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Development of the Real-time On-road Emission (ROE v1.0) model for street-scale air quality modeling based on dynamic traffic big data

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SUPPLEMENTARY

Table and figure List

S1 Emission factors and correction factors

Table S1. The on-road emission factors of petrol vehicle (unit: g/km)

Vehicle Category	Emission Standard	CO	HC	NO_x	$PM_{2.5}$	PM_{10}
LDV	Pre-China I	25.72	2.685	1.971	0.028	0.031
	China I	6.71	0.663	0.409	0.026	0.029
	China II	2.52	0.314	0.324	0.011	0.012
	China III	1.18	0.191	0.100	0.007	0.008
	China IV	0.68	0.075	0.032	0.003	0.003
	China V	0.46	0.056	0.017	0.003	0.003
MDV	Pre-China I	39.13	3.695	2.938	0.099	0.110
	China I	21.43	2.567	1.781	0.060	0.067
	China II	15.37	1.443	1.461	0.018	0.020
	China III	4.33	0.373	0.474	0.011	0.012
	China IV	1.98	0.107	0.196	0.006	0.007
	China V	1.98	0.107	0.147	0.006	0.007
HDV	Pre-China I	100.74	5.144	5.156	0.293	0.326
	China I	62.09	5.255	2.645	0.159	0.177
	China II	16.64	1.980	2.562	0.072	0.080
	China III	8.25	0.869	1.520	0.044	0.049
	China IV	3.77	0.418	0.775	0.044	0.049
	China V	3.77	0.418	0.582	0.044	0.049
LDT	Pre-China I	47.83	4.987	3.310	0.099	0.110

	China I	26.16	3.324	2.006	0.060	0.067
	China II	21.54	2.210	1.656	0.018	0.020
	China III	5.61	0.610	0.534	0.011	0.012
	China IV	2.37	0.169	0.229	0.006	0.007
	China V	2.37	0.169	0.172	0.006	0.007
MDT	Pre-China I	123.13	6.884	5.807	0.293	0.326
	China I	75.79	6.777	2.979	0.159	0.177
	China II	23.32	3.023	2.905	0.072	0.080
	China III	10.71	1.371	1.713	0.044	0.049
	China IV	4.50	0.573	0.907	0.044	0.049
	China V	4.50	0.573	0.680	0.044	0.049
HDT	Pre-China I	123.13	6.749	5.807	0.293	0.326
	China I	75.79	6.759	2.979	0.159	0.177
	China II	23.32	3.006	2.905	0.072	0.080
	China III	10.71	1.354	1.713	0.044	0.049
	China IV	4.50	0.555	0.907	0.044	0.049
	China V	4.50	0.555	0.680	0.044	0.049
MC	Pre-China I	14.20	2.010	0.130	0.030	0.033
	China I	8.96	0.990	0.140	0.018	0.020
	China II	2.58	0.530	0.150	0.008	0.009
	China III	1.11	0.210	0.100	0.003	0.003

LDV: light-duty vehicle, MDV: middle-duty vehicle, HDV: heavy-duty vehicle, LDT: light-duty truck, MDT: middle-duty truck, HDT: heavy-duty truck, MC: motorcycle.

Table S2. The on-road emission factors of diesel vehicle (unit: g/km)

Vehicle Category	Emission Standard	CO	HC	NO_x	$PM_{2.5}$	PM_{10}
LDV	Pre-China I	1.34	0.785	1.324	0.179	0.199
	China I	0.36	0.071	0.976	0.063	0.070
	China II	0.45	0.046	0.976	0.052	0.058
	China III	0.14	0.024	0.841	0.032	0.036
	China IV	0.13	0.016	0.679	0.031	0.034
	China V	0.13	0.016	0.679	0.031	0.034
MDV	Pre-China I	3.91	1.493	5.470	1.603	1.781
	China I	3.44	1.425	4.787	0.464	0.516
	China II	2.82	0.425	5.693	0.157	0.174
	China III	2.12	0.364	3.347	0.148	0.164
	China IV	1.84	0.364	2.678	0.106	0.118
	China V	1.84	0.364	2.276	0.053	0.059
HDV	Pre-China I	10.53	2.668	12.421	1.286	1.429
	China I	9.86	0.576	11.156	0.983	1.092
	China II	8.68	0.351	9.892	0.882	0.980
	China III	6.74	0.283	9.892	0.395	0.439

	China IV	3.25	0.107	9.892	0.252	0.280
	China V	1.62	0.054	8.640	0.126	0.140
LDT	Pre-China I	3.28	2.097	6.758	0.435	0.483
	China I	4.19	2.040	5.578	0.269	0.299
	China II	3.22	1.305	5.578	0.261	0.290
	China III	1.88	0.368	3.765	0.130	0.144
	China IV	1.48	0.186	2.636	0.058	0.064
	China V	1.48	0.186	2.240	0.012	0.013
MDT	Pre-China I	12.05	3.560	10.782	1.322	1.450
	China I	4.24	1.612	7.479	0.905	1.006
	China II	4.63	0.421	6.221	0.273	0.303
	China III	2.09	0.203	6.221	0.171	0.190
	China IV	1.65	0.103	4.354	0.099	0.110
	China V	1.65	0.103	3.701	0.020	0.022
HDT	Pre-China I	13.60	4.083	13.823	1.322	1.450
	China I	5.79	0.897	9.589	0.623	0.692
	China II	3.08	0.520	7.934	0.502	0.558
	China III	2.79	0.255	7.934	0.243	0.270
	China IV	2.20	0.129	5.554	0.138	0.153
	China V	2.20	0.129	4.721	0.027	0.030

LDV: light-duty vehicle, MDV: middle-duty vehicle, HDV: heavy-duty vehicle, LDT: light-duty truck, MDT: middle-duty truck, HDT: heavy-duty truck.

Table S3. HC evaporation factors of petrol vehicle

	evaporation factors	unit
Driving	11.6	g/h
Parking	6.5	g/day

Table S4. Temperature correction factors of petrol vehicle

	Low Temperature (< 10 ºC)	High Temperature (< 10 ºC)
CO	1.36	1.23
HC	1.47	1.08
NO_x	1.15	1.31

Table S5. Temperature correction factors of diesel vehicle

	Vehicle Category	Low Temperature (< 10 ºC)	High Temperature (> 25 ºC)
CO	LDV	1.00	1.33
	LDT	1.00	1.33
	MDV, LDV, MDT, LDT	1.00	1.30
HC	LDV	1.00	1.07
	LDT	1.00	1.06
	MDV, LDV, MDT, LDT	1.00	1.06
NO_x	LDV	1.06	1.17
	LDT	1.05	1.17
	MDV, LDV, MDT, LDT	1.06	1.15
$PM_{2.5}$, PM_{10}	LDV	1.87	0.68
	LDT	1.27	0.90
	MDV, LDV, MDT, LDT	1.70	0.74

LDV: light-duty vehicle, MDV: middle-duty vehicle, HDV: heavy-duty vehicle, LDT: light-duty truck, MDT: middle-duty truck, HDT: heavy-duty truck.

Table S6. Relatively humidity correction factors of petrol vehicle

	Low Relatively Humidity (<50%)		High Relatively Humidity (>50%)	
	Low Temperature (< 24 ºC)	High Temperature (> 24 ºC)	Low Temperature (< 24 ºC)	High Temperature (> 24 ºC)
CO	1.00	0.97	1.00	1.04
HC	1.00	0.99	1.00	1.01
NO_x	1.06	1.13	0.92	0.87

Table S7. Relatively humidity correction factors of diesel vehicle

	Low Relatively Humidity (<50%)		High Relatively Humidity (>50%)	
	Low Temperature (< 24 ºC)	High Temperature (> 24 ºC)	Low Temperature (< 24 ºC)	High Temperature (> 24 ºC)
CO	1.00	1.00	1.00	1.00
HC	1.00	1.00	1.00	1.00
NO_x	1.04	1.12	0.94	0.88

Table S8. High altitude (>1500 m) correction factors of vehicle

Vehicle Category	Fuel Type	CO	HC	NO_x
LDT, LDV	Petrol	1.58	2.46	3.15
LDT, LDV	Diesel	1.20	1.32	1.35
MDV, MDT, LDV, LDT	Petrol	3.95	2.26	0.88
MDV, MDT, LDV, LDT	Diesel	2.46	2.05	1.02

LDV: light-duty vehicle, MDV: middle-duty vehicle, HDV: heavy-duty vehicle, LDT: light-duty truck, MDT: middle-duty truck, HDT: heavy-duty truck.

Table S9. Traffic condition correction factors of petrol vehicle

	Traffic Speed (km/h)				
	<20	20–30	30–40	40–80	>80
CO	1.69	1.26	0.79	0.39	0.62
HC	1.68	1.25	0.78	0.32	0.59
NO_x	1.38	1.13	0.90	0.96	0.96
$PM_{2.5}$, PM_{10}	1.68	1.25	0.78	0.32	0.59

Table S10. Traffic condition correction factors of diesel vehicle

	Emission Standard	Traffic Speed (km/h)				
		<20	20–30	30–40	40–80	>80
CO	Pre-China I to China III	1.43	1.14	0.89	0.84	0.61
	China IV, China V	1.29	1.10	0.93	0.70	0.61
HC	Pre-China I to China III	1.41	1.13	0.90	0.61	0.41
	China IV, China V	1.38	1.12	0.91	0.64	0.48
NO_x	Pre-China I to China III	1.31	1.08	0.93	0.74	0.66
	China IV, China V	1.39	1.12	0.91	0.60	0.28
$PM_{2.5}$, PM_{10}	Pre-China I to China III	1.22	1.08	0.93	0.71	0.49
	China IV, China V	1.36	1.12	0.91	0.65	0.48

S2 Uncertainty analysis of the emission factors

In order to estimate the uncertainty of emission factors, some previous results were collected and compared with the emission factors applied in this study. As shown in Figure S1, the uncertainties for each pollutant of petrol vehicles were much larger than that of diesel vehicle. Overall, the uncertainties of LDVs for CO, HC, and NO_x were larger than those of all other vehicle categories, irrespective of the use of petrol or diesel as the fuel. There were maximum 8.9 and 9.8 times higher for CO emission factors, 13.5 and 21.9 for HC, and 10.5 and 2.0 times for NO_x than that of the emission factors applied in this study. For $PM_{2.5}$ and PM_{10}, HDTs had showed the largest uncertainty range, at a maximum of 11.9 and 11.3 times higher for petrol HDT, and 3.5 and 16.1 times for higher diesel HDT, compared with the emission factors used in this study, respectively. However, it should be indicated more comprehensive emissions factor measurements are required to analyze the uncertainty and improve the accuracies of the emission factors in the future.

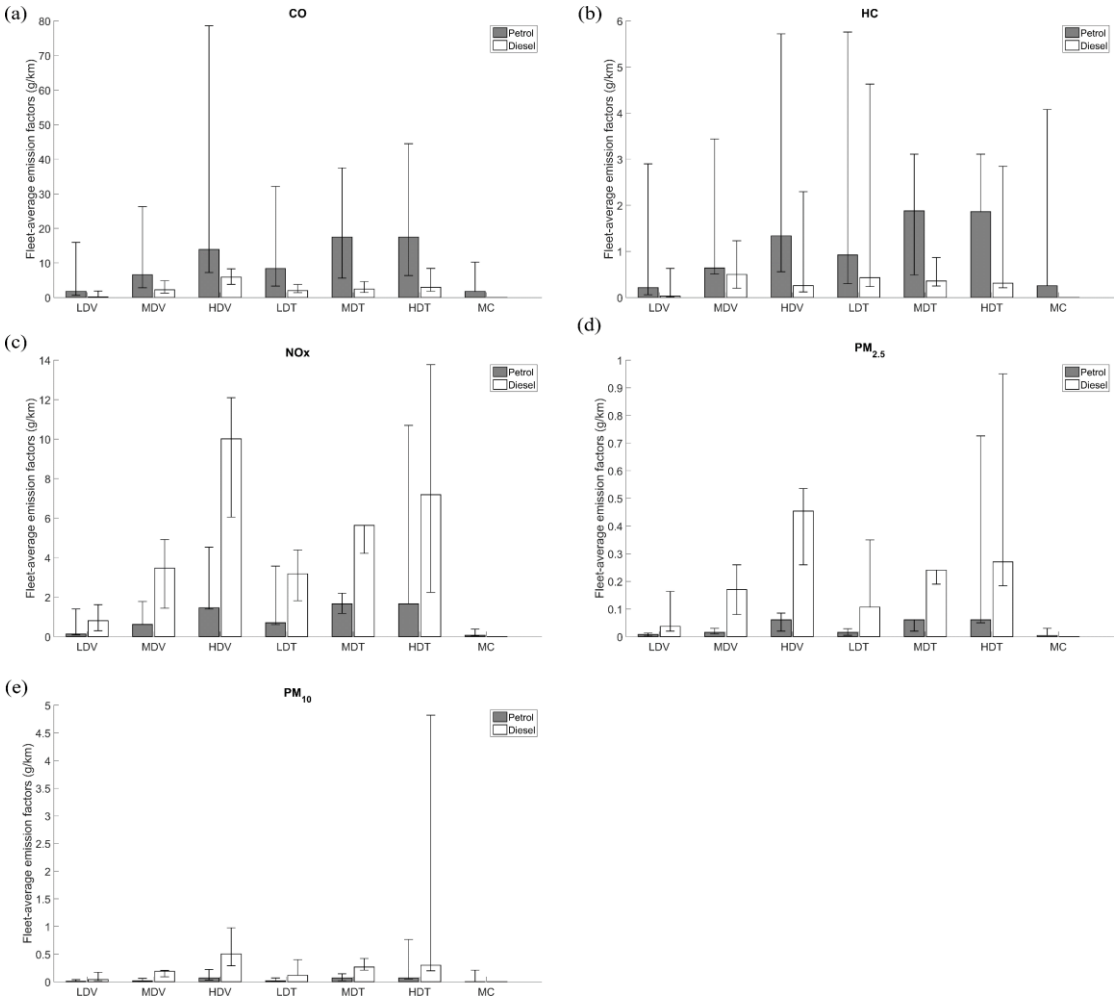

Figure S1. Fleet-average emission factors of (a) CO, (b) HC, (c) NO_x, (d) $PM_{2.5}$, and (e) PM_{10} (the value of the histogram represented the fleet-average emission factors in the study, the range represented the emission factors from other literatures).

S3 Sensitivity analysis of air quality modeling simulation

In order to identify the factors that affected the simulation results, the modeling sensitivity was tested in this study. As per the diurnal variations shown in Figure S2, the NO_2 concentrations were underestimated, while the O_3 concentrations were overestimated at night. However, the daytime model predictions, which indicated the overprediction of NO_2 concentrations and the underprediction of O_3 concentrations, were opposite to the nighttime predictions. Combined with the observation and background concentrations data in Figure S3, the daytime NO_2 and nighttime O_3 overprediction may be caused by the overestimation of background concentrations.

To evaluate the impact of background concentrations on the simulation results, the no-emission sensitivity case was devised for enhancing the background effect. This case was run without any emissions, and the results are shown in Figure S4. For NO_2, daytime concentrations were still overestimated compared with the observational data, especially for May 2nd, with the maximum daytime overestimation during the simulation being 23.7%. Nighttime O_3 concentrations were also overpredicted in this case, showing that the overestimation was mostly due to the overestimation of the background O_3 concertation. In contrast, since only vehicle emissions were considered, the underestimation of daytime O_3 concentrations should relate to the lack of other sectors of emission in the simulation street network.

Another case was set up to evaluate the nighttime NO_x titration. Since NO_2 concentrations were underestimated at night but overestimated during daytime, NO_2 titration was not underpredicted and was probably overpredicted at night. The overestimation of nighttime should be due to the underestimation of the NO concentrations. Thus, the double-background-NO case was set up with double background NO concentrations to evaluate the NO titration. As the background NO concentration increased, the nighttime NO_2 concentrations increased, offsetting the underestimated concentration in the base case. O_3 concentrations decreased due to the enhancement of NO titration. These results show that, on the one hand, the overestimation of background O_3 concentrations could lead to the overprediction of O_3 at night. On the other hand, the underestimated NO titration was also a reason for the nighttime overprediction of O_3 concentrations.

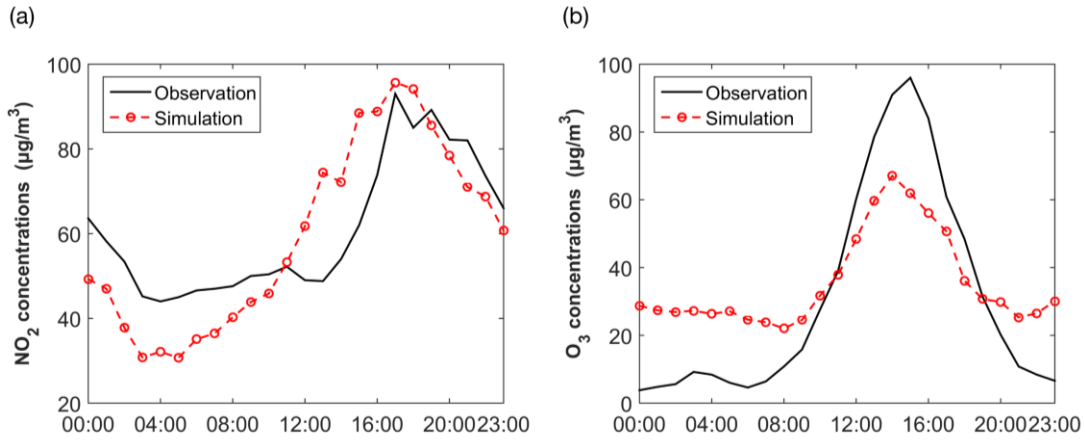

Figure S2. Diurnal variations of (a) NO_2 and (b) O_3 during the simulation period. (black solid line: observation; red dashed line: simulation).

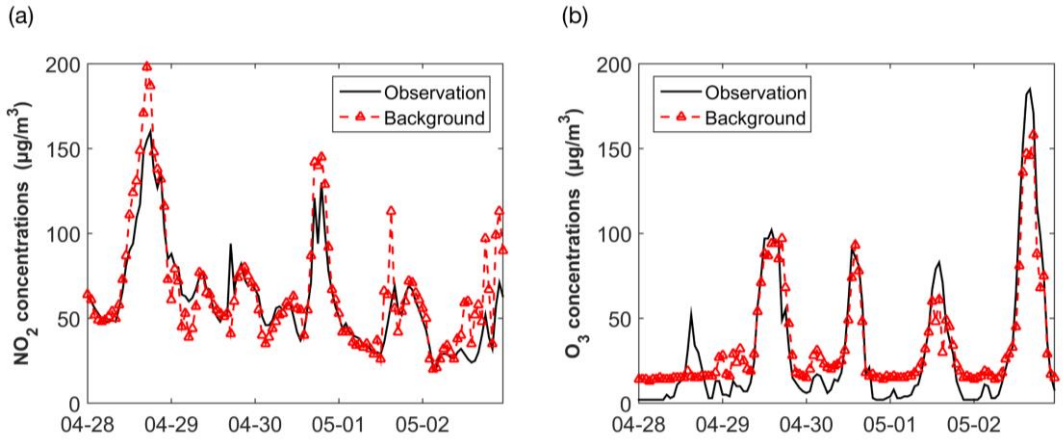

Figure S3. Time series of observational and background concentrations for (a) NO_2 and (b) O_3 during the simulation period (black solid line: observation; red dashed line: background).

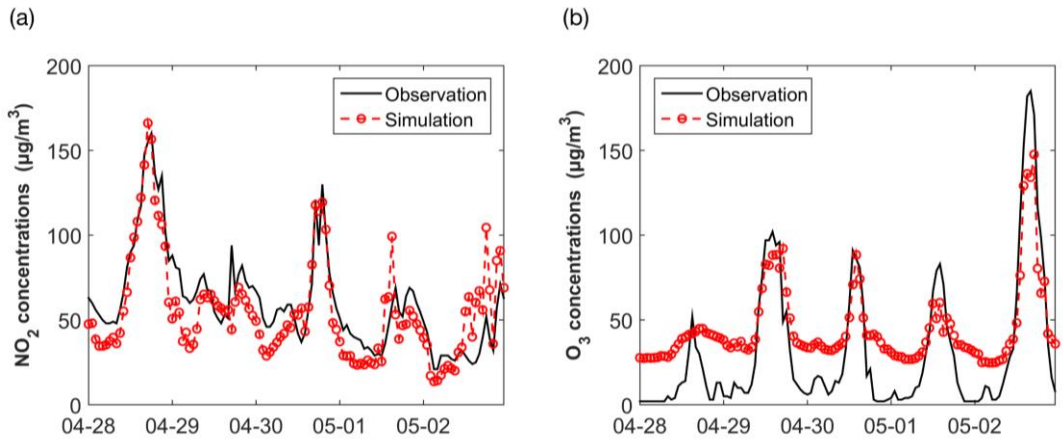

Figure S4. Time series of (a) NO_2 and (b) O_3 during the simulation period in no-emission sensitivity case. (black solid line: observation; red solid line: simulation).

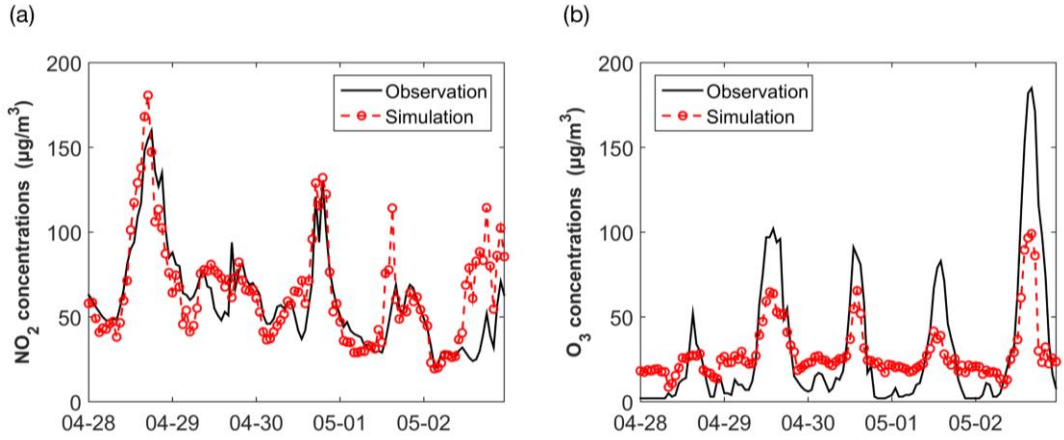

Figure S5. Time series of (a) NO_2 and (b) O_3 during the simulation period in double-background-NO case. (black solid line: observation; red solid line: simulation).