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Direct thermal enhancement dominates over emission-mediated pathways in heatwave-induced O_3 and SOA increases across China

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S1. Adjustment of MEIC emissions for 2021 and 2022

The transportation, industrial and power sectors are major sources of emissions and the latest emissions inventory of MEIC is only updated until 2020, so adjustments need to be made for 2021 and 2022 emissions. For the transportation sector, we used passenger turnover and cargo turnover (https://www.mot.gov.cn/tongjishuju/gonglu/index.html, last access: April 2023) to adjust NO_x and VOCs emissions (see Tables S4 and S5 for adjustment factors). For the industry sector, the same adjustment ratio was also applied to VOC emission, and an average annual NO_x reduction rate of 2% was used according to a previous study [1]. For the SO_2 and particulate matter (PM), we used the change rates between 2017 and 2019 to adjust the emission in 2022, assuming the same rate of change within 2020 to 2022 as Eq.1.2:

$$\delta_{i,j,k,2022} = \frac{E_{i,j,k,2019}}{E_{i,j,k,2017}} \quad (1.1)$$

$$E_{i,j,k,2022} = \delta_{i,j,k,2022} \times E_{i,j,k,2020} \quad (1.2)$$

where, $E_{i,j,k,t}$ and $\delta_{i,j,k,t}$ (t=2017, 2019, 2020, 2022) are the emission rates and the adjustment factor of pollutant k (SO_2, PM) in year t at the grid (i, j).

For the power sector, the adjustment factor δ_{power} is calculated based on the national thermal power generation (https://cec.org.cn/detail/index.html, last access: April 2023) as shown in Eq.1.3:

$$\delta_{power} = \frac{E_{power,2021}}{E_{power,2020}} = 1.01 \quad (1.3)$$

where $E_{power,2021}$, and $E_{power,2020}$ are the national thermal power generation in 2021 and 2020, respectively. The residential and agricultural sectors remained the same with MEIC 2020.

S2. statistical equations

The mean bias (MB), gross error (GE), and root mean square error (RMSE) were used for the evaluation of WRF model performance, while the mean normalized bias (MNB), mean normalized error (MNE), mean fractional bias (MFB) and mean fractional error (MFE) were used for the validation of CMAQ model performance.

$$MB = \frac{1}{N}\sum_{i=1}^{N}\left(C_{m,i} - C_{o,i}\right) \quad \text{(s1)}$$

$$GE = \frac{1}{N}\sum_{i=1}^{N}\left|C_{m,i} - C_{o,i}\right| \quad \text{(s2)}$$

$$RMSE = \left(\frac{1}{N}\sum_{i=1}^{N}\left(C_{m,i} - C_{o,i}\right)^{2}\right)^{\frac{1}{2}} \quad \text{(s3)}$$

$$MNB = \frac{1}{N}\sum_{i=1}^{N}\frac{C_{m,i} - C_{o,i}}{C_{o,i}} \quad \text{(s4)}$$

$$MNE = \frac{1}{N}\sum_{i=1}^{N}\frac{\left|C_{m,i} - C_{o,i}\right|}{C_{o,i}} \quad \text{(s5)}$$

$$MFB = \frac{2}{N}\sum_{i=1}^{N}\frac{C_{m,i} - C_{o,i}}{C_{m,i} + C_{o,i}} \quad \text{(s6)}$$

$$MFE = \frac{2}{N}\sum_{i=1}^{N}\frac{\left|C_{m,i} - C_{o,i}\right|}{C_{m,i} + C_{o,i}} \quad \text{(s7)}$$

where $C_{m,i}$ and $C_{o,i}$ refer to the i^{th} predicted and observed value, respectively. *N* is the number of prediction-observation pairs drawn from all measurement sites.

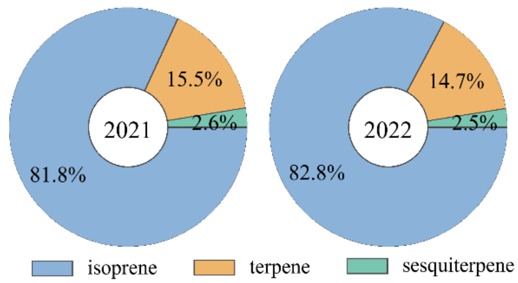

Figure S1. Components of biogenic terpenoid emissions. Contribution of isoprene, terpene and sesquiterpene to total biogenic terpenoids emissions from 2021 to 2022 in China.

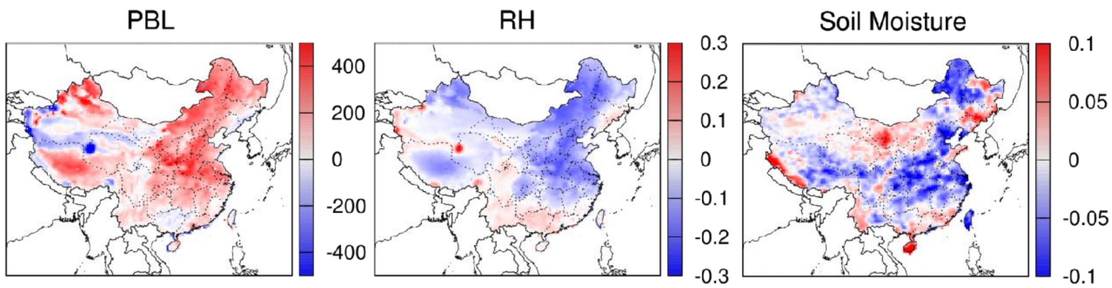

Figure S2. The differences of simulated planetary boundary layer (PBL), relative humidity (RH) and soil moisture between 2022 and 2021 (2022−2021). The units are m (meter), % (percentage) and m^3 m^{-3}, respectively.

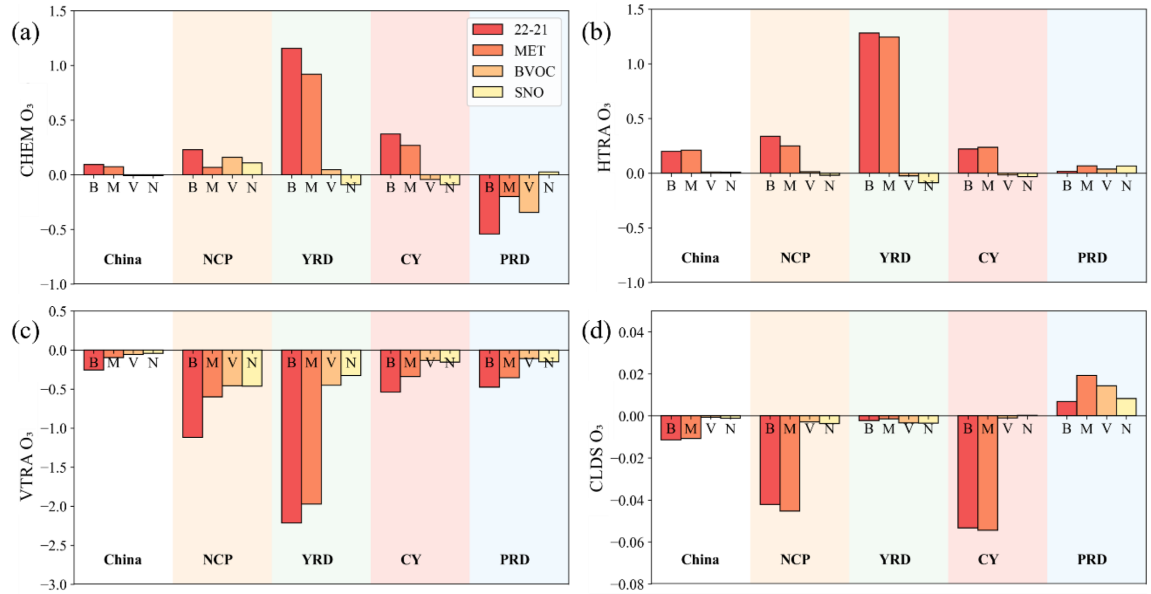

Figure S3. (a) Differences in impacts of gas-chemistry on O_3 concentrations (unit: ppb h^{-1}) between different cases (11:00-18:00 BJT). (b-d) Same with panel a but for horizontal transport, vertical transport and cloud processes. Units are ppb h^{-1}.

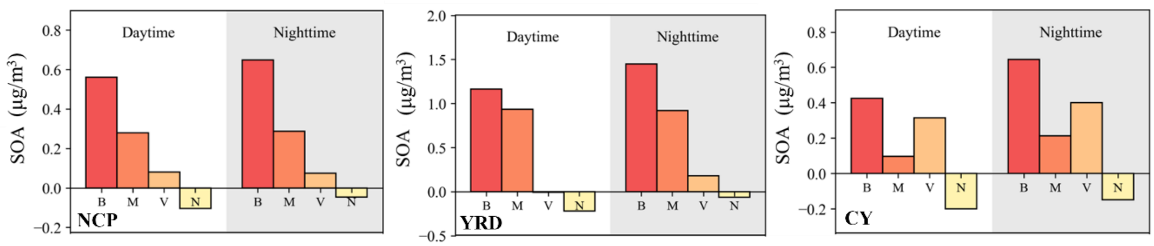

Figure S4. Diurnal differences of SOA in the NCP, YRD, and CY regions, respectively. Daytime is from 8:00 to 20:00 and nighttime is from 20:00 to 8:00.

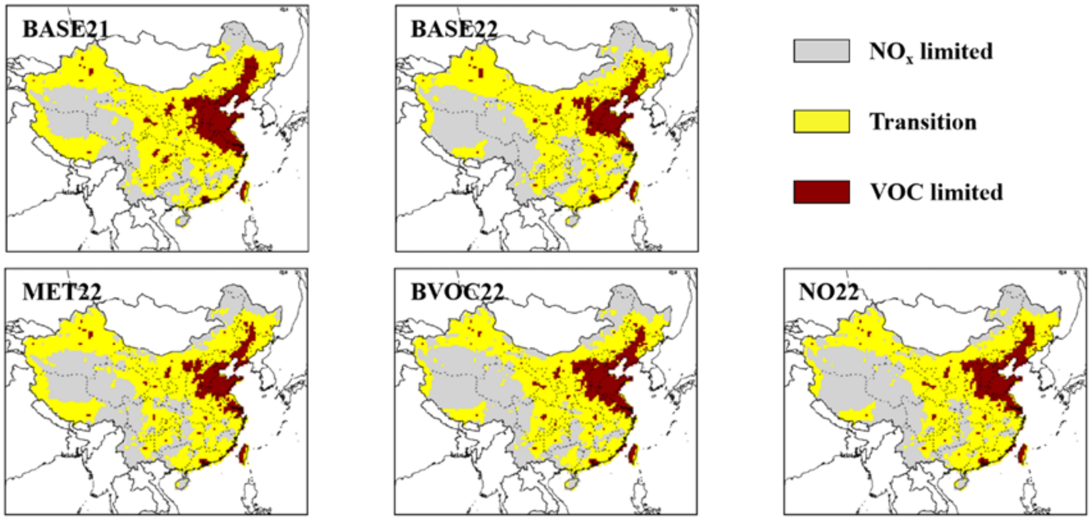

Figure S5. Sensitivity regime of BASE case in 2021 and 2022, MET22, BVOC22 and SNO22 based on the indicator of HCHO/NO_y. A value below 0.303 indicates a VOC-limited regime, above 1.26 indicates a NO_x-limited regime, and values in between are transition area (Wang et al., 2022). The grey, yellow and brick red areas are NO_x-limited, transition and VOC-limited regimes. The threshold of different regimes is referenced from Wang, Zhu [5].

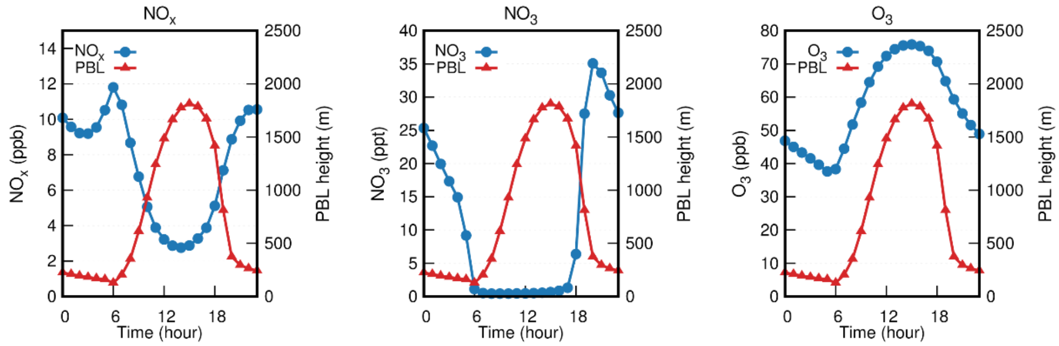

Figure S6. Diurnal variations of key chemical species and PBL height in the NCP under the BVOC22 scenario.

Table S1. Correlation coefficient of MDA8 O_3 and SOA to daily maximum temperature (T_{max}), daily average temperature (T), BVOC emissions (BVOC), and SNO emissions (NO) in different regions.

	Variable	China	NCP	YRD	CY	PRD
MDA8 O_3	T_{max}	0.28	0.44	0.62	0.48	0.43
	T	0.28	0.45	0.65	0.50	0.45
	BVOC	0.16	0.56	0.31	0.27	-0.16
	SNO	0.25	0.65	0.53	0.39	0.15
SOA	T_{max}	0.50	0.58	0.86	0.80	0.18
	T	0.53	0.60	0.89	0.82	0.05
	BVOC	0.62	0.54	0.59	0.63	0.12
	SNO	0.70	0.61	0.82	0.77	0.25

Table S2. Adjustment factors for MEIC by sector and species.

	NO_x	SO_2	VOCs	CO	PM
Industry	0.98	$\delta_{i,j,k,2022}$*	Table S7	——	$\delta_{i,j,k,2022}$
Transportation	Table S7	——	Table S7	——	——
Power			1.01		
Residential			——		
Agriculture			——		

*: The details of $\delta_{i,j,k,2022}$ is from Section S1.

Table S3. NO_x and VOCs adjustment factors by province. The abbreviation adopts 'Administrative Division Names' regulated by the Ministry of Industry and Information Technology in China.

Province	Abbreviation	NO_x-May	NO_x-Jun	NO_x-Jul	NO_x-Aug	VOCs
Beijing	BJ	0.87	0.90	1.17	0.93	0.99
Tianjin	TJ	0.89	0.96	0.88	0.84	0.97
Hebei	HE	0.78	0.70	0.77	0.74	0.97
Shanxi	SX	0.75	0.71	0.75	0.57	0.98
Inner Mongolia	NM	0.80	0.75	0.87	0.75	0.99
Liaoning	LN	0.72	0.65	0.74	0.73	0.98
Jilin	JL	0.87	1.62	0.69	0.65	0.96
Heilongjiang	HL	1.53	1.53	1.06	1.01	0.99
Shanghai	SH	0.47	0.89	0.89	0.96	0.99
Jiangsu	JS	0.42	0.64	0.68	0.72	0.96
Zhejiang	ZJ	0.84	0.91	0.99	0.93	0.97
Anhui	AH	0.75	0.65	0.74	0.74	0.98
Fujian	FJ	0.92	1.10	1.03	0.98	0.98
Jiangxi	JX	0.66	0.69	0.75	0.75	0.99
Shandong	SD	1.03	0.83	0.89	0.88	0.96
Henan	HA	1.12	0.99	1.02	1.04	0.97
Hubei	HB	1.18	0.84	1.01	0.83	0.98
Hunan	HN	0.86	1.06	0.98	0.96	0.98
Guangdong	GD	0.68	0.74	0.67	0.66	0.96
Guangxi	GX	0.84	0.86	0.83	0.80	0.99
Hainan	HI	1.03	0.94	0.85	0.38	0.99
Chongqing	CQ	0.84	0.92	0.70	0.62	0.99
Sichuan	SC	0.95	1.00	0.93	0.81	0.98
Guizhou	GZ	0.79	0.81	0.74	0.77	0.97
Yunnan	YN	1.15	1.10	1.26	1.10	0.99
Tibet	XZ	1.47	1.67	1.30	0.41	0.99
Shaanxi	SN	0.82	0.65	0.74	0.67	0.98
Gansu	GS	0.71	0.76	0.81	0.77	0.99
Qinghai	QH	0.70	0.84	1.06	0.62	1.00
Ningxia	NX	0.90	1.05	1.12	1.04	0.99
Xinjiang	XJ	2.36	2.31	1.95	1.59	0.99

Note: National Statistical Yearbook lacks relevant traffic data for Tibet in August 2022, which is substituted by the Tibet adjustment coefficients for August 2021.

Table S4. Model performance of WRF model: temperature (T2), wind speed (WS), wind direction (WD), and relative humidity (RH) in June, July and August in 2021 and 2022 (PRE: mean prediction; OBS: mean observation; MB: mean bias; GE: gross error; RMSE: root mean square error). The values that do not meet the criteria are denoted in bold.

		2021			2022			
		Jun	Jul	Aug	Jun	Jul	Aug	Benchmark
T2 (K)	OBS	296.2	298.5	296.8	296.6	298.7	298.1	
	PRE	296.1	298.5	296.6	296.4	298.7	298.1	
	MB	-0.1	0.0	-0.2	-0.2	0.0	0.0	≤ ±0.5
	GE	**2.3**	**2.3**	**2.1**	**2.2**	**2.3**	**2.4**	≤ 2.0
	RMSE	3.2	3.1	2.9	3.1	3.1	3.3	
WS (m s^{-1})	OBS	3.2	3.1	3.0	3.4	3.2	3.2	
	PRE	3.9	3.9	3.6	4.1	3.9	3.8	
	MB	0.8	0.8	0.6	0.7	0.7	0.6	≤ ±0.5
	GE	1.5	1.5	1.4	1.6	1.4	1.4	≤ 2.0
	RMSE	2.0	2.0	1.8	2.1	1.9	1.9	≤ 2.0
WD (°)	OBS	175.2	166.6	166.2	173.2	174.1	171.9	
	PRE	181.9	170.5	168.4	179.7	181.4	175.7	
	MB	**8.1**	**6.0**	**5.3**	**7.9**	**8.3**	**5.9**	
	GE	46.4	45.1	45.6	44.5	45.3	43.9	≤ ±30
	RMSE	63.5	62.3	62.5	61.4	62.2	60.6	
RH (%)	OBS	68.2	70.9	72.7	68.8	68.9	68.4	
	PRE	63.7	66.8	69.1	64.6	63.5	62.4	
	MB	-4.6	-4.2	-3.5	-4.2	-5.4	-6.0	
	GE	**12.2**	**11.7**	**11.0**	**11.7**	**12.2**	**13.2**	
	RMSE	15.9	15.3	14.6	15.3	16.1	17.1	

Table S5. Model performance of O_3-1h (ppb), $PM_{2.5}$ (μg m^{-3}), PM_{10} (μg m^{-3}), CO (ppm), NO_2 (ppb) and SO_2 (ppb) of BASE case in China in June, July and August in 2021 and 2022. MNB: mean normalized bias, MNE: mean normalized error, MFB: mean fractional bias, MFE: mean fractional error. The performance criteria are suggested by *Emery, Liu* [2]. The values that do not meet the criteria are denoted in bold.

		2021			2022			
		Jun	Jul	Aug	Jun	Jul	Aug	Criteria
O_3-1h (ppb)	OBS	61.73	57.29	57.76	62.31	58.63	57.21	
	PRE	67.51	64.01	64.74	67.15	65.18	61.98	
	MFB	0.09	0.11	0.11	0.12	0.14	0.11	
	MFE	0.20	0.21	0.20	0.21	0.23	0.20	
	MNB	0.13	0.15	0.15	0.08	0.10	0.08	≤ ±0.15
	MNE	0.22	0.23	0.22	0.19	0.20	0.18	≤ 0.3
$PM_{2.5}$ (μg m^{-3})	OBS	27.31	22.33	25.04	25.97	23.71	24.02	
	PRE	25.10	21.62	28.63	22.52	21.47	21.01	
	MFB	-0.17	-0.10	0.00	0.01	0.06	0.00	≤ ±0.6
	MFE	0.50	0.44	0.48	0.53	0.49	0.45	≤ 0.75
	MNB	0.07	0.10	0.31	-0.21	-0.13	-0.16	
	MNE	0.57	0.52	0.67	0.49	0.45	0.43	
PM_{10} (μg m^{-3})	OBS	46.41	36.14	39.39	44.58	39.00	37.50	
	PRE	29.22	24.71	31.65	25.21	25.65	25.05	
	MFB	-0.46	-0.40	-0.27	-0.26	-0.18	-0.19	
	MFE	0.68	0.60	0.57	0.58	0.53	0.53	
	MNB	-0.18	-0.17	-0.02	-0.54	-0.40	-0.41	
	MNE	0.60	0.54	0.58	0.71	0.60	0.60	
CO (ppm)	OBS	0.47	0.44	0.49	0.44	0.44	0.45	
	PRE	0.24	0.21	0.25	0.22	0.22	0.22	
	MFB	-0.64	-0.71	-0.70	-0.42	-0.41	-0.43	
	MFE	0.73	0.78	0.77	0.54	0.54	0.55	
	MNB	-0.41	-0.45	-0.44	-0.66	-0.66	-0.68	
	MNE	0.54	0.56	0.55	0.73	0.74	0.76	
NO_2 (ppb)	OBS	18.81	16.93	17.20	17.94	16.78	16.11	
	PRE	22.61	21.40	22.38	21.19	21.36	22.03	

	MFB	0.14	0.18	0.21	0.32	0.39	0.48
	MFE	0.42	0.40	0.42	0.54	0.57	0.61
	MNB	0.34	0.38	0.43	0.12	0.19	0.25
	MNE	0.56	0.56	0.60	0.40	0.41	0.42
SO_2 (ppb)	OBS	15.07	14.56	15.92	15.10	15.02	16.71
	PRE	15.07	13.07	16.14	14.77	14.06	14.76
	MFB	0.01	-0.10	0.02	0.08	0.03	0.02
	MFE	0.32	0.28	0.34	0.34	0.28	0.29
	MNB	0.13	-0.03	0.14	-0.01	-0.03	-0.06
	MNE	0.38	0.27	0.39	0.32	0.28	0.30

References

1. Zhong M, Tian J, Ye D. 14th Five-Year Period
China's Total VOCs Control Program Research and Suggestions during the 14th Five-Year Period. *Environmental Impact Assessment* 2021, **43**(02)**:** 1-6.

2. Emery C, Liu Z, Russell AG, Odman MT, Yarwood G, Kumar N. Recommendations on statistics and benchmarks to assess photochemical model performance. *Journal of the Air & Waste Management Association* 2017, **67**(5)**:** 582-598.

3. Ji X, Chen G, Chen J, Xu L, Lin Z, Zhang K*, et al.* Meteorological impacts on the unexpected ozone pollution in coastal cities of China during the unprecedented hot summer of 2022. *Science of The Total Environment* 2024, **914:** 170035.

4. Lyu X, Li K, Guo H, Morawska L, Zhou B, Zeren Y*, et al.* A synergistic ozone-climate control to address emerging ozone pollution challenges. *One Earth* 2023, **6**(8)**:** 964-977.

5. Wang P, Zhu S, Vrekoussis M, Brasseur G, Wang S, Zhang H. Is atmospheric oxidation capacity better in indicating tropospheric O3 formation? *Frontiers of Environmental Science & Engineering* 2022, **16:** 65.