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The role of chemical boundary conditions in simulating summer ozone and cross-boundary transport over China

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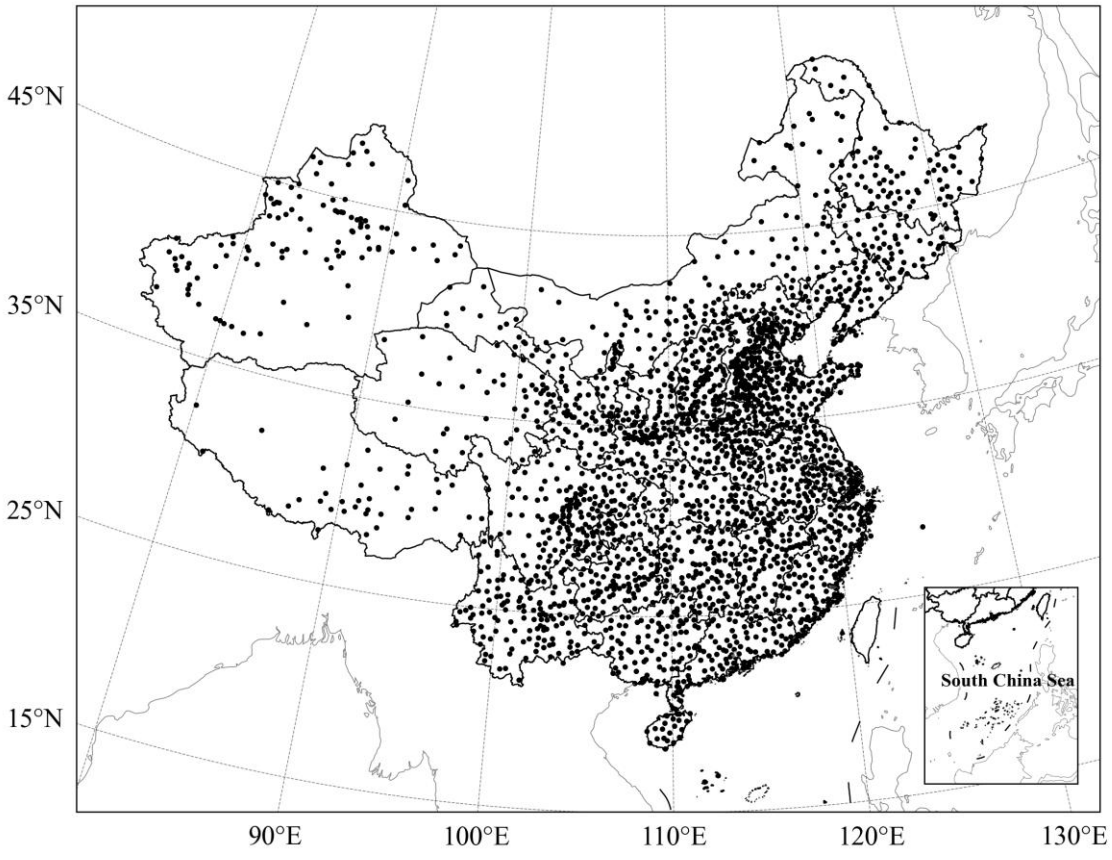

Fig. S1. Surface meteorological observation station location.

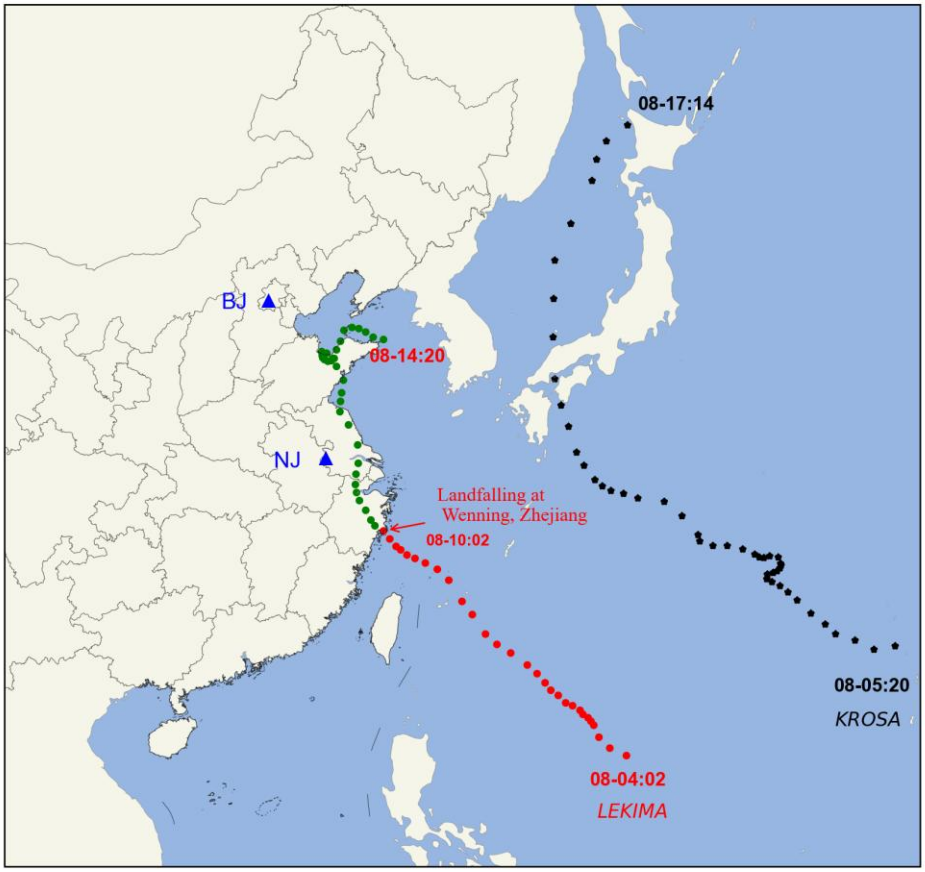

Fig. S2. Trajectories of Typhoons Lekima and Krosa. Green dots mark Lekima's path after landfall. Blue triangles indicate the locations of Beijing (BJ) and Nanjing (NJ). All times are shown in local time.

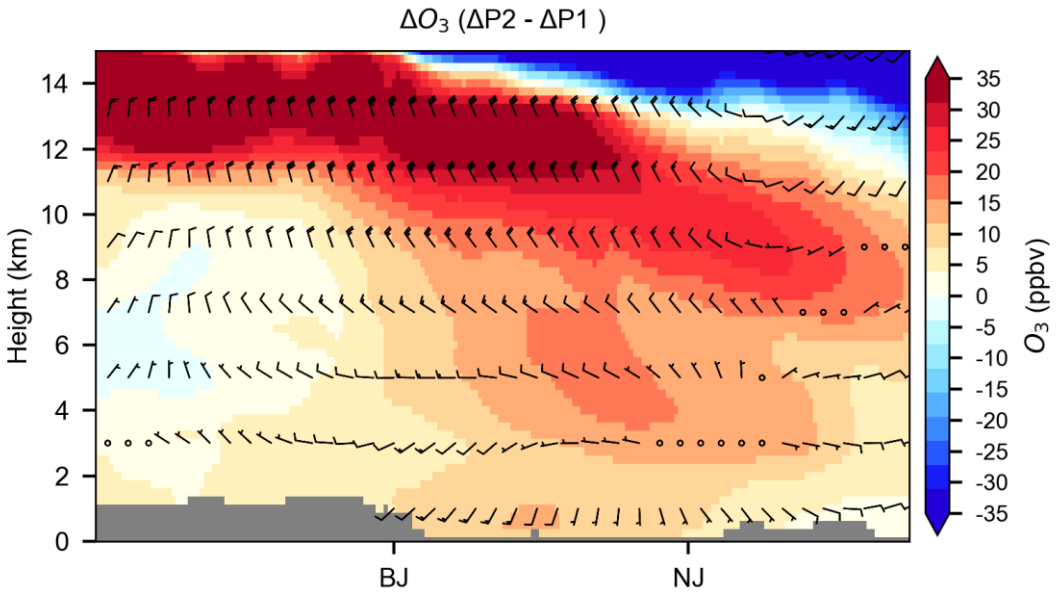

Fig. S3. Vertical cross-sectional analysis of the O_3 and wind difference between P2 (Fig. 9c) and P1 (Fig. 9a).

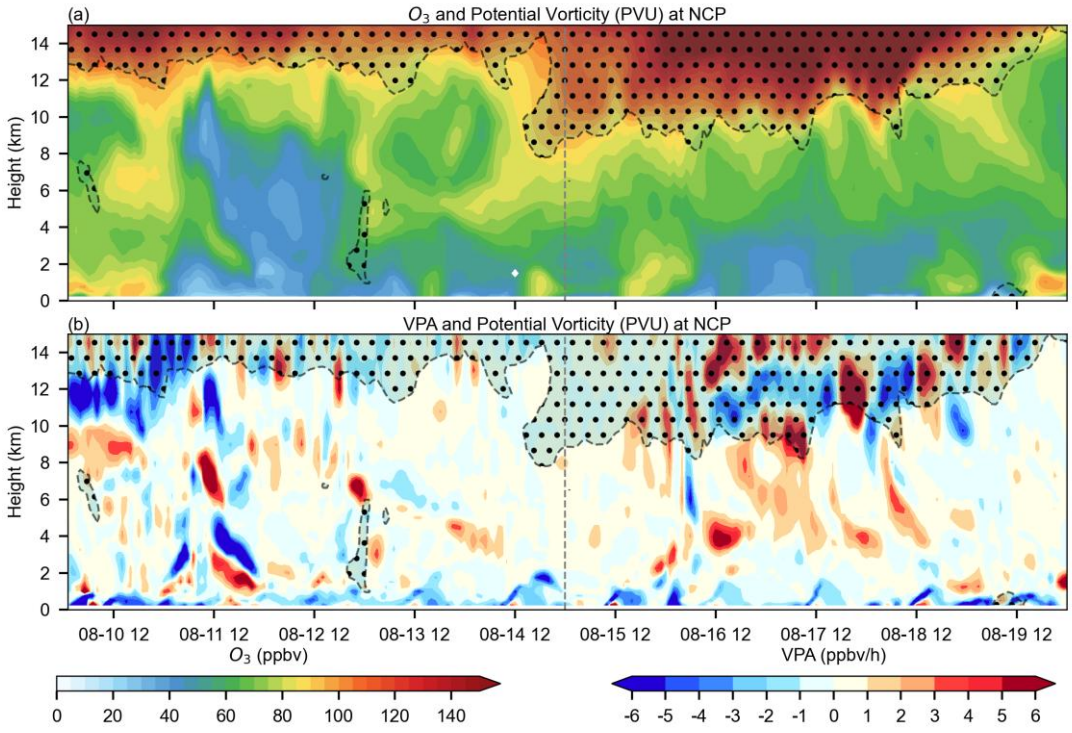

Fig. S4. The Vertical time cross-sectional analysis of the O_3 and VPA (calculated by CMAQ process analysis as the sum of vertical diffusion and vertical advection) during P1 and P2 processes in the North China Plain (NCP) region. The black dots areas represent regions where PVU > 2, and the black contour lines represent PVU = 2.

Table S1. Subregions and the provinces included in each subregion.

subregion	Provinces included
South China	Fujian, Guangdong, Guangxi, Hainan, Jiangxi
East China	Anhui, Jiangsu, Shanghai, Shandong, Zhejiang
North China	Beijing, Hebei, Neimenggu, Shanxi, Tianjin
Central China	Henan, Hubei, Hunan
Northeast China	Heilongjiang, Jilin, Liaoning
Northwest China	Gansu, Ningxia, Qinghai, shannxi, Xinjiang
Southwest China	Sichuan, Chongqing, Guizhou, Yunnan, Xizang

Table S2. Surface and vertical observation data.

Surface Observation Data						
Dataset Name	**Stations number**	**Variables**	**Temporal Resolution**	**Source**		**Data Periods**
Meteorological Observations	2394	T2, T2max, RH2, WS10, PRS,PRECIP	hourly	National Meteorological Information Center (http://data.cma.cn)		July–August 2019
O_3 Observations	1480	O_3	hourly	China National Environmental Monitoring Center (https://air.cnemc.cn:18007/)		
O_3 Vertical Observation Data						
Site Name	**Location**	**Altitude Above Sea Level (m)**	**Launching Time (LST)**	**number of profiles**	**Source**	**Data Periods**
Hongkong	114.17E, 22.31N	66	13:00-14:00	9	World Ozone and Ultraviolet Radiation Data Centre (WOUDC, https://woudc.org/data.php)	03/07/2019 to 28/08/2022
Nanjing	118.90E, 31.93N	20	14:00	4	China Air Pollution Data Center (CAPDC, https://www.capdatabase.cn)	23/07/2019, 25/07/2019, 31/08/2020, 01/09/2020
Lhasa	91.14E, 29.66N	3650	23:00 to 02:00	12	National Tibetan Plateau Data Center (TPDC, https://data.tpdc.ac.cn/home, Bai, Z., 2022)	31/07/2019 to 21/08/2019, 04/08/2020 to 19/08/2020
Lijiang	100.22E, 26.85N	2389	23:00 to 02:00	5		02/07/2022 to 30/08/2022

Golmud	94.91E, 36.42N	2754	23:00 to 02:00	8		30/07/2020 to 30/08/2020, 27/06/2021 to 28/08/2021
Tropospheric Ozone Column (TOC) Data						
Satellite	**Area**	**Variables**	**Spatial Resolution**	**Sensor**	**Source**	**Data Periods**
Gaofen-5 satellite	China Mainland	Tropospheric Ozone (TOC) Column	1 km × 1 km	ultraviolet-visible hyperspectral spectrometer	University of Science and Technology of China (USTC), Zhao et al. (2024).	July–August 2019

Table S3. The average of observed and simulated avg-O3MDA8 and 90th-O3MDA8 for China and seven regions in July-August 2019. (Number of monitoring sites in parentheses).

		China (1480)	E (319)	N (181)	S (256)	C (204)	NE (166)	NW (154)	SW (200)
Avg-O3MDA8 (ppbv)	**OBS**	59.4	64.7	73.5	46.9	66.7	49.5	64.1	51.0
	BASE	56.0	59.6	57.3	51.4	66.6	44.7	52.9	55.7
	H-CMAQ	58.7	60.4	62.9	51.7	68.0	47.5	60.6	59.3
	GEOS-Chem	59.2	61.5	64.3	51.2	68.8	48.5	60.8	58.7
	CESM2.2	62.3	63.0	68.4	52.9	70.7	50.7	68.7	63.4
90th-O3MDA8 (ppbv)	**OBS**	82.8	93.2	98.6	68.9	89.4	71.3	78.9	75.2
	BASE	75.0	85.4	79.1	71.9	83.8	62.9	63.4	68.6
	H-CMAQ	78.1	87.3	82.6	73.2	85.7	65.8	70.7	73.4
	GEOS-Chem	78.9	89.1	83.7	73.7	86.8	67.3	70.6	73.1
	CESM2.2	82.3	90.6	87.2	75.6	89.1	69.2	79.4	79.5

Table S4. Evaluation of avg-O3MDA8 model performance in China and seven regions across four scenarios, using the metrics MB, and RMSE (in ppbv), and IOA, r and NMB (unitless).

		China (1480)	E (319)	N (181)	S (256)	C (204)	NE (166)	NW (154)	SW (200)
MB	**BASE**	-3.39	-5.14	-16.16	4.46	-0.01	-4.84	-11.21	4.68
	H-CMAQ	-0.65	-4.26	-10.54	4.84	1.39	-2.08	-3.50	8.30
	GEOS-Chem	-0.19	-3.24	-9.13	4.31	2.16	-1.07	-3.34	7.73
	CESM2.2	2.90	-1.68	-5.10	5.99	4.09	1.15	4.59	12.40
NMB	**BASE**	-5.7%	-8.7%	-27.2%	7.5%	0.0%	-8.2%	-18.9%	7.9%
	H-CMAQ	-1.1%	-7.2%	-17.8%	8.2%	2.3%	-3.5%	-5.9%	14.0%
	GEOS-Chem	-0.3%	-5.5%	-15.4%	7.3%	3.6%	-1.8%	-5.6%	13.0%
	CESM2.2	4.9%	-2.8%	-8.6%	10.1%	6.9%	1.9%	7.7%	20.9%
RMSE	**BASE**	10.81	10.46	17.80	6.78	7.16	10.26	13.77	7.71
	H-CMAQ	9.34	9.76	13.17	7.08	6.98	9.55	7.34	10.24
	GEOS-Chem	8.75	9.09	11.86	6.78	6.83	9.10	7.17	9.62
	CESM2.2	9.49	8.67	9.66	7.99	7.64	9.40	7.67	14.22
IOA	**BASE**	0.77	0.59	0.58	0.79	0.77	0.71	0.48	0.86
	H-CMAQ	0.82	0.64	0.65	0.78	0.80	0.71	0.66	0.78
	GEOS-Chem	0.85	0.68	0.70	0.79	0.82	0.74	0.68	0.80
	CESM2.2	0.83	0.71	0.74	0.75	0.80	0.71	0.66	0.67
r	**BASE**	0.66	0.44	0.73	0.77	0.78	0.66	0.42	0.84
	H-CMAQ	0.73	0.49	0.69	0.77	0.79	0.63	0.54	0.85
	GEOS-Chem	0.77	0.53	0.72	0.76	0.81	0.65	0.56	0.86
	CESM2.2	0.75	0.54	0.66	0.76	0.81	0.63	0.57	0.78

Table S5. Evaluation of 90th-O3MDA8 model performance in China and seven regions across four scenarios, using the metrics MB, and RMSE (in ppbv), and IOA ,r and NMB (unitless).

		China (1480)	E (319)	N (181)	S (256)	C (204)	NE (166)	NW (154)	SW (200)
MB	**BASE**	-7.75	-7.74	-19.50	3.03	-5.51	-8.41	-15.56	-6.65
	H-CMAQ	-4.70	-5.83	-16.03	4.31	-3.67	-5.51	-8.25	-1.85
	GEOS-Chem	-3.85	-4.11	-14.93	4.82	-2.56	-4.06	-8.37	-2.18
	CESM2.2	-0.43	-2.55	-11.44	6.73	-0.24	-2.11	0.43	4.28
NMB	**BASE**	-13.1%	-13.0%	-32.9%	5.1%	-9.3%	-14.2%	-26.2%	-11.2%
	H-CMAQ	-7.9%	-9.8%	-27.0%	7.3%	-6.2%	-9.3%	-13.9%	-3.1%
	GEOS-Chem	-6.5%	-6.9%	-25.2%	8.1%	-4.3%	-6.8%	-14.1%	-3.7%
	CESM2.2	-0.7%	-4.3%	-19.3%	11.3%	-0.4%	-3.6%	0.7%	7.2%
RMSE	**BASE**	14.57	15.48	22.16	10.25	10.11	13.41	17.29	11.23
	H-CMAQ	12.91	14.79	19.38	10.50	9.29	11.97	10.84	10.33
	GEOS-Chem	12.39	14.08	18.43	10.62	8.89	11.17	10.85	9.66
	CESM2.2	12.31	13.78	16.19	11.49	8.78	10.74	8.22	13.61
IOA	**BASE**	0.78	0.48	0.62	0.83	0.75	0.78	0.60	0.87
	H-CMAQ	0.81	0.48	0.64	0.83	0.76	0.80	0.73	0.86
	GEOS-Chem	0.83	0.49	0.66	0.83	0.77	0.82	0.73	0.89
	CESM2.2	0.82	0.50	0.67	0.81	0.76	0.83	0.78	0.77
r	**BASE**	0.73	0.25	0.74	0.75	0.68	0.80	0.77	0.88
	H-CMAQ	0.75	0.25	0.73	0.76	0.68	0.81	0.79	0.86
	GEOS-Chem	0.76	0.26	0.73	0.77	0.68	0.82	0.80	0.88
	CESM2.2	0.73	0.27	0.70	0.78	0.66	0.82	0.70	0.70