Supporting Information

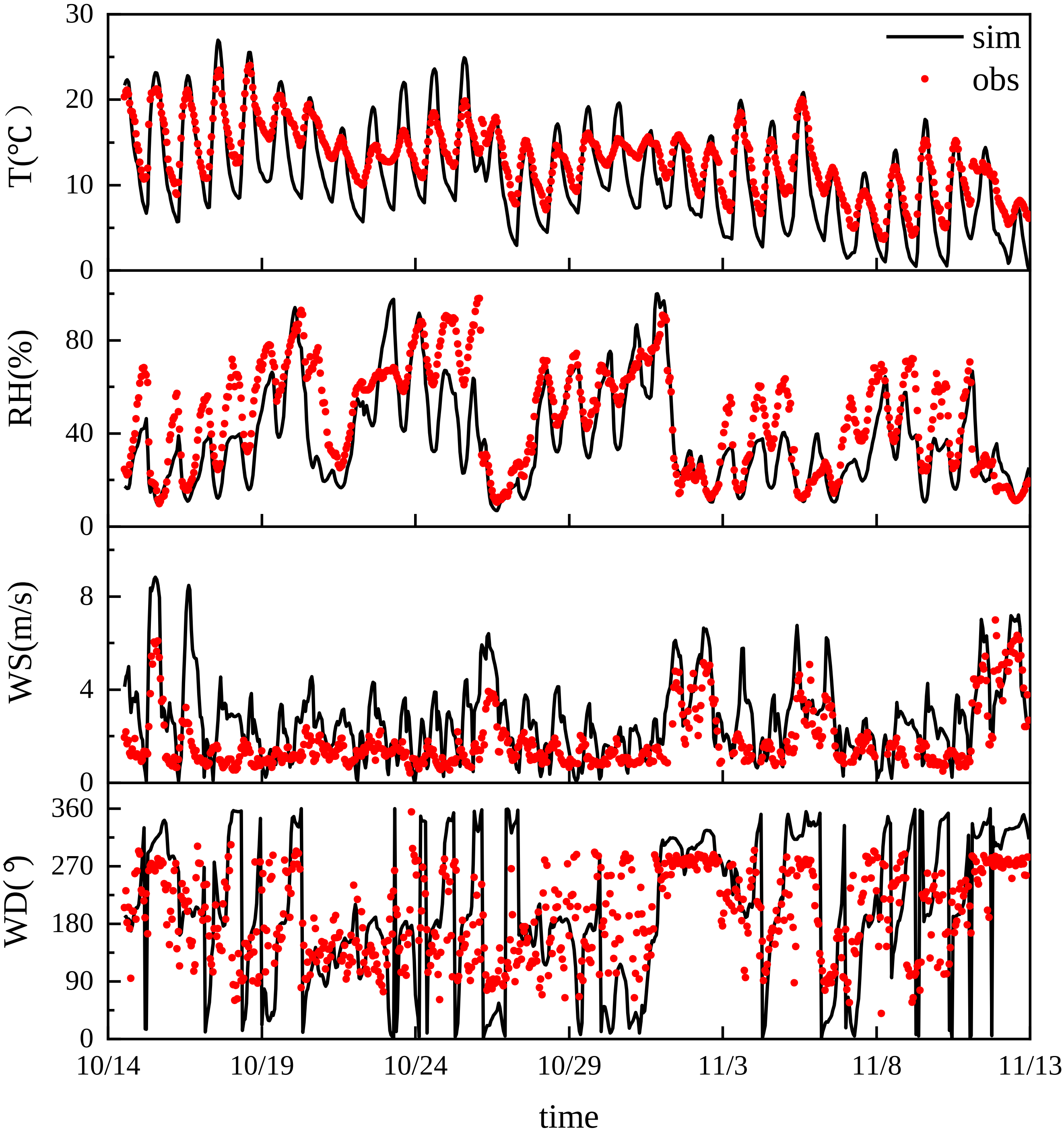

Figure S1. The observed and simulated hourly meteorological variations of temperature (T), relative humidity (RH), wind speed (WS), and wind direction (WD) during the episode from October 14 to November 14, 2014 at the Beijing site.

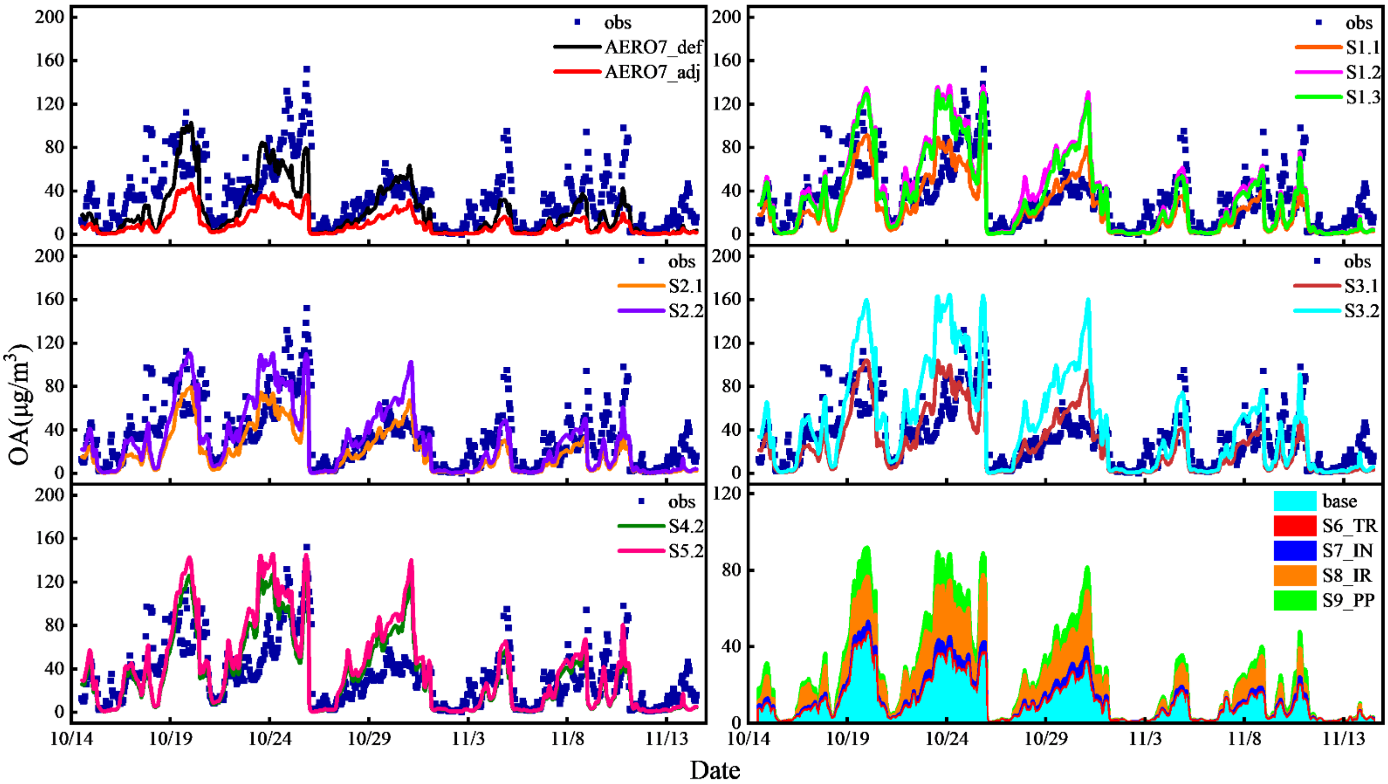

Figure S2. The observed and simulated hourly OA concentrations during the episode from October 14 to November 14 in 2014 at the Beijing site in the sensitivity cases as summarized in Table 3.

Table S1 Model evaluation statistics for meteorological variables including T, RH and WS.

		2014 (October 14 to November 14)						2018 (December 1 to 30)					
Variables		OBS	SIM	MB	GE	RMSE	R	OBS	SIM	MB	GE	RMSE	R
T (□)	Beijing	11.91	11.61	-0.30	2.01	2.52	0.90	-2.15	-3.29	-1.14	2.07	2.63	0.90
	Baoding	11.93	12.83	0.90	2.10	2.65	0.91	-2.35	-1.53	0.82	2.21	2.79	0.90
	Xingtai	13.52	13.84	0.32	1.82	2.35	0.90	-0.06	-0.08	-0.02	1.80	2.22	0.91
	Jinan	14.17	13.04	-1.13	1.68	2.12	0.94	1.16	-0.21	-1.37	1.80	2.29	0.95
	Changsha	18.65	18.90	0.25	2.08	2.76	0.84	5.90	8.82	2.92	3.14	3.66	0.88
	Hangzhou	17.71	17.29	-0.42	1.74	2.12	0.90	7.57	9.01	1.44	1.88	2.52	0.91
	Guangzhou	22.13	24.04	1.91	2.17	2.89	0.86	16.01	17.60	1.59	2.51	3.33	0.85
	Guiyang	14.22	15.45	1.23	2.27	2.84	0.83	4.79	6.15	1.36	2.51	3.27	0.85
	Wulumuqi	6.93	7.54	0.61	1.78	2.27	0.93	-12.65	-10.79	1.86	2.96	3.92	0.74
RH (%)	Beijing	51.30	35.74	-15.56	17.84	23.19	0.75	29.55	35.00	5.45	9.03	11.67	0.85
	Baoding	57.15	37.51	-19.64	21.22	26.13	0.73	46.07	37.66	-8.41	13.03	17.80	0.74
	Xingtai	60.64	38.44	-22.20	23.29	28.42	0.68	45.83	32.91	-12.92	15.87	22.22	0.64
	Jinan	53.37	51.57	-1.80	8.35	11.21	0.89	47.49	49.77	2.28	11.66	15.30	0.82
	Changsha	64.42	58.96	-5.46	11.42	15.18	0.83	84.49	70.71	-13.78	16.72	23.23	0.80
	Hangzhou	70.37	69.19	-1.18	10.79	13.10	0.85	80.97	85.02	4.05	9.43	12.32	0.75
	Guangzhou	75.58	65.30	-9.28	11.94	15.93	0.80	78.90	66.98	-11.92	15.04	19.35	0.74
	Guiyang	85.30	78.05	-7.25	12.37	16.30	0.67	85.31	79.53	-5.78	11.12	16.79	0.72
	Wulumuqi	56.03	43.32	-12.71	14.87	17.62	0.84	73.54	72.89	-0.65	10.30	12.86	0.52
WS (m/s)	Beijing	2.03	2.97	0.94	1.34	1.67	0.62	2.38	3.41	1.03	1.47	1.90	0.56
	Baoding	2.11	2.84	0.73	1.26	1.64	0.57	1.71	2.50	0.79	1.21	1.57	0.53
	Xingtai	1.35	3.43	2.08	2.15	2.66	0.51	2.67	3.09	0.43	1.39	1.81	0.33
	Jinan	2.87	4.51	1.64	1.87	2.28	0.70	2.10	3.61	1.51	1.66	1.99	0.62
	Changsha	1.90	3.23	1.33	1.49	1.82	0.50	3.56	4.11	0.55	1.19	1.43	0.75
	Hangzhou	2.11	2.95	0.84	1.18	1.49	0.48	2.46	3.91	1.45	1.63	2.01	0.67
	Guangzhou	2.16	3.24	1.08	1.40	1.69	0.50	3.01	4.31	1.30	1.54	1.85	0.69
	Guiyang	2.41	3.68	1.27	1.49	1.85	0.43	2.69	4.00	1.31	1.56	1.95	0.34
	Wulumuqi	2.17	3.74	1.57	1.95	3.08	0.21	1.69	2.04	0.35	1.22	1.57	0.37

Note: OBS denotes the observation value; SIM denotes the simulation value; MB denotes mean bias; GE denotes gross error; RMSE denotes root mean square error; R denotes correlation coefficient.

Table S2 Model evaluation statistics for hourly $PM_{2.5}$ concentrations during October 14–November 14, 2014, and daily $PM_{2.5}$ concentrations during December 6–30, 2018, under different sensitivity simulation cases.

Period	City	Species	Cases	N	OBS	SIM	MB	NMB	NME	R
October 14–November 14, 2014	Beijing	$PM_{2.5}$	def	692	83.09	44.45	-38.64	-46.50%	48.00%	0.73
			adj		83.09	33.52	-49.57	-59.66%	59.83%	0.70
			S1.1		83.09	46.88	-36.21	-43.58%	45.85%	0.72
			S1.2		83.09	60.67	-22.42	-26.99%	42.04%	0.72
			S1.3		83.09	57.50	-25.59	-30.80%	42.19%	0.73
December 6–30, 2018	Handan	$PM_{2.5}$	adj	18	89.60	54.79	-34.81	-38.85%	44.36%	0.60
			S1.1		89.60	74.00	-15.60	-17.41%	37.34%	0.59
			S1.3		89.60	92.47	2.87	3.20%	36.17%	0.58
	Shijiazhuang	$PM_{2.5}$	adj	18	89.68	53.45	-36.23	-40.40%	40.41%	0.67
			S1.1		89.68	74.84	-14.84	-16.55%	27.13%	0.67
			S1.3		89.68	97.18	7.50	8.36%	33.83%	0.66
	Xingtai	$PM_{2.5}$	adj	18	83.51	40.73	-42.78	-51.23%	51.77%	0.64
			S1.1		83.51	57.60	-25.91	-31.02%	38.77%	0.63
			S1.3		83.51	74.11	-9.40	-11.26%	32.51%	0.62

Note: OBS and SIM denote mean concentrations ($\mu g\ m^{-3}$) of observations and simulations, respectively; MB: mean bias; NMB: normalized mean bias; NME: normalized mean error; R: correlation coefficient.

Table S3 The collected CPM emission information from a review of references.

emission source		fuel	APCD*	T(°C)	FPM$_{2.5}$ (mg/Nm^3)	CPM (mg/Nm^3)	CPM-organic (mg/Nm^3)	CPM-inorganic (mg/Nm^3)	flue gas volume flow rate	test method	location	reference
coal-fired boiler	A	coal	FF + WFGD		12. 1 ±3. 6	17. 2 ± 1. 7	1%	67%		condensation	CFPP	(Pei, 2015)
	B		ESP + WFGD		33. 4 ±3. 7	23. 6 ± 2. 0						
	C		SCR+ESP+ WFGD		16. 2 ±2. 6	22. 8 ± 2. 3						
coal-fired boiler		coal	SCR+ESP+ BH+WFGD	88	1.04	12.94				condensation filter	CFPP	(Hu et al., 2016)
			integrated purification	40	27.41	22.6					heating plant	
			BH+WFGD	52	9.29	22.55					heating plant	
			integrated purification	43	46.58	35.81					industrial enterprise	
Iron and steel coking plant		coal	DFGD +FF +SCR	169.9	0.3 mg/m^3 0.4 mg/kg coal	1.2 mg/m^3 1.7 mg/kg coal	10.4%		231406 ±28521 m^3/h 168.6 t(coal)/h	indirect dilution		(Zhang et al., 2020)
CFPP	#1	coal	SCR + ESP + WFGD + WESP	51		7.5 5.8 3.5				dry impinger indirect dilution direct dilution	coal-fired power plants	(Wang et al., 2020a)
	#2			48.8		3 2 2.5						
	#3			63.8		5.5 1.5 4						
	#4			50.6		2.5 1 2.5						
	#5			50.3		11 2.5 3						
	#6			52.1		10 1.5 1.3						
coking plant			DFGD +FF +SCR	169.9		24.5 1.2 0.5					iron and steel plant	
sintering plant			ESP+ absorption	129.2		10 5 1.5						

			tower									
WIPP	stack #1	household garbage kitchen waste	SNCR+SDFGD+ DFGD +activated carbon adsorption+ FF	146.5		19 0.5			300 tons/day		waste incineration power plants	
	stack #2			145.3		21 1.0						
WIPP	stack #1	household garbage kitchen waste	SNCR+ SDFGD+ bag filter	146.5	0.87± 0.1 mg/m^3 0.009± 0.001g/kg	19.04± 3.67 mg/m^3 0.201± 0.039g/kg	22.6%	77.1%	131784 m^3/h 300t(solid waste)/d	EPA 201A EPA202	Shandong	(Wang et al., 2018)
	#2			145.3	0.68 ±0.19 0.006± 0.002g/kg	21.09± 3.32 0.178± 0.028g/kg	5.3%	94.4%	105427 m^3/h 300t/d			
WIPP	#3	household garbage kitchen waste coal	ESP+ bag filter	120	3.3 ± 0.65				150 t/d	two–stage virtual impactor	Zhejiang	
circulating fluidized bed boiler		coal	SNCR&SCR +ESP+FGD+ WESP			3.75			220 t/h	parallel sampling system dilution	Ultralow Emission coal-fired Power Plant	(Zheng et al., 2018)
pulverized coal boiler		bituminous coal	SCR+ESP&FF+WFGD		9.8 ± 6.8 g/t(coal)	12 167.83 ± 33.92 g/t(coal)	5.8	6.2	200 t/h	EPA Method 202	Coal-fired power plants (CFPPs) #1 #2 #3 #4	(Wu et al., 2020)
pulverized coal boiler			SCR+FF+WFGD		15.67± 4.12 g/t(coal)	15 138.45 ± 21.89	10.5	4.5	410 t/h			

						g/ t(coal)						
circulating fluidized bed			SNCR+FF+WFGD&WESP		21.76 ± 5.91 g/t(coal)	9.5 109.89 ± 35.76 g/t(coal)	6.5	3	260 t/h			
pulverized coal boiler			SCR+ESP+WFGD&WESP		4.70 ± 1.19 g/t(coal)	10 74.33 ± 13.68 g/t(coal)	3.3	6.7	2209 t/h			
coal-fired boiler		coal	SCR+ ESP+ GGH+WFGD +WESP	80	1.1	7.9	4.3	3.6		ISO 23210-2009 EPA 202	LH CFPP #1unit	(Li et al., 2017a)
coal-fired boiler	stage1	coal	SCR+ LLT-ESP+ MGGH + WFGD+ WESP	130	0.46	18.6	62%		2×10⁶ Nm³/h	ISO 23210-2009 EPA 202	YQ CFPP #1unit	(Li et al., 2017b)
	stage2				0.4	11.9	81%					
	stage3					27.1	87%					
coal-fired boiler	E1	coal		100	3.8	36.3	21.6	14.7		ISO 23210-2009 EPA 202	Zhejiang	(Qi et al., 2017)
	E2			97	3.8	31.8	10.3	21.5				
	E3			93	10.1	40.8	21.7	19.1				
coal-fired boiler	stage1	coal		86	3.5	48.7	44.3	4.4	10 L/min		JX CFPP #7unit	(Li et al., 2019)
	Stage2			95	7.8	35.2	28.8	6.4				
coal-fired boiler		coal			1.81	10.66	5.59	5.07	3688100 Nm³/h 360.88 t(coal)/h		Ultralow-Emission JX CFPP #8unit	(Song et al., 2020)
coal-fired boiler		coal			1.4	32	29.9	2.1		ISO 23210-2009 EPA 202	FT #1unit	(Li, 2018)
					2.2	18.3	13.7	4.6			YQ #2unit	
coal-		coal	SCR+ESP+WFGD		2.54	24.8	23.1	1.69			ZJK #8unit	(Zhou, 2019)
					6.14	16.24	11.4	4.85			WT #2unit	

fired boiler	stage1		SCR+LLT-ESP+WFGD +WESP		1.4	6.66	4.44	2.22			JX #7unit	
	stage2				0.83	6.69	5.51	1.45				
	stage3				1.14	8.93	6.68	2.25				
	stage4				1.77	6.66	4.05	2.61				
					1.81	10.66	5.59	5.07			JX #8unit	
coal-fired power plant		coal	SCR + BH + SWFGD	105	0.45 5.25 g/t(coal)	12.7 ± 1.44 142 g/t(coal)	90 ±3.7%		2300000 Nm^3/h 275 t(coal)/h	EPA 201A EPA 202		(Lu et al., 2019)
coal-fired boiler			SCR + ESP + WFGD	59	1.9 20.1 g/t(coal)	28.0 ± 6.32 307 g/t(coal)		93 ± 2.4%	80000 Nm^3/h 8 t(coal)/h		food processing plant	
Power plant		coal oil	ESP+FGD		0.75	2.15		89%		EPA 201A EPA 202	Taiwan, China	(Yang et al., 2014)
industry boiler		coal	Cyclone+ BH		16.9	29.3		69.4%				
brick manufacturing plant					8.67	83.5		72.3%				
incinerator			BH		0.15	0.17		89.8%				
arc furnace			BH		2.12	2.53		72.8%				
sintering		coke	ESP denitrification de-dioxin	161	1.01	65.3		95.4%	468 t flux/h	EPA 201A EPA 202	iron and steel plants	(Yang et al., 2015)
coke making		coke oven gas		178	0.37	89.7		52%	159 t coal/h			
blast furnace		mixed gas	BH	57.5	0.16	3.84		69.9%	166t steel/h			
Basic oxygen furnace		natural gas	BH	57.8	0.15	1.32		63.6%	15.7t waste steel/h			
electric arc furnace		natural gas	CO convertor + BH	70.5	0.28	2.02		58.4%	144t waste steel/h			
municipal solid waste incinerator		municipal solid	SNCR+ semidry lime	157	FCPM 10.2 ± 0.67 mg/Nm^3		OC+EC 33.1%		4210 Nm^3/h	dilution sampling	central Taiwan,	(Yang et al., 2016)

		waste	scrubber+activated carbon injection+ BH		61.6 ± 4.52 g/ton waste		OC/EC 1.73			method	China	
					0.29 ±0.03	28.1 ±17				in-stack sampling		
coal-fired boilers	1(n=4)	raw coal	cyclone	65.3	18.6± 13.7	22.7 ± 5.61	22.9%	77.1%		EPA 201A EPA 202	industrial plants	(Yang et al., 2018b)
	2(n=5)		EP	44.6	3.83± 1.05	3.92 ± 1.08	45.6%	54.4%				
	3(n=3)		baghouse	83.3	3.51± 3.21	8.61 ± 4.03	41.1%	58.9%				
	4(n=3)		EP	101	0.84± 0.18	5.96 ± 2.21	13.6%	86.4%			power plants	
oil-fired boilers	1(n=8)	heavy oil	no	148	141 ± 76.1	242 ± 131	80.5%	19.5%				
	2(n=2)		cyclone	195	22.6± 5.28	84.2 ± 38.1	62.4%	37.6%				
	3(n=1)		BH	125	2.31	3.16	20.4%	79.6%				
CFBs (n=5)		coal	cyclone+ BH	76.6	19.3± 2.94	27.2 ± 3.49	2.765	6.77 ± 1.74		EPA 201A EPA 202	industrial boilers	(Yang et al., 2018a)
WFBs (n=5)		wood	wet scrubber	70.6	90.8± 40.6	31.4 ± 14.1	3.104	4.98 ± 2.23				
HOFBs (n=4)		heavy oil	no	159	28 ± 5.6	163 ± 62.8	69.686	27.1 ± 23.7				
DFBs (n=1)		diesel	no	162	0.273	7.67	4.324	2.65				
NGFBs (n=3)		natural gas	no	133	0.352 ± 0.157	7.02 ± 3.1	2.349	3.38 ± 1.51				
CFPP	C	coal	SCR+ESP+WFGD+ WESP	47	3.9	7.33	4.04	3.29	119 t(coal)/h	EPA 202	north China around Beijing	(Wang et al., 2020b)
	D		SCR+BF+WFGD+ WESP	46	0.55	6.15	3.51	2.64	150.2 t(coal)/h			
CFPP	A		SCR+ESP+WFGD+ WESP	50.1	2.35	15.92	9.59	6.33		EPA202	Xi’an city, Shaanxi	(Yang et al., 2021)
	B		SCR+LLTe+ESP+ WFGD	53.9	3.96	30.69	8.73	21.96			Urumqi City, Xinjiang	

Note: Air pollution control devices (APCDs) include selective catalytic reduction denitration device (SCR), selective noncatalytic reduction (SNCR), electrostatic precipitator (ESP), gas−gas heat exchanger (GGH), tube type gas−gas heat exchanger (MGGH), wet flue gas desulfurization (WFGD), wet electrostatic precipitator (WESP), low-low temperature electrostatic precipitator (LLT-ESP), fabric filters (FF), baghouse (BH), seawater flue gas desulfurization (SWFGD), and semi-dry flue gas desulphurization(SDFGD).

Table S4 The model species for POA, ASOA (SOA from anthropogenic VOCs), BSOA (SOA from biogenic VOCs), and SISOA (SOA from low volatile S/IVOCs).

	model species
POA	ALVPO1I ASVPO1I ASVPO2I APOCI APNCOMI ALVPO1J ASVPO1J ASVPO2J APOCJ ASVPO3J AIVPO1J APNCOMJ
ASOA	AAVB1J AAVB2J AAVB3J AAVB4J AOLGAJ
BSOA	AISO1J AISO2J AISO3J AMT1J AMT2J AMT3J AMT4J AMT5J AMT6J AMTNO3J AMTHYDJ AGLYJ ASQTJ AOLGBJ
SISOA	ALVOO1I ALVOO2I ASVOO1I ASVOO2I ALVOO1J ALVOO2J ASVOO1J ASVOO2J ASVOO3J APCSOJ
SOA	AAVB1J AAVB2J AAVB3J AAVB4J AOLGAJ AORGCJ AISO1J AISO2J AISO3J AMT1J AMT2J AMT3J AMT4J AMT5J AMT6J AMTNO3J AMTHYDJ AGLYJ ASQTJ AOLGBJ ALVOO1I ALVOO2I ASVOO1I ASVOO2I ALVOO1J ALVOO2J ASVOO1J ASVOO2J ASVOO3J APCSOJ

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