

Continental precursor transport enhances ozone formation over the atmosphere of tropical coastal waters

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Text S1

To evaluate the model performance, index of agreement (IOA), correlation coefficient (COE), and the root mean square error (RMSE) were determined through formulas 1 - 3. IOA indicates the agreement between observations and simulations in the range of 0 - 1, and higher value of IOA represents better agreement. COE measures the strength of the relationship between observed and simulated values, and the perfect negative and positive relationships are shown as values of -1 and 1, respectively. RMSE estimates how well the simulated results fit the observed data, and the lower values of RMSE reflect better fit.

$$IOA = 1 - \frac{\sum_{i=1}^n (O_i - S_i)^2}{\sum_{i=1}^n (|O_i - \bar{O}| + |S_i - \bar{O}|)^2} \quad (1)$$

$$COE = \frac{\sum_{i=1}^n (O_i - \bar{O})(S_i - \bar{S})}{\sqrt{\sum_{i=1}^n (O_i - \bar{O})^2 \sum_{i=1}^n (S_i - \bar{S})^2}} \quad (2)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (O_i - S_i)^2} \quad (3)$$

S_i and O_i denoted the model and observation results, while $\bar{S}$ and $\bar{O}$ denoted the mean values of simulated and observed concentrations, respectively. n represented the number of data points.

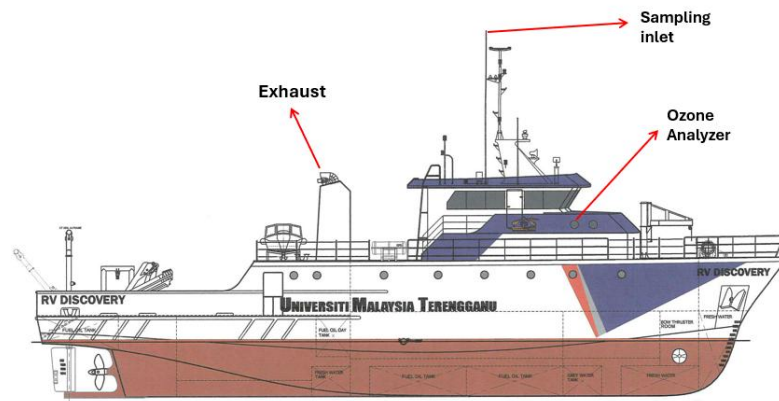


Figure S1 Schematic illustration of the RV Discovery showing the configuration of the shipborne O₃ measurement system during the NESC'16 cruise.

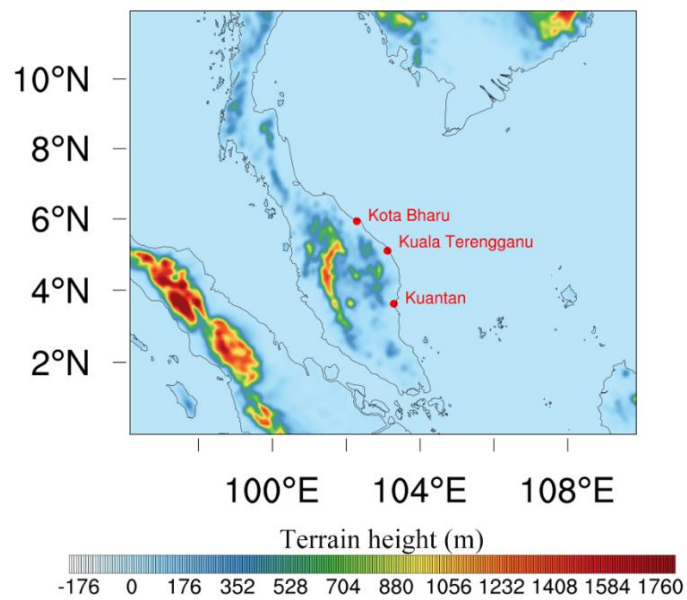


Figure S2 Terrain height (m) in the WRF simulation domain.

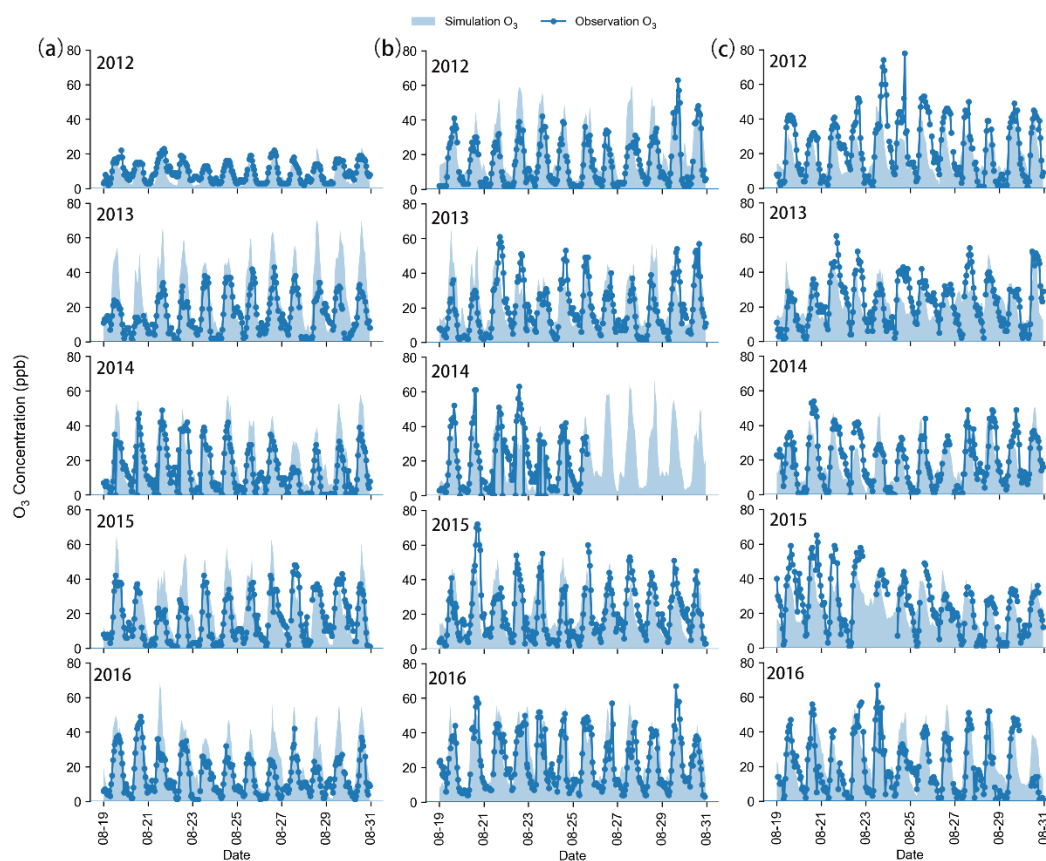


Figure S3 Time series of simulated and observed O₃ in each sampling site of (a) Kota Bharu, (b) Kuala Terengganu, and (c) Kuantan.

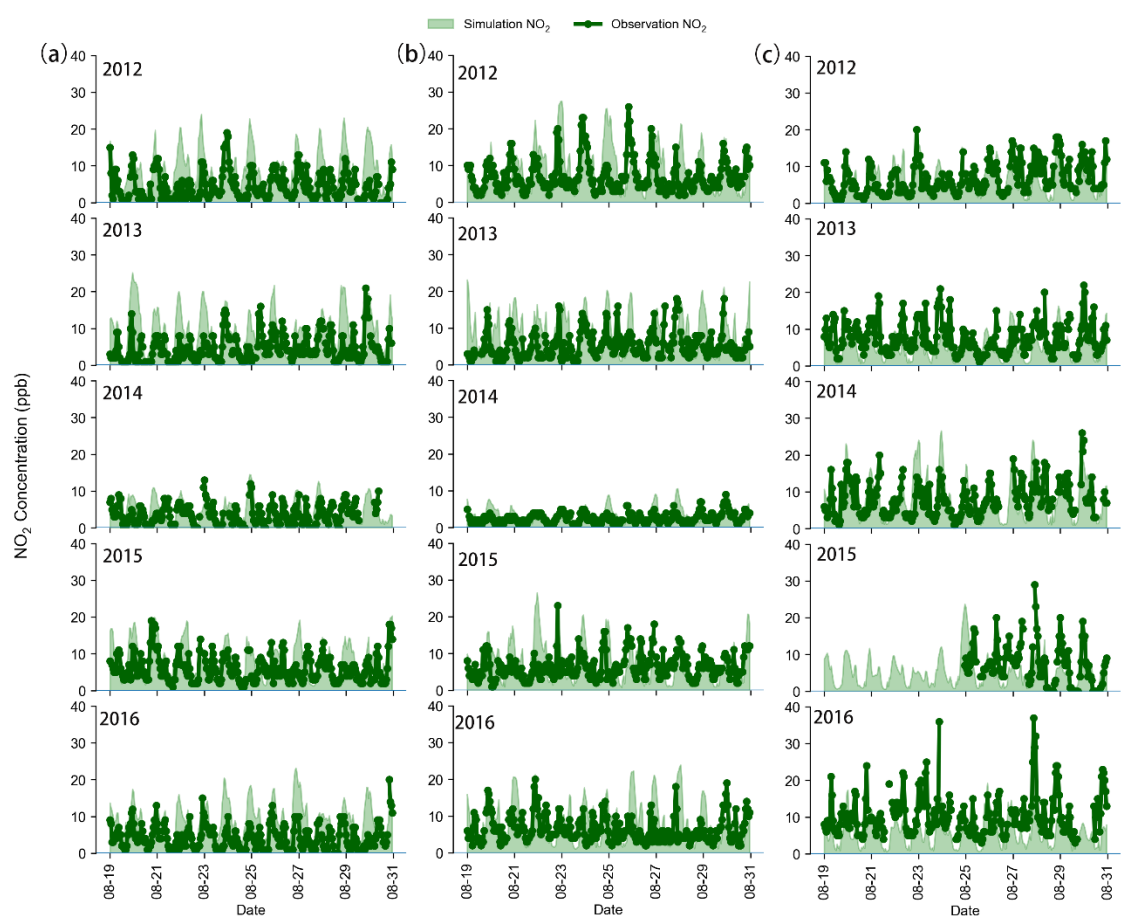


Figure S4 Time series of simulated and observed NO_2 in each sampling site of (a) Kota Bharu, (b) Kuala Terengganu, and (c) Kuantan.

Table S1 Statistical comparison between hourly observed and simulated O₃, NO₂, and meteorological parameters at Kota Bharu.

2012					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	9.44	8.20	0.82	0.89	3.56
NO ₂ (ppb)	7.45	9.02	0.52	0.57	3.73
Temperature (°C)	27.16	26.51	0.88	0.91	1.73
Relative Humidity (%)	77.49	88.08	0.85	0.80	13.22
2013					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	25.81	26.73	0.78	0.72	4.22
NO ₂ (ppb)	6.76	8.98	0.62	0.73	3.91
Temperature (°C)	27.49	26.86	0.89	0.93	1.53
Relative Humidity (%)	74.85	86.25	0.85	0.76	13.37
2014					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	14.35	21.06	0.76	0.82	9.88
NO ₂ (ppb)	3.72	4.66	0.62	0.64	3.23
Temperature (°C)	27.07	26.55	0.83	0.90	1.70
Relative Humidity (%)	77.42	86.17	0.78	0.77	11.62
2015					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	21.16	22.53	0.73	0.82	6.66
NO ₂ (ppb)	6.09	8.37	0.55	0.68	4.76
Temperature (°C)	27.23	27.04	0.84	0.91	1.70
Relative Humidity (%)	79.15	86.83	0.86	0.84	9.86
2016					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	25.09	23.17	0.83	0.79	5.11
NO ₂ (ppb)	6.23	8.45	0.59	0.56	2.04
Temperature (°C)	27.46	27.05	0.84	0.90	1.65
Relative Humidity (%)	79.35	87.65	0.80	0.80	11.18

Table S2 Statistical comparison between hourly observed and simulated O₃, NO₂, and meteorological parameters at Kuala Terengganu.

2012					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	19.06	23.62	0.81	0.83	7.45
NO ₂ (ppb)	7.18	8.40	0.51	0.55	2.59
Temperature (°C)	27.50	26.45	0.90	0.90	1.89
Relative Humidity (%)	79.90	88.25	0.82	0.76	14.61
2013					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	19.57	23.63	0.66	0.79	12.20
NO ₂ (ppb)	6.43	8.25	0.54	0.53	2.16
Temperature (°C)	27.43	26.86	0.85	0.91	1.72
Relative Humidity (%)	85.63	86.32	0.84	0.88	9.21
2014					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	19.63	21.12	0.72	0.84	11.66
NO ₂ (ppb)	2.57	3.15	0.54	0.59	2.20
Temperature (°C)	26.88	26.39	0.82	0.88	1.77
Relative Humidity (%)	88.24	87.80	0.76	0.82	10.26
2015					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	21.19	23.04	0.68	0.81	11.77
NO ₂ (ppb)	6.49	7.19	0.56	0.58	3.15
Temperature (°C)	27.66	27.11	0.86	0.92	1.50
Relative Humidity (%)	86.52	86.09	0.79	0.84	10.66
2016					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	23.69	26.79	0.75	0.85	11.29
NO ₂ (ppb)	6.57	8.14	0.59	0.53	3.91
Temperature (°C)	28.08	27.16	0.81	0.83	2.15
Relative Humidity (%)	80.00	89.04	0.77	0.73	12.39

Table S3 Statistical comparison between hourly observed and simulated O₃, NO₂, and meteorological parameters at Kuantan.

2012					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	21.03	19.54	0.71	0.77	7.33
NO ₂ (ppb)	6.62	6.07	0.59	0.76	2.59
Temperature (°C)	26.82	26.14	0.77	0.85	1.91
Relative Humidity (%)	91.82	90.69	0.78	0.88	6.80
2013					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	23.10	23.49	0.57	0.73	11.30
NO ₂ (ppb)	5.77	5.39	0.56	0.64	1.68
Temperature (°C)	26.68	26.12	0.87	0.92	1.47
Relative Humidity (%)	92.12	89.11	0.84	0.90	6.77
2014					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	20.04	19.12	0.73	0.85	9.85
NO ₂ (ppb)	8.00	8.28	0.59	0.75	1.74
Temperature (°C)	26.22	26.17	0.82	0.89	1.52
Relative Humidity (%)	93.43	90.03	0.70	0.80	7.78
2015.00					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	25.18	24.15	0.72	0.81	11.09
NO ₂ (ppb)	7.09	5.08	0.52	0.58	2.84
Temperature (°C)	26.74	26.77	0.87	0.93	1.30
Relative Humidity (%)	90.50	86.72	0.84	0.87	7.91
2016					
	Sim_mean	Obs_mean	IOA	R	RMSE
O ₃ (ppb)	23.25	24.92	0.77	0.85	9.58
NO ₂ (ppb)	6.29	5.80	0.54	0.56	3.83
Temperature (°C)	27.71	27.10	0.75	0.84	2.05
Relative Humidity (%)	78.11	88.17	0.72	0.72	13.14

Text S2

As shown in the table, the WRF-Chem model demonstrates reasonable reliability in simulating VOC components at the Kuala Terengganu and Kota Bharu stations. The Index of Agreement (IOA) for alkanes (ALK) at both stations exceeds 0.83, while the IOA values for aromatics (ARO) and olefins (OLE) are generally above 0.64, indicating that the model is capable of reproducing the temporal variability of these components with acceptable accuracy. These results are consistent with the findings of Zeren et al. (2022) and Wu et al. (2024), who reported IOA values generally above 0.46 when applying the WRF-Chem model over the Pearl River Estuary region. However, the correlation coefficients (COE) for certain components are relatively low, such as the COE of only 0.28 for ARO at Kota Bharu and 0.37 for OLE at Kuala Terengganu. Moreover, the simulated mean concentration of OLE at Kuala Terengganu (0.02 ppbv) is substantially lower than the observed value (0.14 ppbv), suggesting notable underestimation for more reactive VOC species. Wu et al. (2025) highlighted that uncertainties in emission inventories and incomplete chemical mechanisms are among the primary factors contributing to such model underestimation. Overall, the simulation results are considered acceptable for further analysis of regional VOC sources and their contributions to secondary pollutant formation.

Table S4 Comparison of simulated and observed Concentrations of Aromatic Hydrocarbons (ARO), Alkanes (ALK), and Olefins (OLE) in Kuala Terengganu and Kota Bharu.

Kuala Terengganu									
	MEAN		MAX		MIN		RMSE	COE	IOA
	SIM	OBS	SIM	OBS	SIM	OBS			
ARO	0.71	1.02	16.46	23.16	9.24	10.89	0.66	0.67	0.81
ALK	3.22	3.00	34.83	63.70	34.17	52.61	12.92	0.61	0.83
OLE	0.02	0.14	4.11	4.82	0.77	1.43	8.95	0.57	0.72
Kota Bharu									
	MEAN		MAX		MIN		RMSE	COE	IOA
	SIM	OBS	SIM	OBS	SIM	OBS			
ARO	2.71	2.36	14.05	13.01	8.12	5.54	2.61	0.58	0.64
ALK	13.29	9.69	63.66	46.61	22.68	15.15	9.44	0.66	0.85
OLE	0.15	0.14	1.83	1.59	1.37	1.22	4.97	0.60	0.80

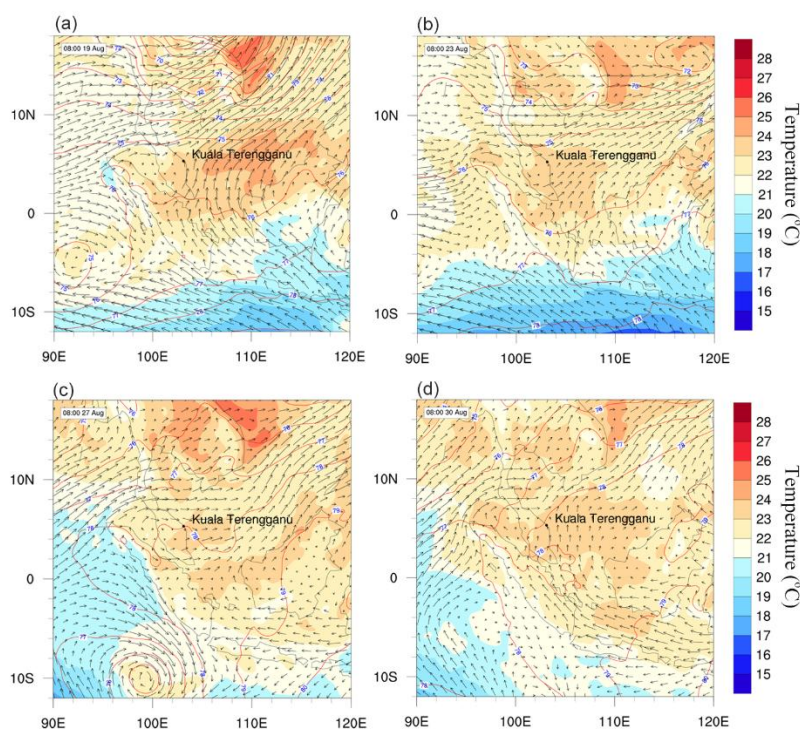


Figure S5 The spatial distributions of geopotential height (red line; units: dagpm), temperature (shaded; units: °C) and overlain by the wind vectors and wind speed (vector; units: $\text{m} \cdot \text{s}^{-1}$) at 925 hPa derived from the NCEP reanalysis data: (a) 08:00 LT on 19 August; (b) 08:00 LT on 23 August; (c) 08:00 LT on 27 August; (d) 08:00 LT on 30 August.

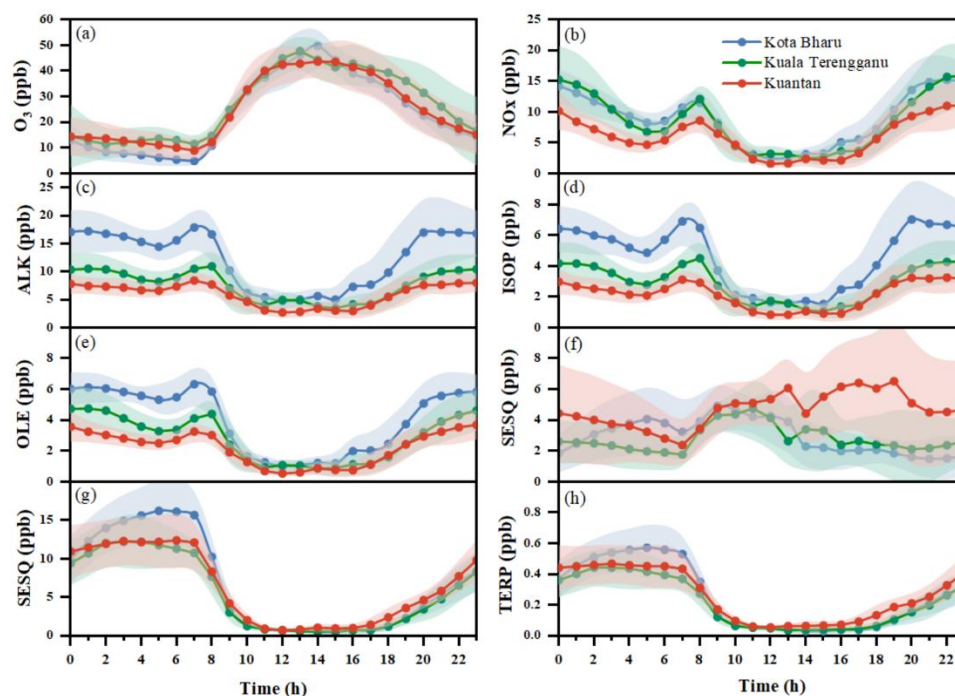


Figure S6 The diurnal variations of O_3 , NO_x , and volatile organic compounds in Kota Bharu, Kuala Terengganu, and Kuantan.

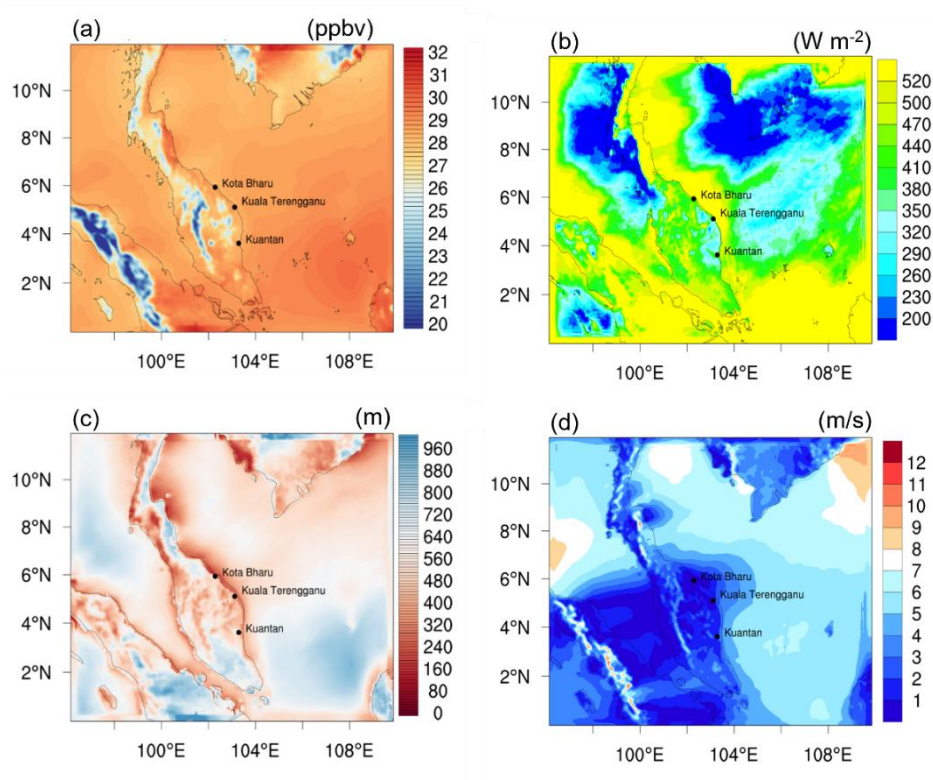


Figure S7 Spatial distribution of simulated surface temperature (a), downward shortwave radiation (b), planetary boundary layer height (c), and wind speed (d) in August 2016.

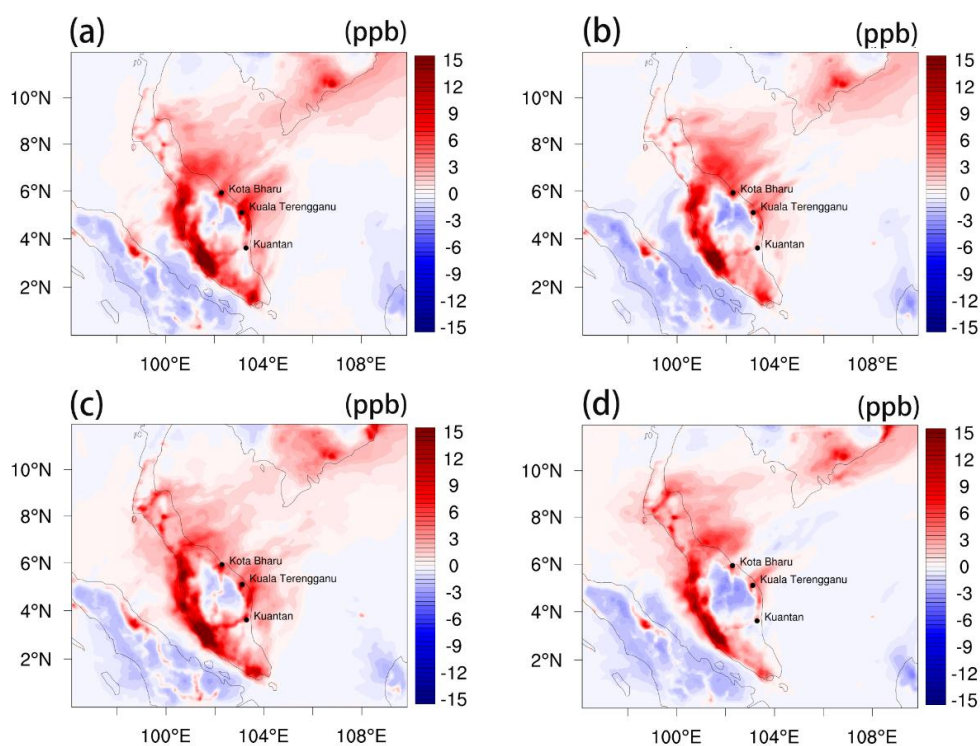


Figure S8 Differences in simulated surface O_3 between the base and case simulations at 1400 LST in August for 2012 - 2015: (a) 2012, (b) 2013, (c) 2014, (d) 2015.

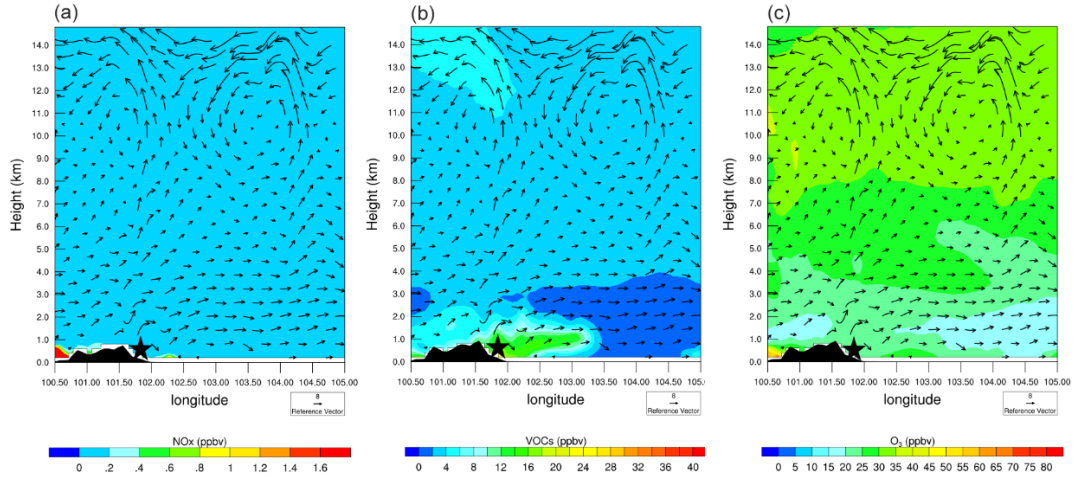


Figure S9 Vertical cross sections of simulated mixing ratios of (a) NO_x , (b) VOCs, and (c) O_3 , with in-plane wind vectors overlaid. The vertical velocity is multiplied by 100. The cross section extends from (6.14°N, 100.25°E) to (6.14°N, 105.25°E), and the black triangle denotes the Kota Bharu site.

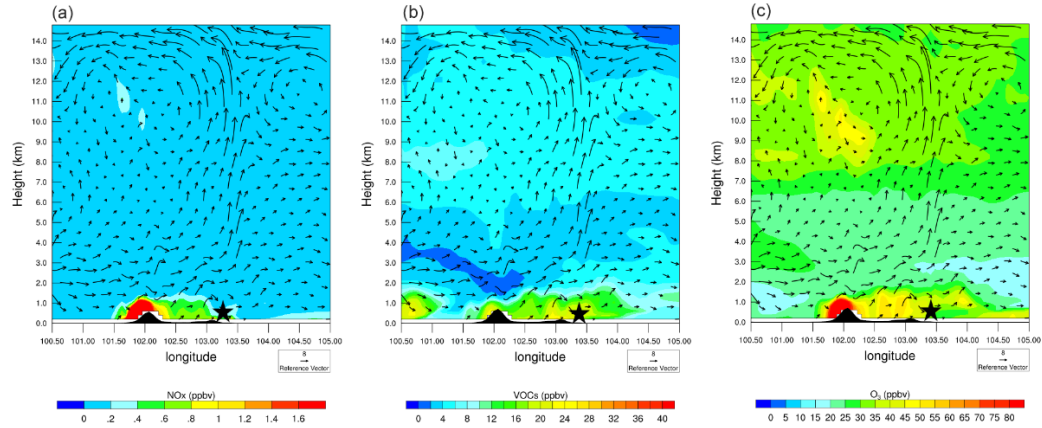


Figure S10 Vertical cross sections of simulated mixing ratios of (a) NO_x , (b) VOCs, and (c) O_3 , with in-plane wind vectors overlaid. The vertical velocity is multiplied by 100. The cross section extends from (3.82°N, 100.30°E) to (3.82°N, 105.30°E), and the black triangle denotes the Kuantan site.

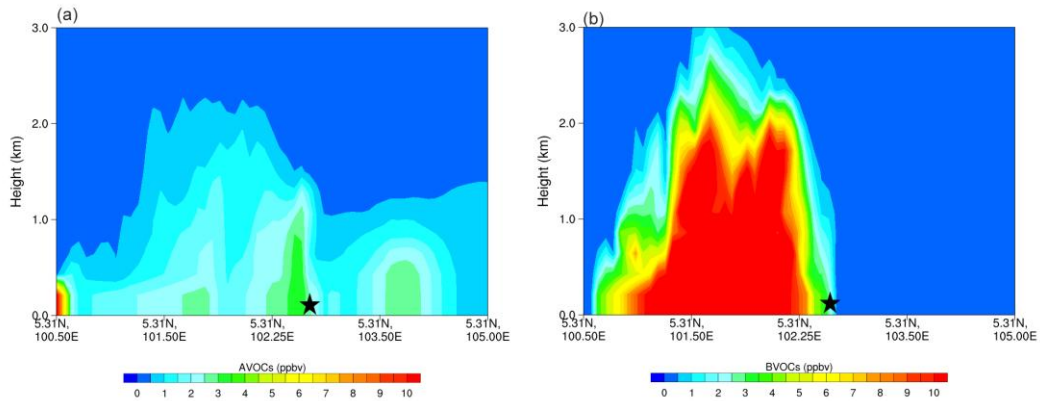


Figure S11 Vertical cross sections of VOCs concentrations (color-filled contours) and in-plane wind vectors (arrows), where the vertical speed is multiplied by 100 along the cross line from (5.10°N, 100.50°E) to (5.10°N, 105.00°E) for different VOCs components: (a) AVOCs, and (b) BVOCs. The black

triangle under the x-axis denotes the location of the Kuala Terengganu site.

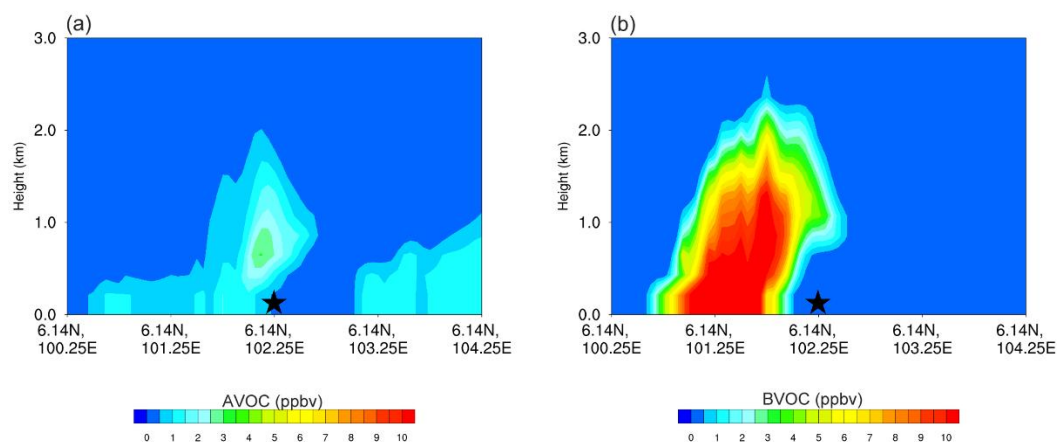


Figure S12 Vertical cross sections of VOCs concentrations (color-filled contours) and in-plane wind vectors (arrows), where the vertical speed is multiplied by 100 along the cross line from (6.14°N, 100.25°E) to (6.14°N, 105.25°E) for different VOCs components: (a) AVOCs, and (b) BVOCs. The black triangle under the x-axis denotes the location of the Kota Bharu site.

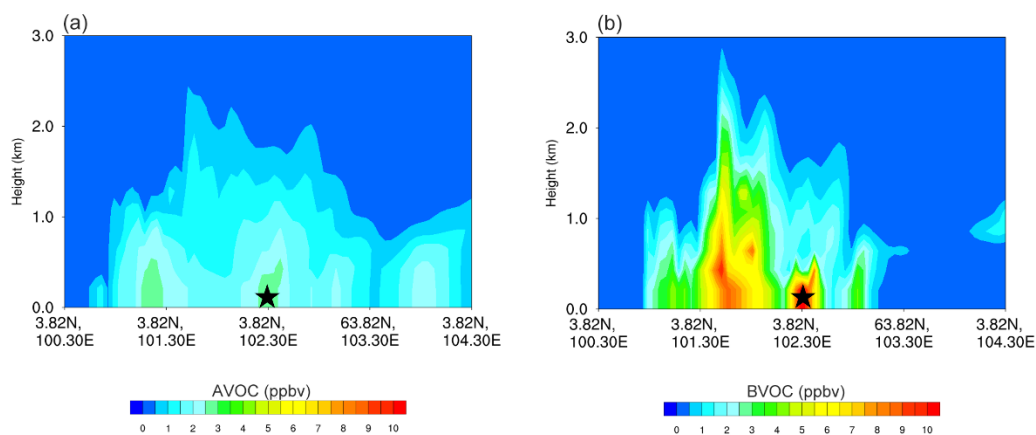


Figure S13 Vertical cross sections of VOCs concentrations (color-filled contours) and in-plane wind vectors (arrows), where the vertical speed is multiplied by 100 along the cross line from (3.82°N, 100.30°E) to (3.82°N, 105.30°E) for different VOCs components: (a) AVOCs, and (b) BVOCs. The black triangle under the x-axis denotes the location of the Kuantan site.

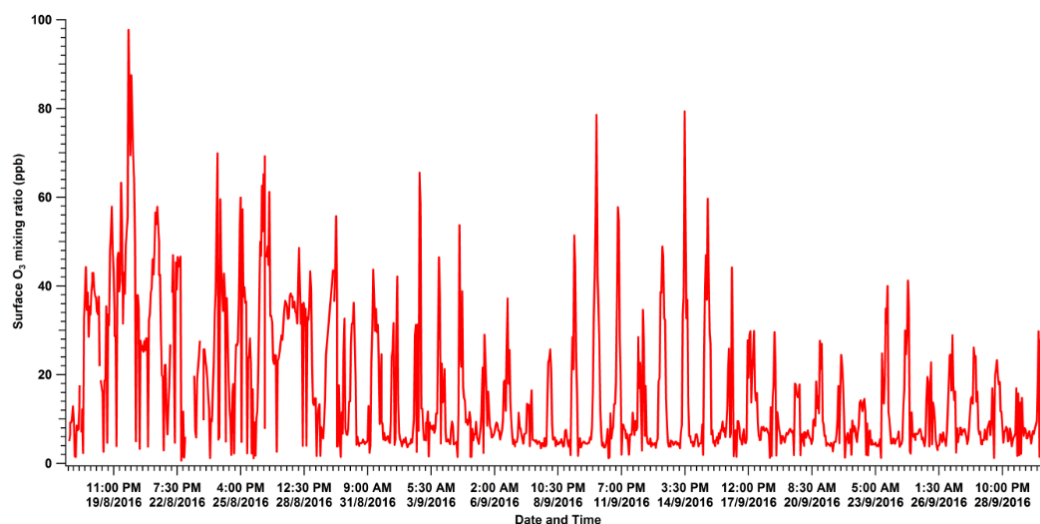


Figure S14 Diurnal distributions of surface O_3 over the maritime area during NESC'16 (19 to 28 August 2016) and at the oil palm plantation at Pekan (31 August to 30 September 2016).

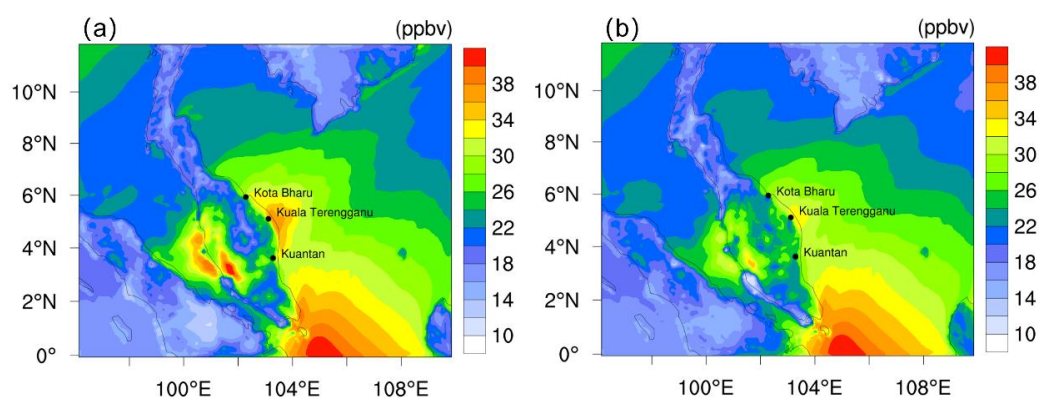


Figure S15 Spatial distribution simulation results of O_3 in Base (a) and Case (b).

Reference

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