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Modeling of aerosol property evolution during winter haze episodes over a megacity cluster in northern China: roles of regional transport and heterogeneous reactions of SO_2

Huiyun Du et al.

Correspondence to: Ji Li (lijie8074@mail.iap.ac.cn)

Supplements

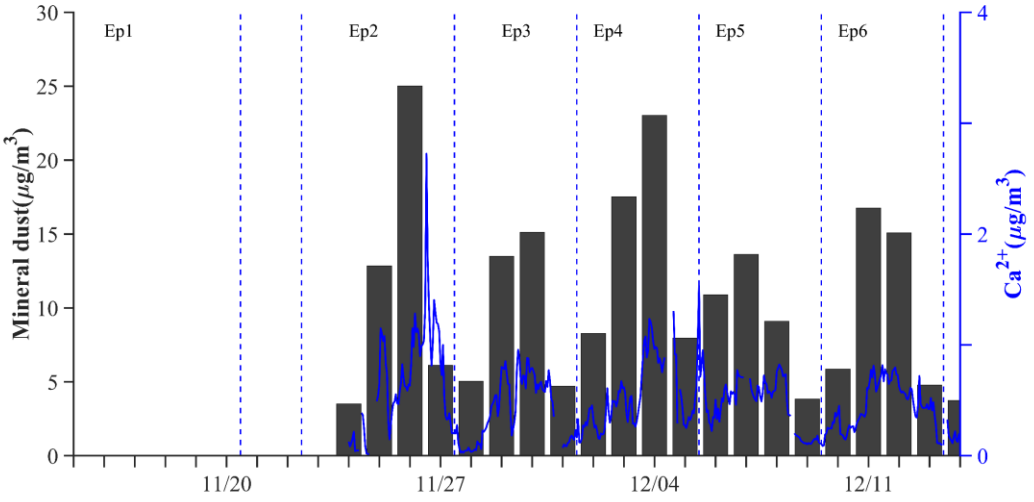

Figure S1. Concentration of mineral dust and Ca^{2+} in $PM_{2.5}$ during the study period. And $\text{Mineral} = 2.2 \times [\text{Al}] + 2.49 \times [\text{Si}] + 1.63 \times [\text{Ca}] + 2.42 \times [\text{Fe}] + 1.94 \times [\text{Ti}]$.

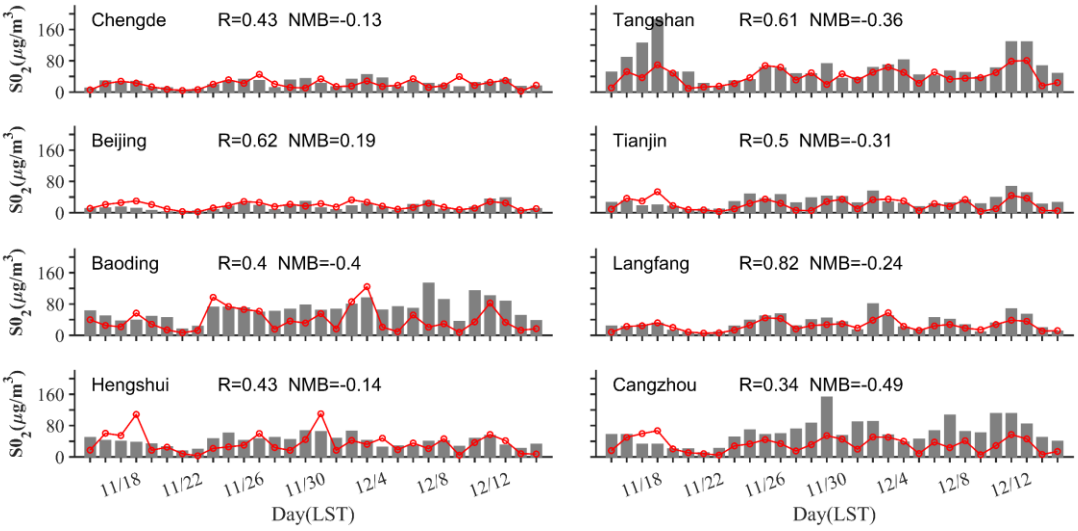

Figure S2. Comparison between the simulated (red) and observed (gray bars) daily concentrations of SO_2.

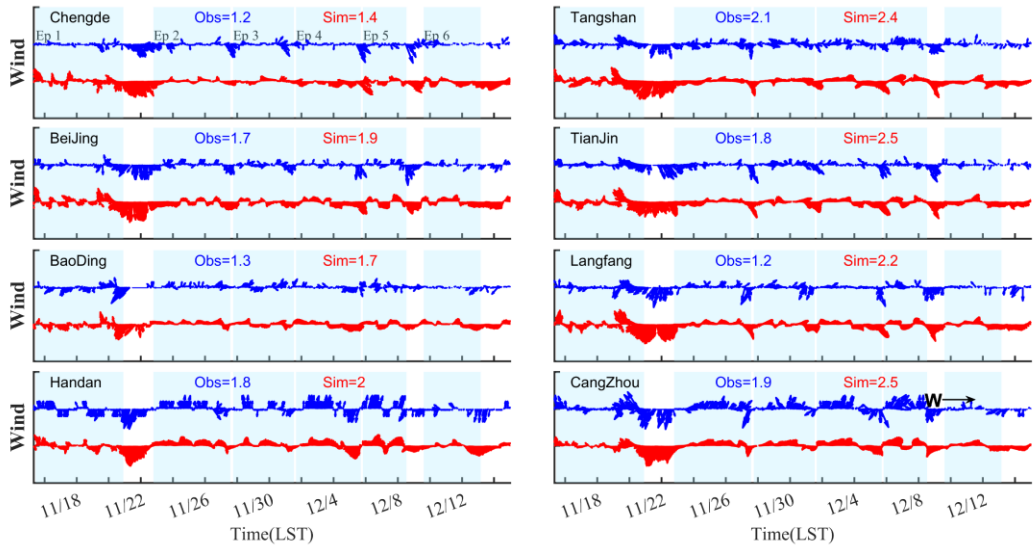

Figure S3. Comparison between simulated (red) and observed (blue) wind vector and wind speeds (data) at cities of BTH.

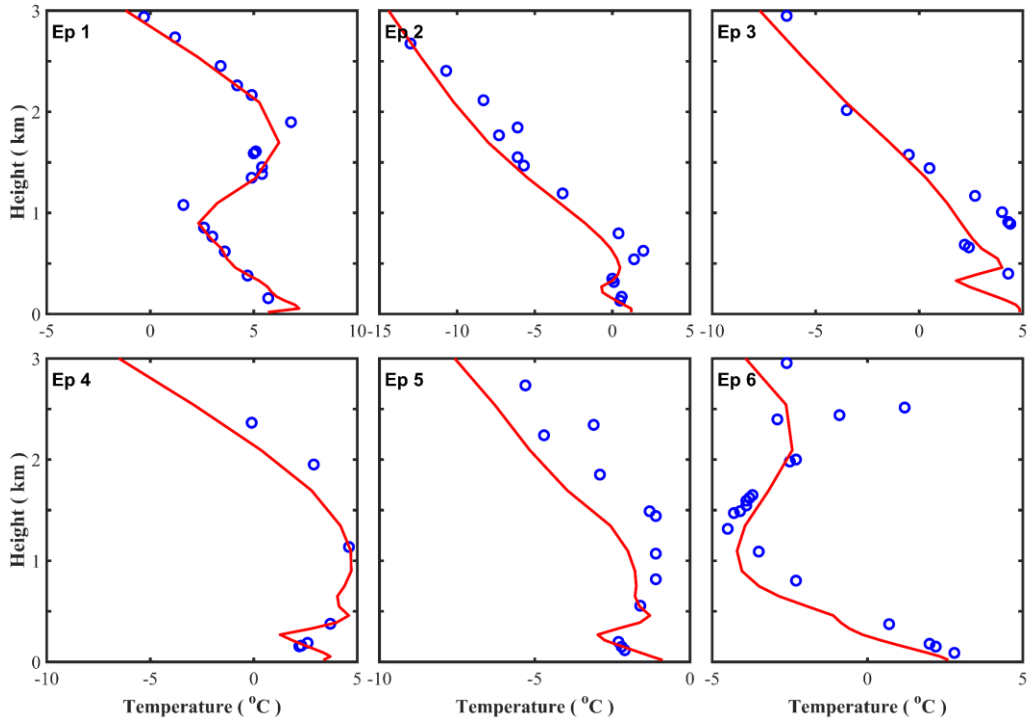

Figure S4. Comparison between simulated (red solid line) and observed (blue dot) temperature profiles during episodes in Beijing.

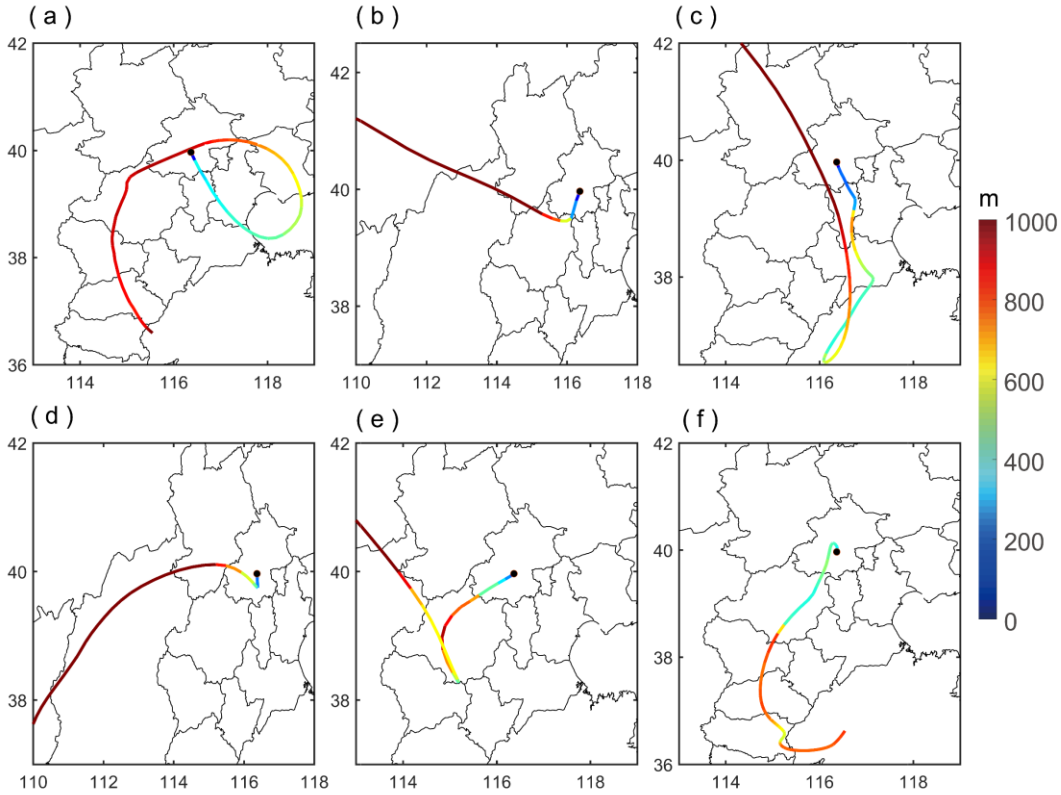

Figure S5. 72 h backward trajectories during different episodes (05:00 on November 20, 18:00 on November 26, 23:00 on November 29, 20:00 on December 03, 05:00 on December 08 and 11:00 on December 12 [LST]) at Beijing at 100m. Line color represents height of trajectories. a-f refer to Ep1-6.

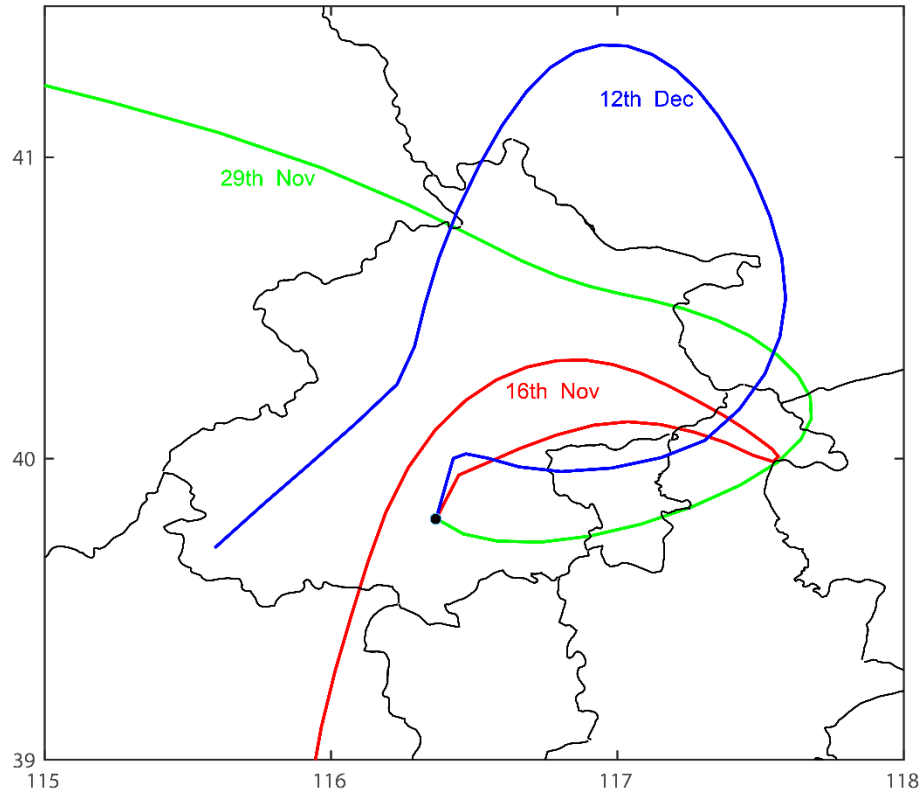

Figure S6. 36 h backward trajectories at different start time (02:00 on November 17, 11:00 on November 29, and 23:00 on December 12 [LST]) at Beijing.

Table S1. Statistics performances of meteorological simulations, including temperature and relative humidity at 2 m, and wind speed at 10 m. Statistical parameters include correlation coefficient (R), Normalized Mean Bias (NMB) and Root Mean Squared Error (RMSE).

		Obs	Sim	NMB	R	RMSE
T2(K)	Beijing	2.42	3.31	0.37	0.88	2.11
	Tianjin	4.05	3.73	-0.08	0.93	1.48
	Langfang	2.13	3.06	0.44	0.89	2.13
	Chengde	-3.39	-1.66	-0.51	0.89	3.31
RH2(%)	Beijing	53.93	39.53	-0.27	0.69	21.87
	Tianjin	56.95	47.58	-0.16	0.73	18.09
	Langfang	60.39	46.54	-0.23	0.71	21.54

WS10(m/s)	Chengde	61.56	55.96	-0.09	0.47	20.26
	Beijing	1.68	1.93	0.15	0.65	1.30
	Tianjin	1.76	2.46	0.39	0.70	1.50
	Langfang	1.23	2.15	0.74	0.57	1.56
	Chengde	1.16	1.41	0.21	0.63	1.22

Table S2. Aerosol properties along transport, including geometric mean diameter (GMD [nm]), mass ratio of coating to BC (R_{BC}), number concentration (N) and contribution of region source to BC (Cr [%]). T_0 means ending points of back trajectories and T_n means n hours before arriving at the ending point.

Period	Property	T_{-24}	T_{-18}	T_{-12}	T_{-6}	T_0
Ep1	R_{BC}	3.6	4.0	5.2	7.8	8.7
	GMD	97	115	128	139	134
	N	28994	15494	15204	15592	19242
	Cr	40	93	75	7	34
Ep2	R_{BC}	2.1	3.6	2.3	5.7	3.8
	GMD	91	104	102	119	106
	N	23909	15189	17961	10994	20121
	Cr	1.2	0.14	0.01	95	13
Ep3	R_{BC}	6.9	13.2	3.2	4.1	7.6
	GMD	13	74	96	95	126
	N	22234	11880	13481	14241	12945
	Cr	59	81.4	6.2	8.8	1
Ep4	R_{BC}	2.3	6.2	3.6	5.4	6.9
	GMD	102	98	95	111	117
	N	19754	12805	21116	10536	17199
	Cr	98	56	68	25	1
Ep5	R_{BC}	69	10.0	2.9	2.1	6.6
	GMD	29	114	99	95	124
	N	8617	8086	16494	28211	13696
	Cr	100	100	50	4	78
Ep6	R_{BC}	1.8	2.4	4.6	5.9	4.6
	GMD	98	103	111	129	116
	N	31691	23691	17885	12897	21955
	Cr	54	0.17	0.01	65	19