## Text S1. Identification of ozone episodes

Ozone exceedance days were identified according to surface measurements from the TCEQ CAMS (onshore) and the boats (offshore). The criteria used in this study are (1) any onshore site from the CAMS network in Houston and Galveston or (2) offshore boat ozone observations that registered daily maximum 8-hour average (MDA8) ozone in exceedance of 70 ppbv, the current air quality standard for ozone. The highest MDA8 ozone of each ozone episode is shown in Table S1.

Table S1. Dates of selected ozone episodes a	and the associated MDA8 O3 maximum.
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Enicodos	Highest MDA8 O <sub>3</sub> (ppbv)					
Episodes	Onshore (CAMS)	Offshore (Boat)				
09/06 - 09/11	89	79				
09/23 - 09/26	81	65				

## Text S2. Description of WRF nudging

We used observation nudging together with surface analysis nudging (also known as surface grid nudging) in WRF as the data assimilation method. In observation nudging, the modeled fields are nudged to match better with observations at individual locations with a radius of influence. The data used for observation nudging are ground-based hourly measurements of temperature, relative humidity as well as wind speed and direction from the Texas Commission on Environmental Quality (TCEQ) continuous ambient monitoring stations (CAMS). Based on site elevations, most nudging is performed within 500m above sea level in eastern Texas, as shown in Figure S1. There are around 155, 98, and 49 observations ingested into WRF domains 1, 2 and 3, respectively. In analysis nudging, temperature, moisture and wind fields are nudged toward gridded analysis above the PBL (~1 km). The OBSGRID program was used for both observation nudging and surface analysis nudging. The program generated merged input files so that observation nudging and surface analysis nudging were conducted simultaneously when running the model. In addition to data assimilation, we adopted objective analysis in OBSGRID to provide better initial and boundary conditions, where first-guess meteorological fields are updated by incorporating observational data. The combined adoption of observation nudging, surface analysis nudging, and objective analysis in the [Nudged] simulation was to maximize the benefits of assimilating observations, as recommended by Chapter 7 of the WRF user guide.



**Figure S1.** Elevation of the Texas Commission on Environmental Quality (TCEQ) continuous ambient monitoring stations (CAMS) used as observational data for WRF nudging methods.

## Text S3. Evaluation of all model experiments

All WRF simulations are shown in Table S2. We evaluated the spatial and temporal variabilities of all simulations against the onshore TCEQ CAMS (Figure S2; Figure S3; Table S3) and the offshore boat measurements (Figure S4; Figure S5; Table S4). Considering both onshore and offshore evaluations, [HRRR] was selected as the best simulation to represent campaign-wide statistics.

Simulations	BC Meteorology	PBL	Microphysics	Nudging	Reinitializing
[Base]	NCEP FNL	MYNN	2M	No	No
[WSM6]	NCEP FNL	MYNN	WSM6	No	No
[YSU]	NCEP FNL	YSU	2M	No	No
[ACM2]	NCEP FNL	ACM2	2M	No	No
[ERA5]	ECMWF ERA5	MYNN	2M	No	No
[HRRR]	HRRR	MYNN	2M	No	No
[Nudged2]	NCEP FNL	MYNN	2M	Yes	No
[Reinit]	NCEP FNL	MYNN	2M	No	Yes

Table S2. List of model experiments.



**Figure S2.** Spatial distribution of CAMS-observed and modeled mean meteorology during ozone episodes.



**Figure S3.** Hourly time series of (a) air temperature, (b) relative humidity, (c) wind speed and (d) wind direction between CAMS observations and WRF model simulations during ozone episodes.

**Table S3.** Performance metrics of spatiotemporal variability between CAMS-observed and WRF-modeled meteorology for five ozone episodes. Hourly meteorology at all stations is used for the calculation of performance metrics below. All metrics have the same unit as meteorological variables, except that the correlation coefficient (R) and normal mean bias (NMB) are unitless.

Variables	Simulation	OBS	MOD	R	NMB	MB	MAE	RMSE
	[Base]	26.19	25.82	0.88	-0.01	-0.36	1.69	2.15
	[WSM6]		25.84	0.89	-0.01	-0.35	1.57	1.99
	[YSU]		26.29	0.89	0.00	0.11	1.65	2.11
Temperature	[ACM2]		25.95	0.86	-0.01	-0.23	1.76	2.23
(°C)	[ERA5]	20.16	24.91	0.85	-0.05	-1.28	2.17	2.71
	[HRRR]		26.12	0.89	0.00	-0.06	1.59	2.05
	[Nudged]		25.92	0.92	-0.01	-0.26	1.43	1.84
	[Re-init]		25.69	0.92	-0.02	-0.49	1.41	1.77
	[Base]		60.94	0.76	0.01	0.82	10.25	13.04
	[WSM6]		62.21	0.78	0.03	2.09	9.85	12.28
	[YSU]		58.45	0.80	-0.03	-1.68	9.54	12.31
Relative humidity	[ACM2]	60.12	62.73	0.71	0.04	2.60	11.40	14.71
(%)	[ERA5]	00.12	64.21	0.77	0.07	4.08	10.55	12.76
	[HRRR]		57.82	0.79	-0.04	-2.30	9.13	12.13
	[Nudged]		64.63	0.82	0.08	4.51	9.54	12.05
	[Re-init]		62.57	0.84	0.04	2.45	8.37	10.66
	[Base]		1.29	0.35	0.59	1.01	1.40	1.70
	[WSM6]		1.67	0.37	0.61	1.04	1.39	1.72
	[YSU]		0.80	0.39	0.75	1.29	1.55	1.87
Wind speed	[ACM2]	0.67	1.16	0.38	0.66	1.12	1.44	1.77
(m/s)	[ERA5]	0.07	1.76	0.43	0.64	1.09	1.38	1.66
	[HRRR]		1.00	0.54	0.49	0.83	1.12	1.36
	[Nudged]		0.89	0.55	0.30	0.51	0.96	1.20
	[Re-init]		1.14	0.61	0.48	0.82	1.07	1.31
	[Base]		72.32	0.43	-0.05	-7.67	56.5	73.36
	[WSM6]		72.56	0.38	-0.04	-5.51	56.41	72.93
Wind direction (deg)	[YSU]	87.76	53.26	0.41	-0.08	-12.14	60.30	77.29
	[ACM2]		54.87	0.37	-0.07	-10.64	64.15	81.29
	[ERA5]		47.32	0.43	-0.07	-10.92	58.05	74.83
	[HRRR]		92.51	0.61	-0.02	-3.43	40.16	57.55
	[Nudged]		93.29	0.48	0.02	3.00	46.05	64.70
	[Re-init]		109.03	0.47	0.00	-0.32	39.99	57.67



Figure S4. Spatial distribution of boat-observed and modeled meteorology during ozone episodes.



Figure S4 (continued). Spatial distribution of boat-observed and modeled meteorology during ozone episodes.



**Figure S5.** Hourly time series of (a) air temperature, (b) relative humidity, (c) wind speed, (d) wind direction and (e) boundary layer height between boat observations and WRF model simulations during ozone episodes.

**Table S4.** Performance metrics of spatiotemporal variability between boat-observed and WRFmodeled meteorology for five ozone episodes. 1-minute meteorology is used for the calculation of performance metrics below. All metrics have the same unit as meteorological variables, except that the correlation coefficient (R) and normal mean bias (NMB) are unitless.

Variables	Simulation	OBS	MOD	R	NMB	MB	MAE	RMSE
	[Base]	26.55	26.45	0.77	0.00	-0.11	1.71	2.14
	[WSM6]		26.50	0.75	0.00	-0.05	1.77	2.20
	[YSU]		26.78	0.78	0.01	0.22	1.71	2.10
Temperature	[ACM2]		26.51	0.75	0.00	-0.04	1.78	2.21
(°C)	[ERA5]		24.85	0.75	-0.06	-1.70	2.21	3.00
	[HRRR]		26.30	0.75	-0.01	-0.25	1.89	2.29
	[Nudged]		26.30	0.87	-0.01	-0.25	1.26	1.65
	[Re-init]		26.53	0.76	0.00	-0.02	1.71	2.15
	[Base]		70.24	0.64	0.15	9.28	11.95	14.59
	[WSM6]		71.09	0.61	0.17	10.14	11.76	14.38
	[YSU]		68.20	0.65	0.12	7.24	10.96	13.29
Relative humidity	[ACM2]	60.06	69.35	0.56	0.14	8.40	12.75	15.33
(%)	[ERA5]	00.90	74.38	0.60	0.22	13.42	14.66	17.23
	[HRRR]		69.20	0.70	0.14	8.24	10.38	12.68
	[Nudged]		73.35	0.75	0.20	12.39	12.87	14.92
	[Re-init]		69.68	0.67	0.14	8.72	10.25	12.42
	[Base]		2.47	0.16	0.74	1.67	2.20	2.78
	[WSM6]		2.62	0.14	0.82	1.85	2.33	2.92
	[YSU]		2.17	0.13	0.99	2.22	2.63	3.19
Wind speed	[ACM2]	0.73	1.99	0.15	0.92	2.07	2.49	3.09
(m/s)	[ERA5]	0.75	1.89	0.22	0.78	1.74	2.21	2.72
	[HRRR]		1.68	0.52	0.59	1.32	1.69	2.05
	[Nudged]		1.75	0.37	0.41	0.92	1.57	1.96
	[Re-init]		2.02	0.30	0.69	1.55	2.00	2.41
	[Base]		118.78	0.32	-0.08	-11.45	57.74	75.38
	[WSM6]		113.5	0.26	-0.13	-19.10	60.40	77.29
	[YSU]		135.77	0.26	-0.11	-16.44	63.52	81.13
Wind direction (deg)	[ACM2]	144 15	125.25	0.27	-0.11	-17.20	68.93	85.92
	[ERA5]	144.13	96.69	0.18	-0.17	-25.20	69.00	85.30
	[HRRR]		137.93	0.58	-0.08	-12.53	41.54	58.16
	[Nudged]		146.95	0.45	-0.05	-7.68	47.87	65.51
	[Re-init]		146.96	0.62	-0.10	-14.98	42.98	59.66
Boundary layer	[Base]	855 58	499.27	0.32	-0.42	-356.30	529.63	699.67
height (m)	[WSM6]	055.50	526.69	0.30	-0.38	-328.88	526.38	691.82

[YSU]		322.22	0.30	-0.62	-533.36	612.29	817.16
[ACM2]		443.60	0.30	-0.48	-411.97	562.12	747.06
[ERA5]		464.75	0.47	-0.46	-390.83	507.51	680.30
[HRRR]		671.27	0.38	-0.22	-184.31	461.30	637.68
[Nudged]		462.09	0.41	-0.46	-393.48	516.18	696.37
[Re-init]		569.57	0.25	-0.33	-286.00	518.21	689.22

**Text S4. Vertical ozone distribution at University of Houston** Similar to the TROPOZ lidar in the main text, the Langley Mobile Ozone Lidar (LMOL) is part of the ground-based Tropospheric Ozone Lidar Network (TOLNet, <u>https://www-air.larc.nasa.gov/missions/TOLNet/</u>). The LMOL has been used to provide continuous, high-resolution profile measurements of ozone during various campaigns. Figure S6 shows the vertical ozone distribution measured by the LMOL at University of Houston during the two ozone episodes.



**Figure S6.** Time series of the vertical ozone profile from (a, c) the LMOL ozone lidar and (b, d) the WRF-GC [HRRR] simulation at the University of Houston site during September 8–11 and September 23–26 of 2021.