



Supplement of

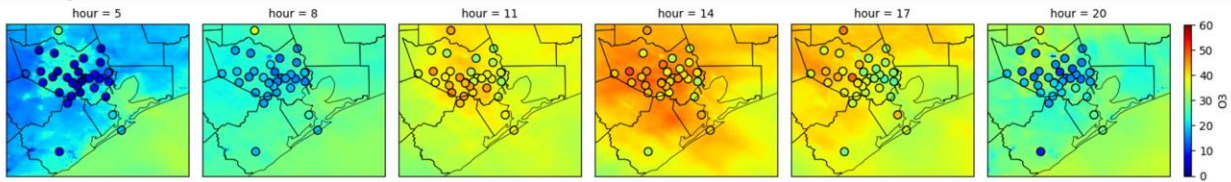
Understanding offshore high-ozone events during TRACER-AQ 2021 in Houston: insights from WRF–CAMx photochemical modeling

Wei Li et al.

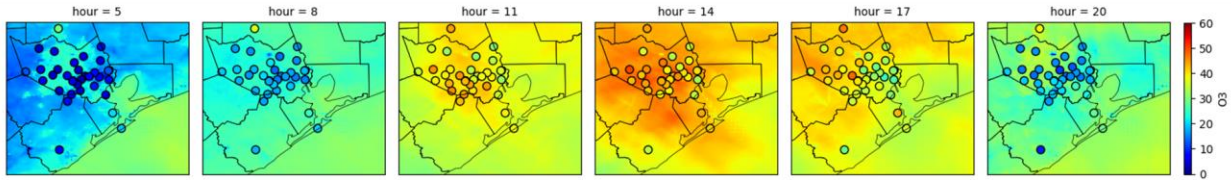
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(a) O₃ concentrations (ppb) using redistributed emissions



(b) O₃ concentrations (ppb) using CAMx Flexi-nesting option



(c) O₃ concentration (ppb) differences (a - b)

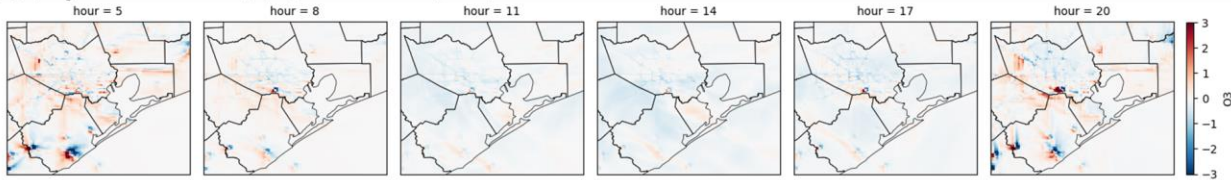


Figure S1. Average O₃ concentrations from August 25-31 in three hour intervals for simulations using redistributed emissions (a) and CAMx Flexi-nesting option (b), and the differences between these two simulations (c). The overlaid dots in a and b show O₃ concentrations at the CAMS sites.

Table S1. Performance metrics of regional-mean hourly O₃ between CAMS observations and simulations from August 25-31. All metrics have the same unit as their corresponding variables, except that correlation coefficient (R) and normal mean bias (NMB) are unitless.

Variables	Simulation	OBS	MOD	R	NMB	MB	MAE	RMSE
O ₃ (ppb)	Flexi-nesting	23.71	29.01	0.87	22.38	5.31	7.41	8.59
	Redistribution		28.90	0.87	21.90	5.19	7.34	8.54

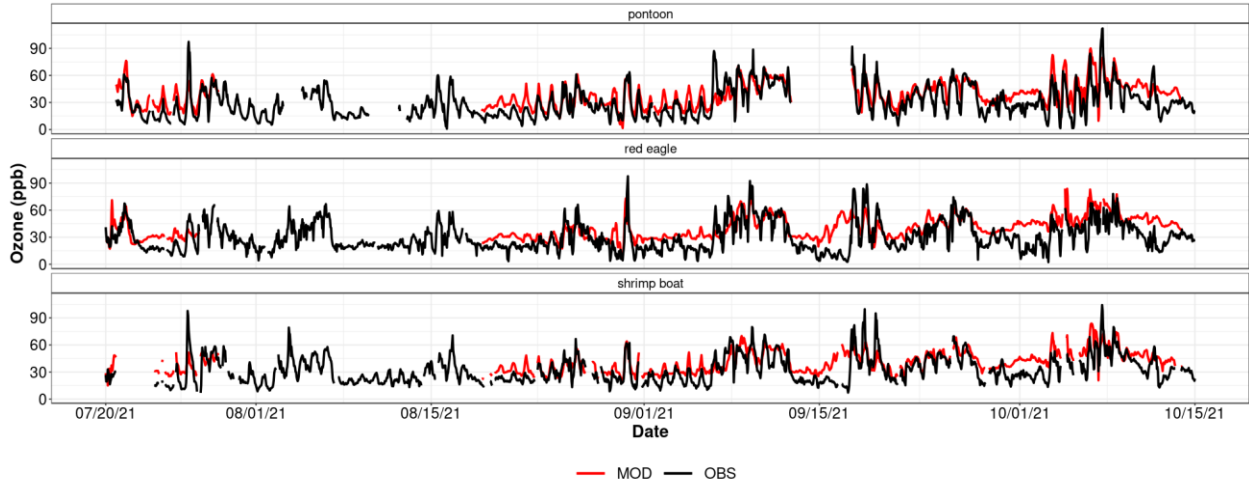


Figure S2. Time series of hourly ozone for observations at three boats (OBS; black line) and simulations (MOD; red line).

Table S2. Hourly ozone evaluation metrics at three boats.

Boat	Period	Observed mean (ppb)	Simulated mean (ppb)	R	MB (ppb)	NMB (%)	MAE (ppb)	RMSE (ppb)
pontoon	all days	31.50	38.60	0.77	7.10	22.53	10.69	13.12
	ozone episode	43.34	45.99	0.69	2.65	6.12	10.15	13.88
	clean days	25.36	34.76	0.76	9.40	37.08	10.97	12.71
Red Eagle	all days	30.39	39.79	0.64	9.39	30.91	12.77	15.82
	ozone episode	44.05	47.87	0.55	3.82	8.66	11.99	15.63
	clean days	24.45	36.27	0.52	11.82	48.34	13.11	15.90
shrimp boat	all days	33.43	40.81	0.71	7.36	22.04	10.68	13.32
	ozone episode	46.13	48.39	0.56	2.26	4.91	10.36	14.24
	clean days	26.54	36.68	0.66	10.14	38.21	10.86	12.80

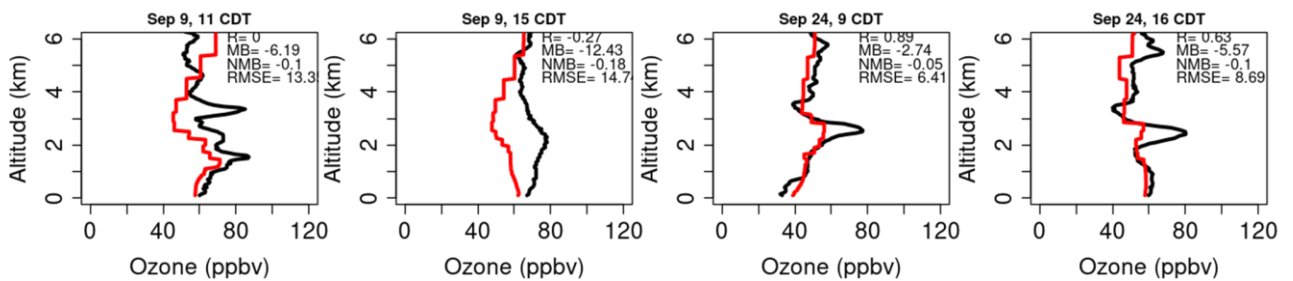


Figure S3: Ozone vertical distributions observed by ozonesondes (black) and simulated by the model (red) over Galveston Bay on September 9th and 24th.

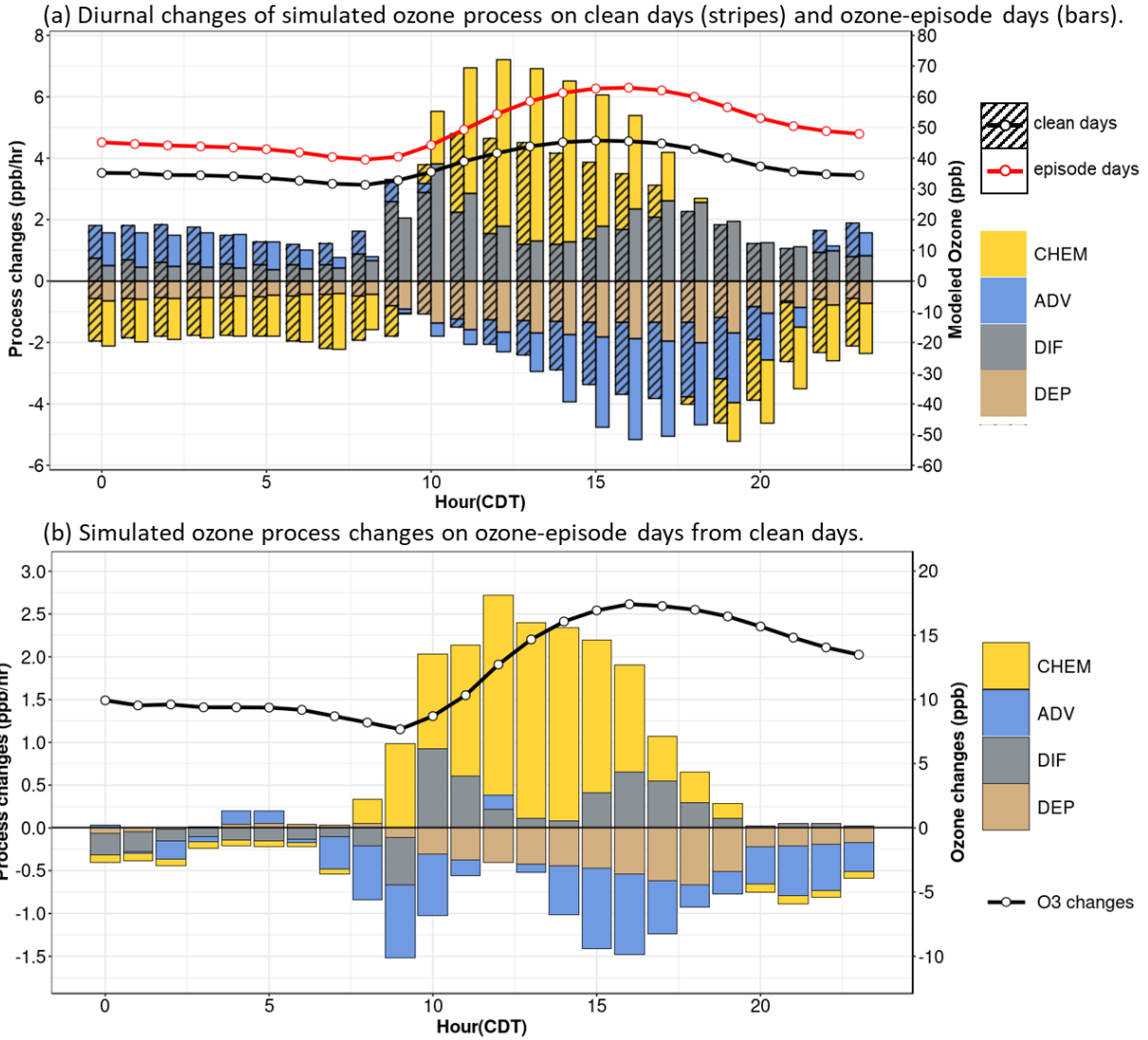


Figure S4. (a) Diurnal changes of simulated ozone processes over the land (black box in Figure 3), including chemistry (CHEM), advection (ADV), diffusion (DIF), and deposition (DEP) on clean days (stripes) and ozone-episode days (bars) integrated across the lowest five model layers. Overlaid lines and points are simulated hourly ozone on clean (black) and ozone-episode (red) days. (b) Process (filled bars) and O₃ (black line) changes during high-O₃ episodes from clean days.

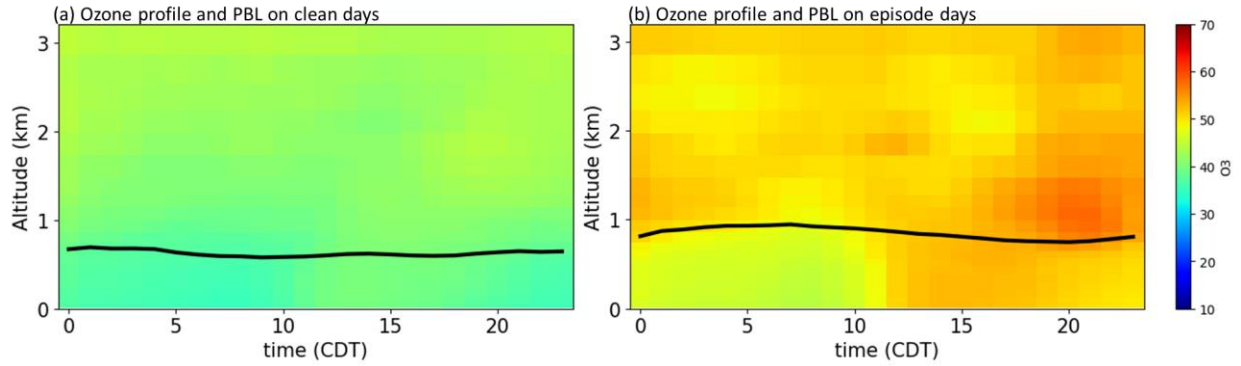


Figure S5. Model simulated diurnal O_3 profiles (background) overlaid with PBL (black lines) averaged over the Gulf of Mexico on clean (a) and episode (b) days.

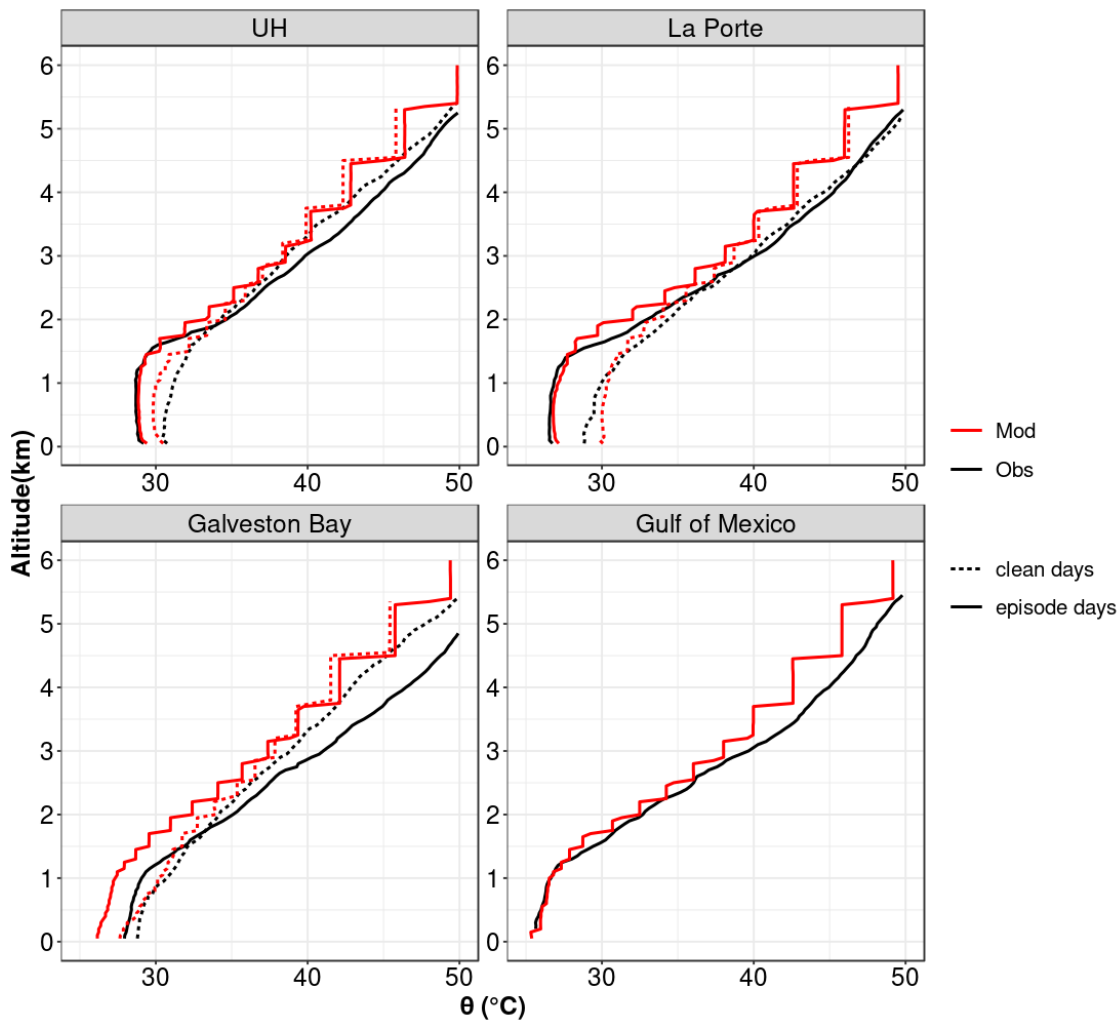


Figure S6. Potential temperature (θ) vertical distribution from the afternoon (12:00-18:00) ozonesonde launches (Obs; black lines) and simulations (Mod; red lines) at UH, LaPorte and Galveston Bay averaged on clean days (dashed lines) and ozone-episode days (solid lines). The Gulf of Mexico only sampled ozone on episode days.

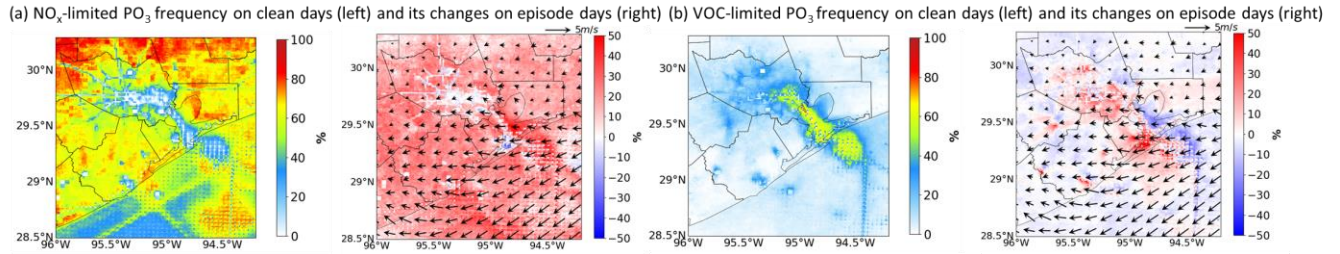


Figure S7. The frequency of ozone production (PO_3) rate under NO_x -limited (a) and VOC-limited (b) regimes on clean days (left) and its changes under episode days (right) during midday (11:00-15:00) hours of the study period.

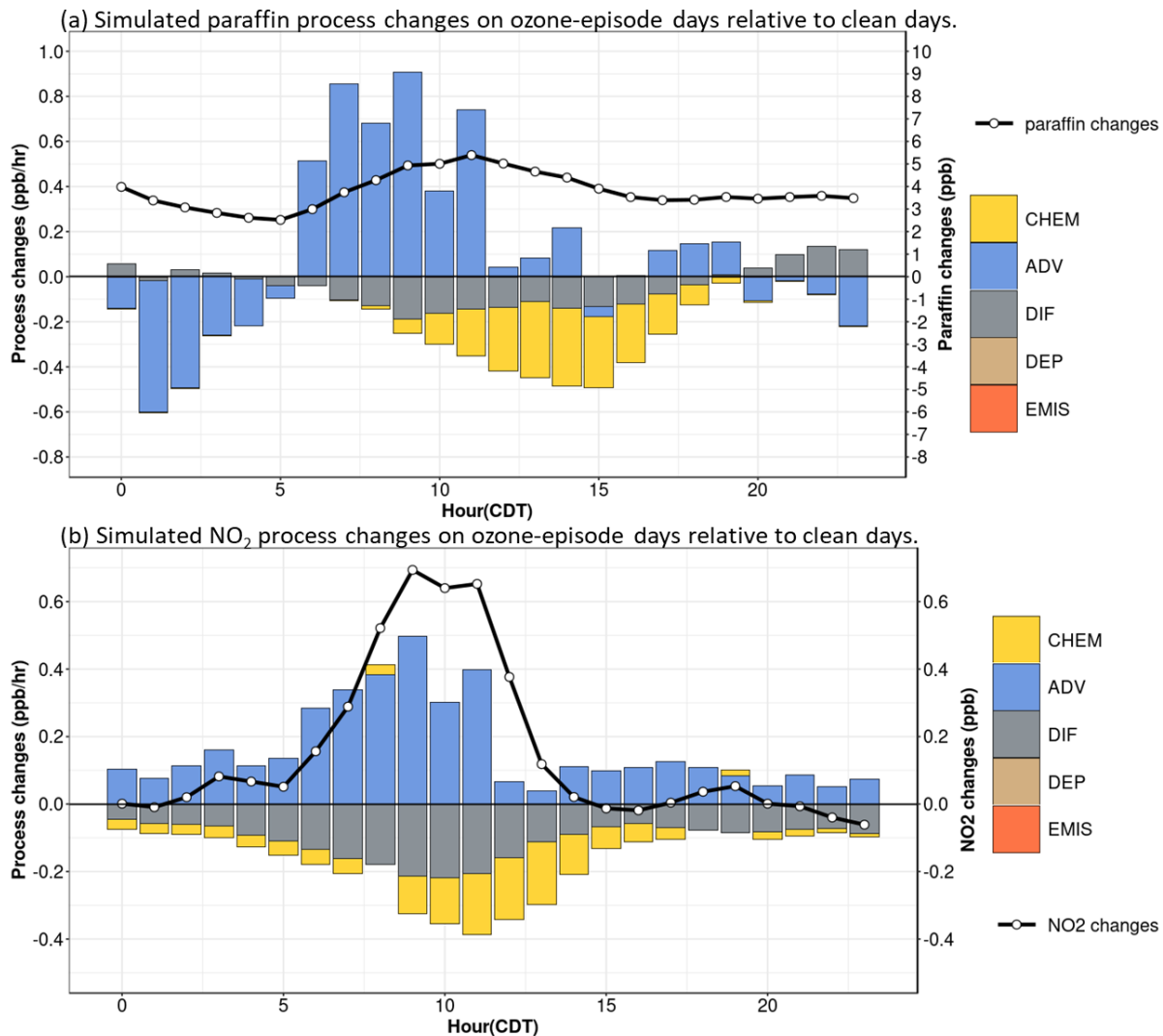


Figure S8. Diurnal changes of simulated processes over the Gulf of Mexico (black box in Figure 2b), including chemistry (CHEM), advection (ADV), diffusion (DIF), deposition (DEP), and emissions (EMIS) on ozone-episode days relative to clean days integrated across the lowest five model layers for paraffin (a) and NO_2 (b). Overlaid lines and points are simulated hourly paraffin (a) and NO_2 (b) changes.

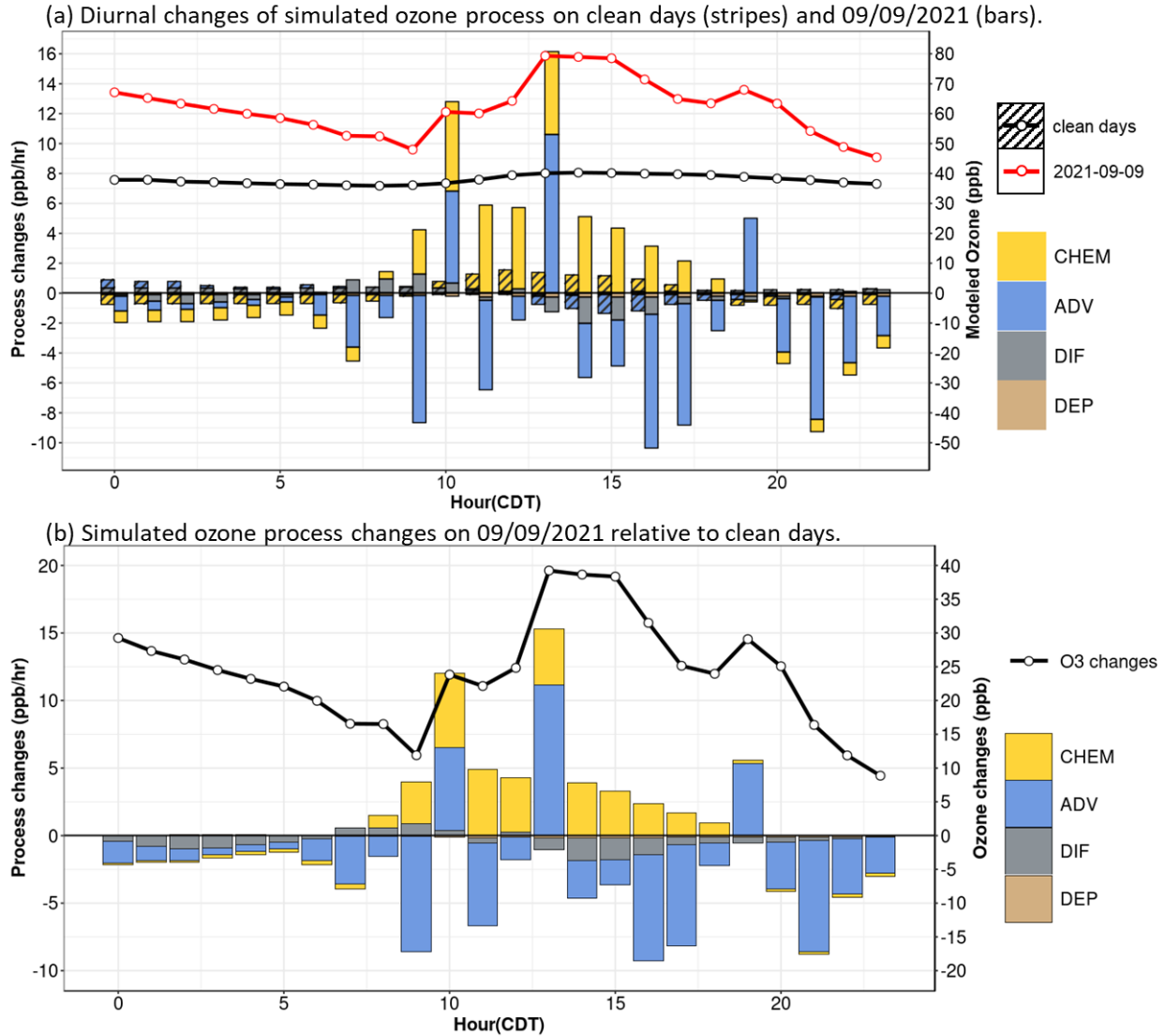


Figure S9. (a) Diurnal changes of simulated ozone processes over the Gulf of Mexico (black box in Figure 2), including chemistry (CHEM), advection (ADV), vertical diffusion (DIF), and deposition (DEP) on clean days (stripes) and 09/09/2021 (bars) integrated across the lowest five model layers. Overlaid lines and points are simulated hourly ozone on clean (black) and 09/09/2021 (red) days. (b) Process (filled bars) and O₃ (black line) changes on 09/09/2021 relative to clean days.

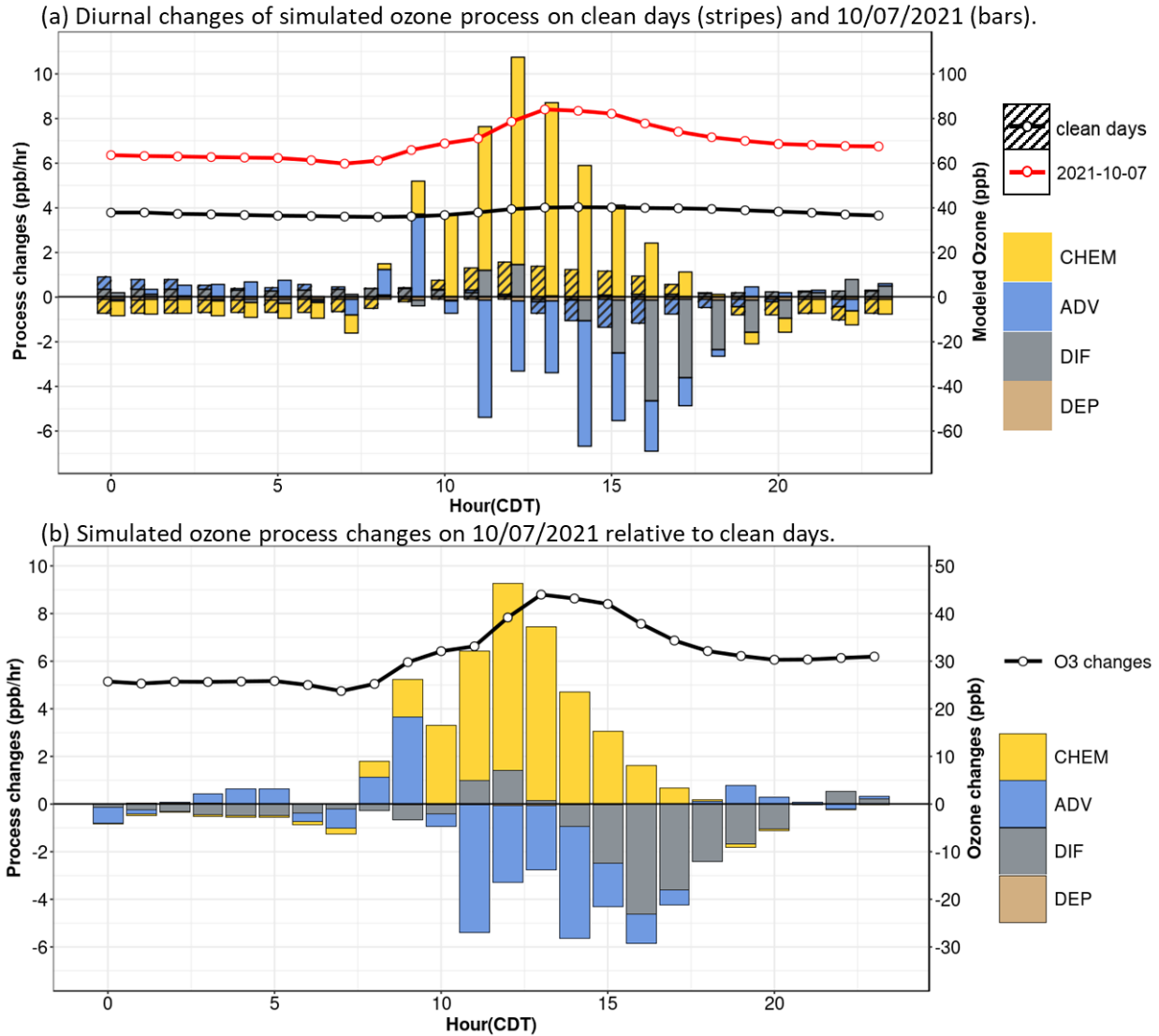


Figure S10. (a) Diurnal changes of simulated ozone processes over the Gulf of Mexico (black box in Figure 2), including chemistry (CHEM), advection (ADV), vertical diffusion (DIF), and deposition (DEP) on clean days (stripes) and 10/07/2021 (bars) integrated across the lowest five model layers. Overlaid lines and points are simulated hourly ozone on clean (black) and 10/07/2021 (red) days. (b) Process (filled bars) and O₃ (black line) changes on 10/07/2021 relative to clean days.