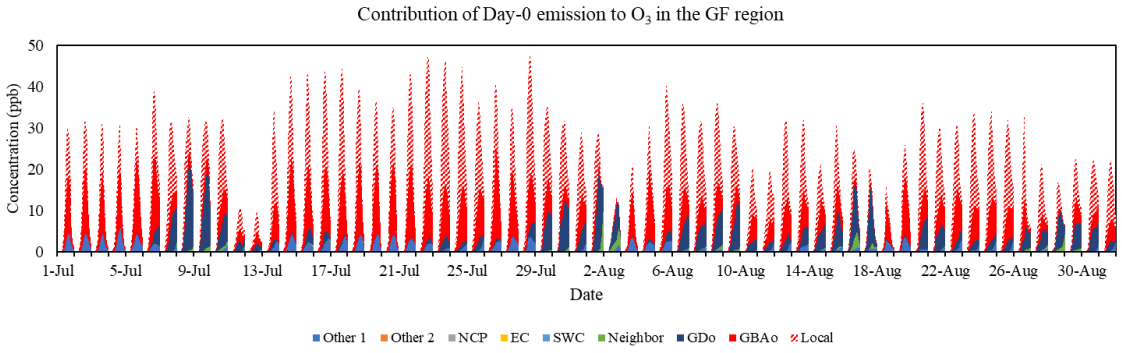
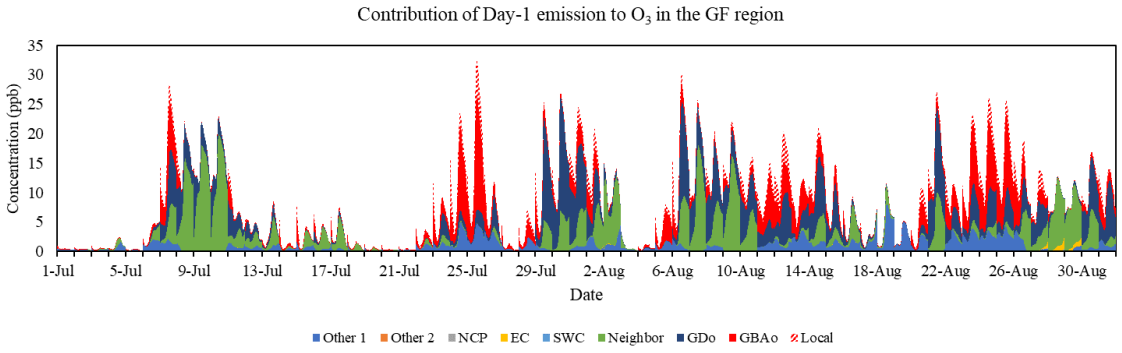
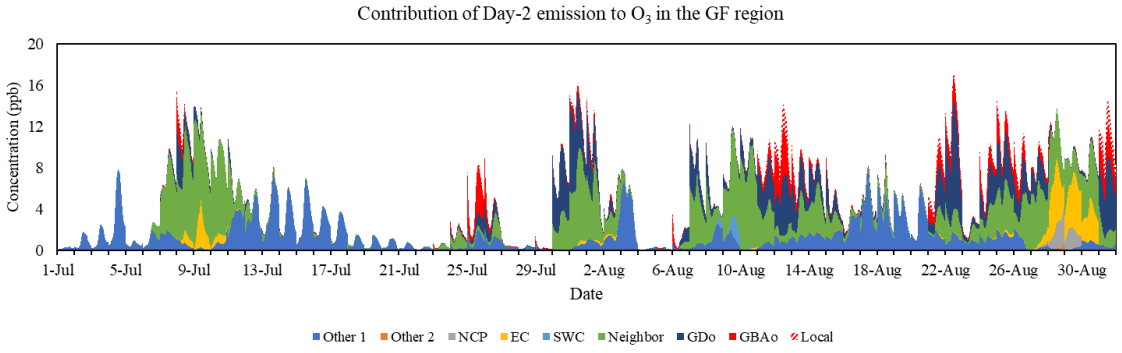
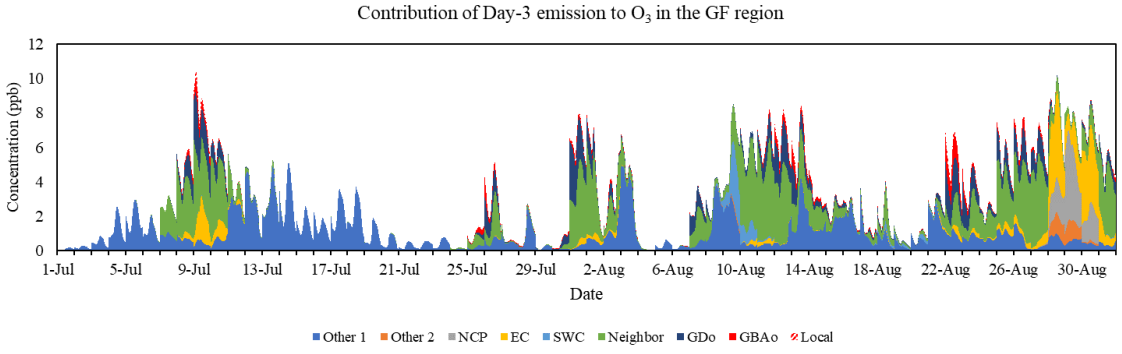


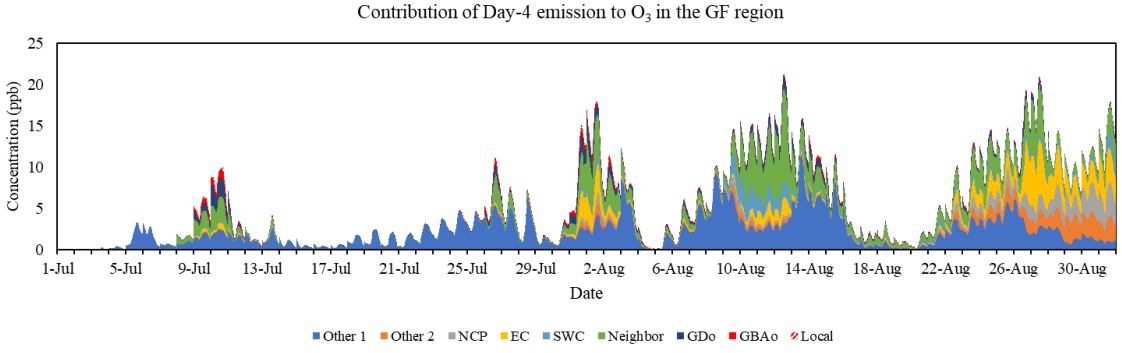
Figure S7. The daily average of 10-m wind field for 23rd – 25th August and 28th – 30th August.


Contribution of Day-0 emission to O_3 in the GF region
Concentration (ppb)
0
10
20
30
40
50
1-Jul
5-Jul
9-Jul
13-Jul
17-Jul
21-Jul
25-Jul
29-Jul
2-Aug
6-Aug
10-Aug
14-Aug
18-Aug
22-Aug
26-Aug
30-Aug
Date
Other 1
Other 2
NCP
EC
SWC
Neighbor
GDo
GBAo
Local

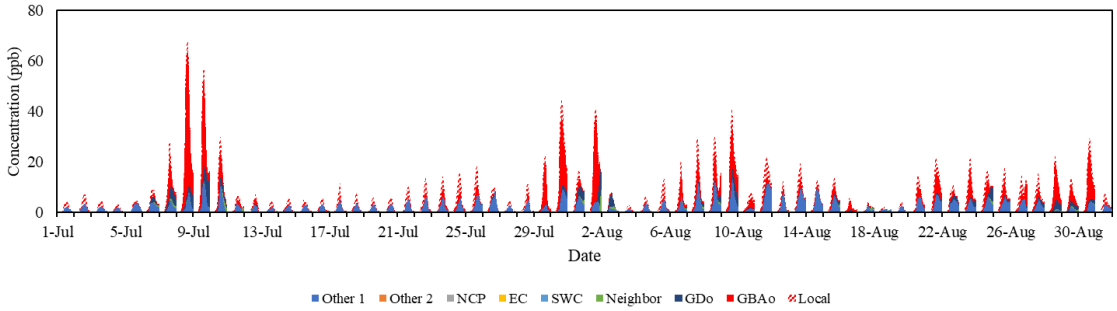

Contribution of Day-1 emission to O_3 in the GF region
Concentration (ppb)
0
5
10
15
20
25
30
35
1-Jul
5-Jul
9-Jul
13-Jul
17-Jul
21-Jul
25-Jul
29-Jul
2-Aug
6-Aug
10-Aug
14-Aug
18-Aug
22-Aug
26-Aug
30-Aug
Date
Other 1
Other 2
NCP
EC
SWC
Neighbor
GDo
GBAo
Local


Contribution of Day-2 emission to O_3 in the GF region
Concentration (ppb)
0
4
8
12
16
20
1-Jul
5-Jul
9-Jul
13-Jul
17-Jul
21-Jul
25-Jul
29-Jul
2-Aug
6-Aug
10-Aug
14-Aug
18-Aug
22-Aug
26-Aug
30-Aug
Date
Other 1
Other 2
NCP
EC
SWC
Neighbor
GDo
GBAo
Local

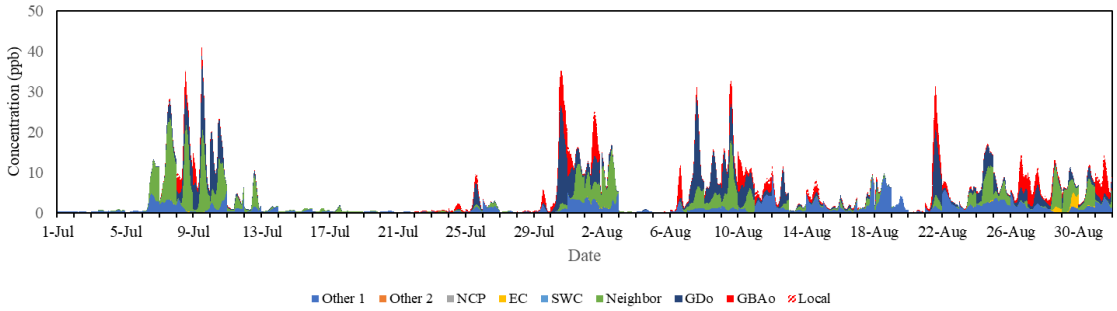

Contribution of Day-3 emission to O_3 in the GF region
Concentration (ppb)
0
2
4
6
8
10
12
1-Jul
5-Jul
9-Jul
13-Jul
17-Jul
21-Jul
25-Jul
29-Jul
2-Aug
6-Aug
10-Aug
14-Aug
18-Aug
22-Aug
26-Aug
30-Aug
Date
Other 1
Other 2
NCP
EC
SWC
Neighbor
GDo
GBAo
Local


Contribution of Day-4 emission to O_3 in the GF region
Concentration (ppb)
0
5
10
15
20
25
1-Jul
5-Jul
9-Jul
13-Jul
17-Jul
21-Jul
25-Jul
29-Jul
2-Aug
6-Aug
10-Aug
14-Aug
18-Aug
22-Aug
26-Aug
30-Aug
Date
Other 1
Other 2
NCP
EC
SWC
Neighbor
GDo
GBAo
Local

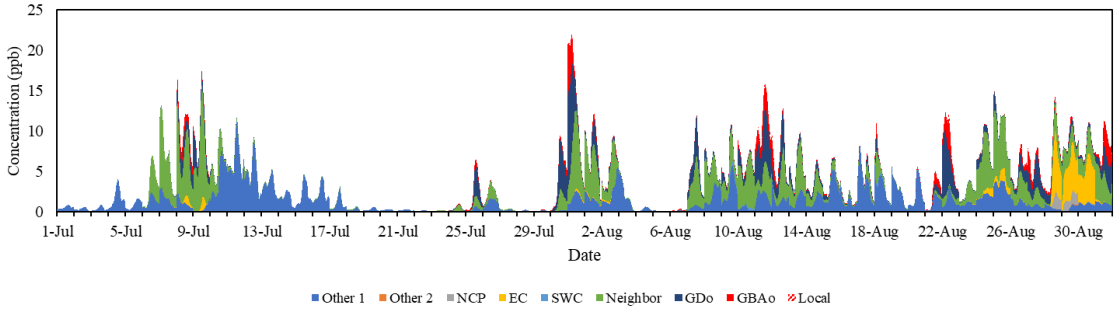
Contribution of Day-0 emission to O_3 in the HK



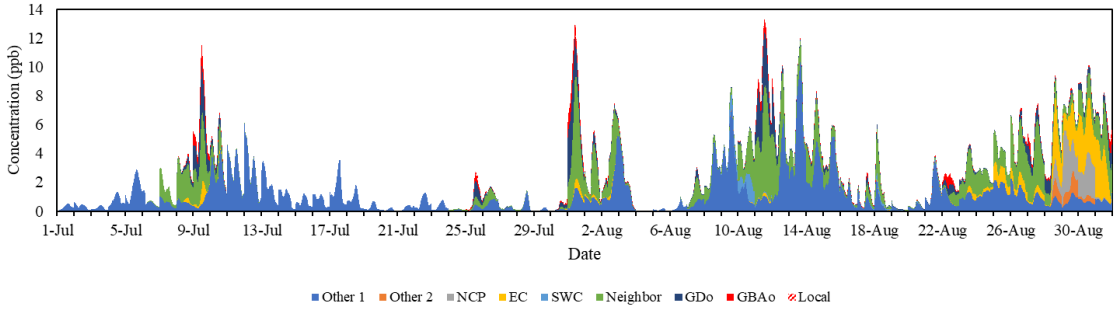
Contribution of Day-1 emission to O_3 in the HK



Contribution of Day-2 emission to O_3 in the HK



Contribution of Day-3 emission to O_3 in the HK



Contribution of Day-4 emission to O_3 in the HK

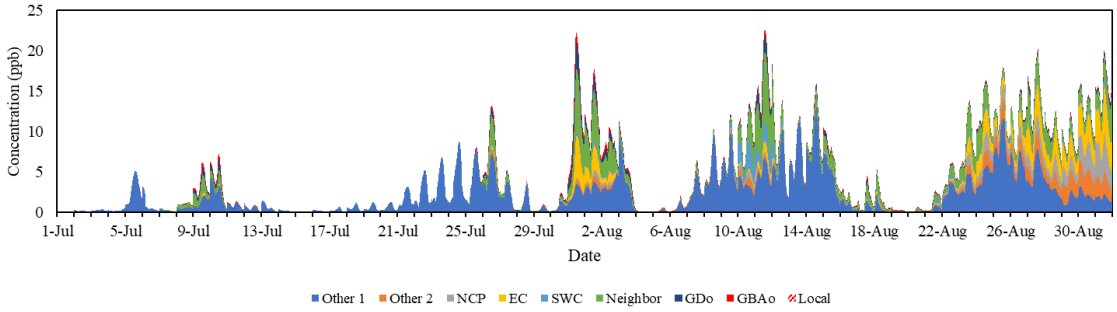


Figure S8. Time series of contributions from different source areas and emitting periods to the O_3 concentrations over the GF region and HK city. (GBAo represent the area outside the target region but within the GBA. GDo represents areas outside the GBA but within Guangdong province. Neighbor represents the provinces around Guangdong province. Other 1 represents ocean, other countries and regions. Other 2 represents other area within the mainland China in the simulation domain.)

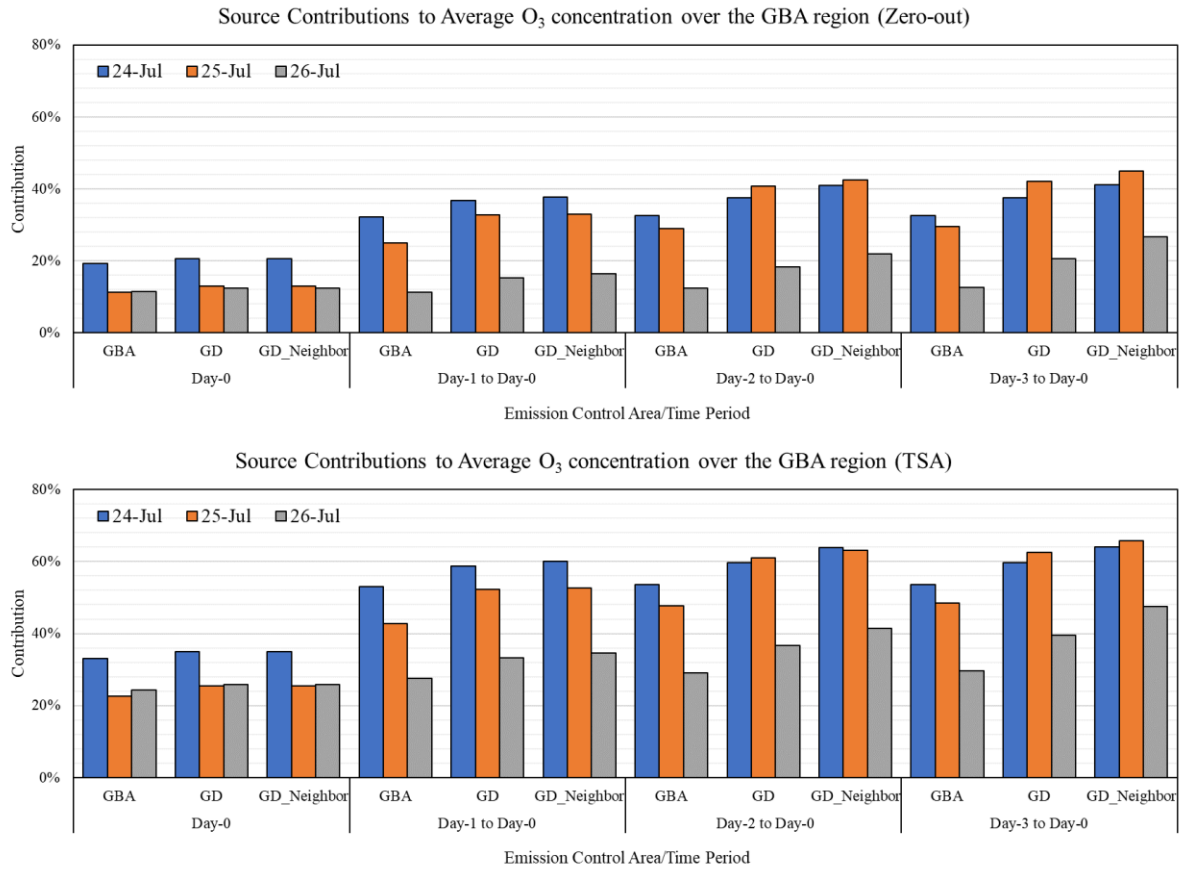


Figure S9. The contribution of different source areas and time periods to the O_3 concentration over the GBA in the sub-tropical high case using the zero-out and TSA methods. (Different colors represent different target dates; Upper: Zero-out; Bottom: TSA)

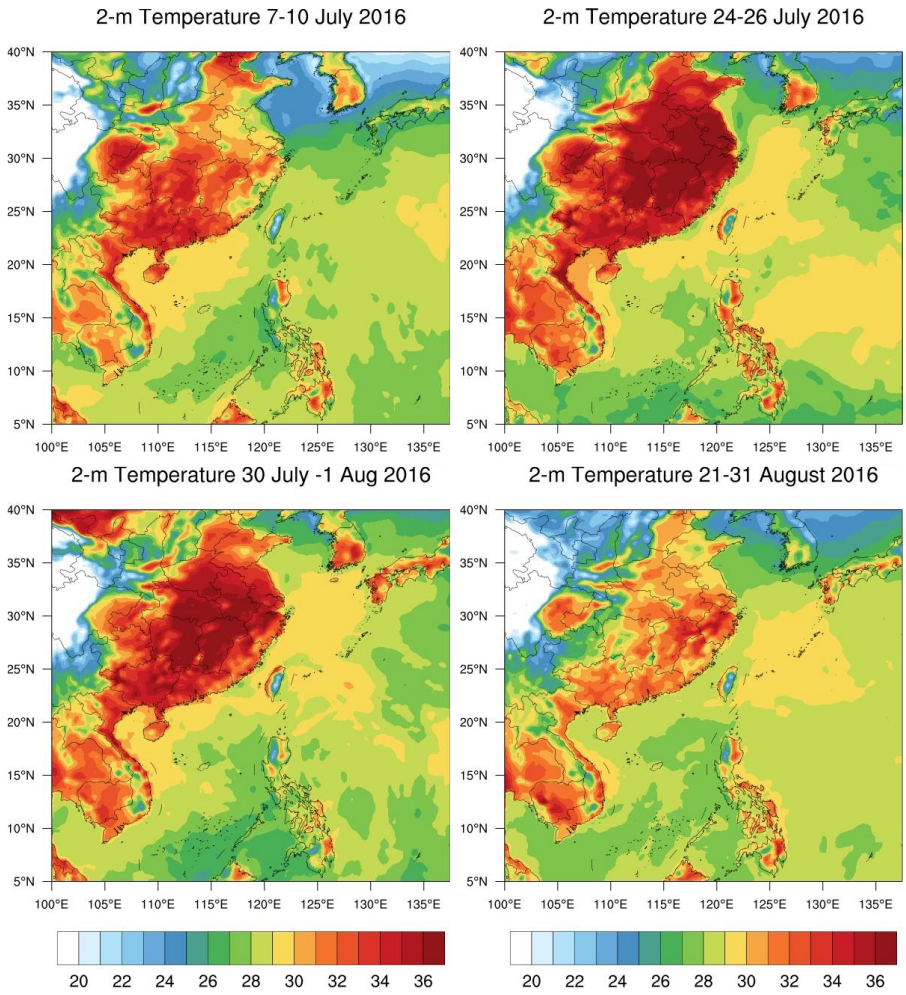


Figure S10. The 2-m temperature at the at 14:00 (Local Time) for O_3 episodes. (The figures were plotted using the ERA5 reanalysis data)

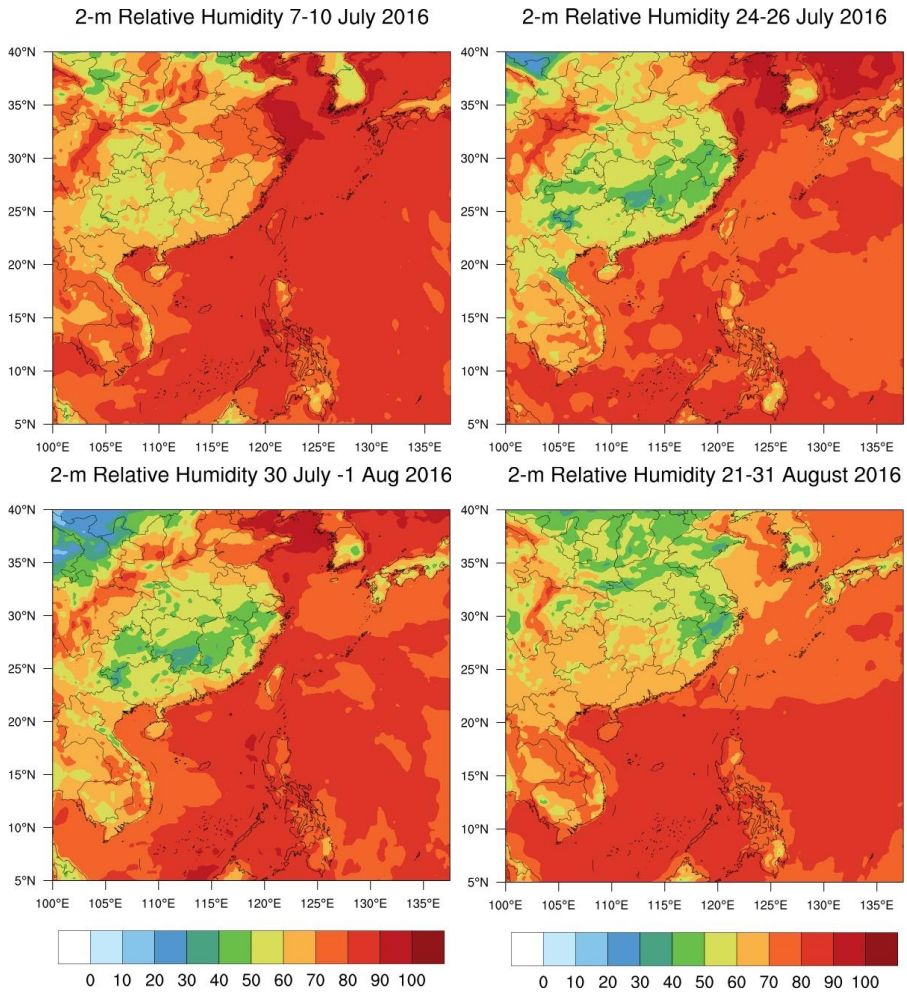


Figure S11. The 2-m relative humidity at the at 14:00 (Local Time) for O_3 episodes. (The figures were plotted using the ERA5 reanalysis data)

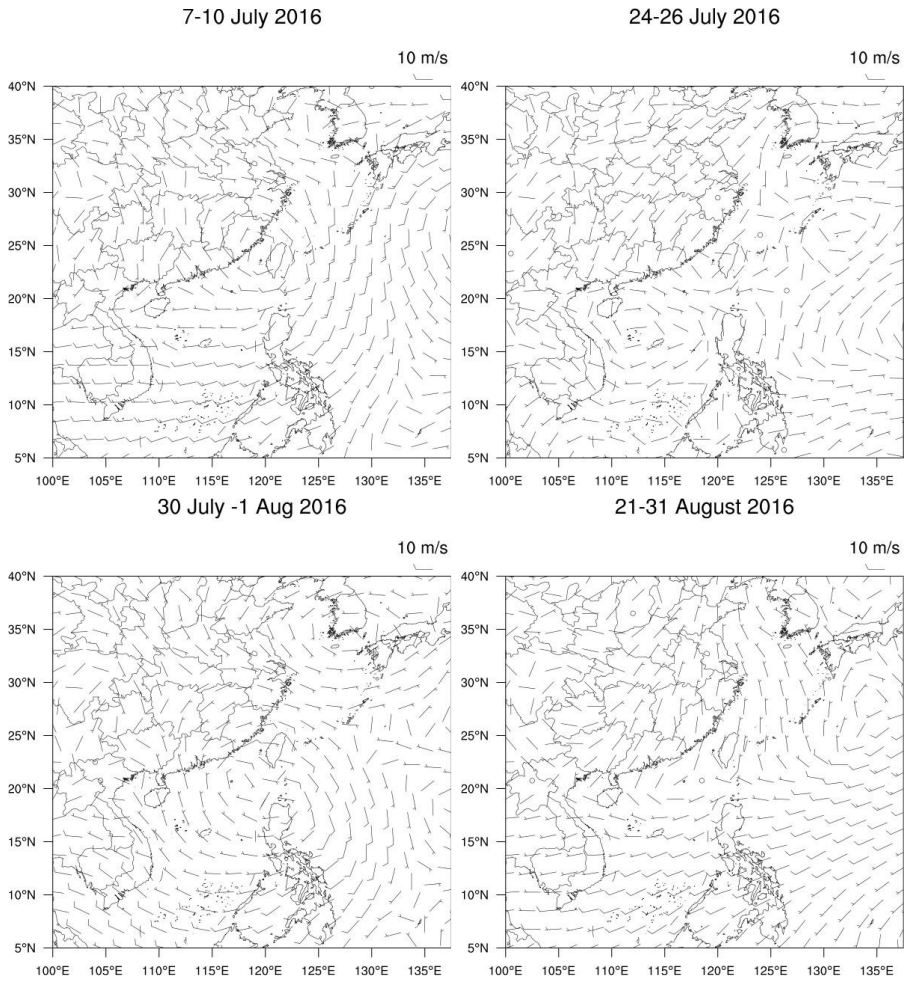


Figure S12. The wind fields at the height of 850 hPa at 14:00 (Local Time) for O_3 episodes. (The figures were plotted using the ERA5 reanalysis data)

References

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Huang, L., Zhu, Y., Zhai, H., Xue, S., Zhu, T., Shao, Y., Liu, Z., Emery, C., Yarwood, G., Wang, Y., Fu, J., Zhang, K., and Li, L.: Recommendations on benchmarks for numerical air quality model applications in China – Part 1: $PM_{2.5}$ and chemical species, Atmospheric Chemistry and Physics, 21, 2725-2743, https://10.5194/acp-21-2725-2021, 2021.