Supplement of Atmos. Chem. Phys., 17, 211–233, 2017
http://www.atmos-chem-phys.net/17/211/2017/
doi:10.5194/acp-17-211-2017-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Development of a high-resolution emission inventory and its evaluation and application through air quality modeling for Jiangsu Province, China

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Tables

Table S1. Source categories and the activity data sources of the emission inventory for Jiangsu Province, China.

Sector	Subsector	Fuel/product/process	Technology/type	Burner/engine	Main sources of activity data
Power plant	-	Coal/oil/gas	Pulverized coal boiler/grate stoker/ circulating fluidized bed combustion	Tangentially-fired/ swirl burner/W-flame	Official environmental statistics; Pollution Source Census; On-site survey; Official energy and industrial statistics (NBSC, 2013a; b; JSBNS, 2013)
Industry	Iron & steel	Coke/sintering/pig iron/ crude steel/casting	Blast furnace/electric furnace/ basic oxygen furnaces		
	Nonferrous metal smelting	Copper/zinc/aluminum/lead			
	Nonmetal mineral production	Cement	Precalciner kilns/shaft kilns/rotary kilns		
		Brick			
		Lime			
	Oil refinery& chemical industry	Oil refinery/sulfuric acid/nitrate acid/ ammonia production/resin/rubber/fiber			
	Other industry	Glass/food/paper			
Solvent use	Industrial use	Textile/printing/metal work/ wood processing/shoe/leather			Official environmental statistics; Pollution Source Census; Official industrial statistics (NBSC, 2013b; JSBNS, 2013)
	Domestic use	Building paint/dry-cleaning/ household use/pesticide application			Official statistics (JSBNS, 2013)
Transportation	On-road	Gasoline/diesel	Light/heavy/Motorcycle	Stage I /II /III/IV/V	Local survey (Zhao et al., 2015) ; Cai and Xie (2007); Wang et al. (2008); He (2015)
	Non-road	Aviation/ships/train/agriculture machine/ tractor/construction machine			Official statistics (JSBNS, 2013)

Table S1 (continued).

Sector	Subsector	Fuel/product/process	Technology/type	Burner/engine	Main source of activity data
Residential & commercial	Fossil fuel combustion	Coal/gas/ liquefied petroleum gas	Stoker furnace/stove		Official energy statistics (NBSC, 2013a)
	Biofuel	Rice straw/wheat residue/corn residue/ bean residue/tuber residue/cotton residue			Official statistics (JSBNS, 2013)
	Open biomass burning	Rice straw/wheat residue/corn residue			
Agriculture	Livestock	Cow/horse/donkey/mule/pig/sheep/rabbit			Official statistics (JSBNS, 2013)
		Poultry	Meat hen/laying hen/duck/goose		
	Fertilizer use	Fertilizer-N/fertilizer-P/fertilizer-K			
Other sources	Cooking				Official statistics (JSBNS, 2013)
	Waste treatment	Wastewater treatment/landfill			
	Human excrement				

Table S2. The penetration rates of FGD, SCR/SNCR, and dust collectors, and the corresponding average removal efficiencies for SO_2, NOx, and TSP for selected emission sources.

Sector	Device	Penetration	Removal efficiency
Power plant	FGD	96.6%	83.3%
	SCR/SNCR	57.4%	37.1%
	Dust collector	98.9%	98.0%
Iron & steel plant			
Sintering	FGD	64.3%	78.0%
Pig iron production	Dust collector	99.9%	95.7%
Steel making	Dust collector	99.3%	94.0%
Cement plant	Dust collector	99.2%	97.3%
Brick plant	Dust collector	7.1%	78.2%
Other industry combustion	FGD	73.4%	62.0%
	SCR/SNCR	4.5%	47.5%
	Dust collector	90.5%	90.4%

Table S3 Emission factors of typical industrial processes (units: kg/t-product unless noted).

Sources		SO_2	NOx	CO	CO_2	VOC	NH_3	TSP	Fraction of TSP			Fraction of $PM_{2.5}$	
									$PM_{>10}$	$PM_{2.5-10}$	$PM_{2.5}$	BC	OC
Cement	Kiln		13.7	12.5[a]	1731/549[a]	0.177[e]		117	0.58	0.24	0.18	0.01[b]	0.02[b]
	Grinding							140[b]	0.76	0.17	0.07		
Iron & steel	Coke	0.7	1.7[b]	0.4	2067[a]	2.4[c]	0.07[b]	5	0.58	0.16	0.26	0.4	0.35
	Sintering	2.9	1.0	22		0.25[c]		47	0.85	0.08	0.07	0.01	0.05
	Pig iron	0.5	0.2	15				48.8	0.73	0.12	0.15	0.19	0.04
	Crude steel			11.3/9.0		0.06[c]		40/12.2	0.43/0.42	0.13/0.15	0.44/0.43	0.05/0	0.01/0.2
Nonferrous metal smelting	Copper	212.07						258	0.08	0.1	0.82		
	Zinc	80			1720[a]			196	0.08	0.1	0.82		
	Aluminum	61			1600[a]			45	0.43	0.19	0.38		
	Lead	80			520[a]			250	0.08	0.1	0.82		
Brick & lime		16	3.8	150[a]	1731[a]	0.132[f]		3.7	0.8	0.13	0.07	0.4	0.4
Glass		0.98	1.6	115[a]	1731/750[a]	0.177[e]		90	0.88	0.1	0.02	0.02[b]	0.01[b]
Sulfuric acid		3.43											
Nitric acid			7.1				3.8[c]						
Ammonia production		0.53		142[a]	4582/3273/2104[a]	4.72[d]	2.1[c]						

Table S3 (continued).

Sources	SO_2	NOx	CO	CO_2	VOC	NH_3	TSP	Fraction of TSP			Fraction of $PM_{2.5}$	
								$PM_{>10}$	$PM_{2.5-10}$	$PM_{2.5}$	BC	OC
Glass				200[a]	3.15[e]		10.6	0.05	0.04	0.91		
Fertilizer production						2/0.07[c]	2.36	0.1	0.11	0.79		
Oil refinery	0.9	0.3	10			0.16[c]	0.12		0.2	0.8		

Notes: Emission factors without special illustration were derived from Zhao et al. (2013). Numbers for the production of crude steel were the emissions factors for converter/electric steelmaking.

a Zhao et al. (2012). Numbers for CO_2 from cement were the emission factors from process (kg CO_2/t-clinker) and kiln (kg CO_2/t-coal). Emission factors of CO_2 from ammonia production referred to the process using coal/oil/natural gas as energy; the unit of emission factors for brick and lime was kg/t-coal.

b Lei et al. (2011).

c Yin et al. (2010).

d Wei et al. (2008).

e Bo et al. (2008).

f MEP, 2014.

Table S4 Model performance statistics of meteorological parameters in D2 at 9km and D3 at 3km resolution for October 2012.

Variables	Parameters	D2 (9km)	D3 (3km)
WS10 (m/s)	Mean OBS	2.4	2.7
	Mean SIM	3.5	3.9
	Bias	1.1	1.2
	RMSE	1.3	1.4
	IOA	0.85	0.73
WD10 (deg)	Mean OBS	141.3	131.3
	Mean SIM	145.4	135.0
	Bias	4.0	3.6
T2 (℃)	Mean OBS	18.1	19.0
	Mean SIM	18.7	19.1
	Bias	0.6	0.1
	RMSE	1.1	1.1
	IOA	0.97	0.97
RH2 (%)	Mean OBS	65.0	66.2
	Mean SIM	61.4	68.5
	Bias	-3.6	2.3
	RMSE	9.7	9.3
	IOA	0.89	0.90

Note: OBS and SIM indicate the results from observation and simulation, respectively. The Bias, IOA and RMSE were calculated using following equations (*P* and *O* indicates the results from modeling prediction and observation, respectively):

$$Bias = \frac{1}{n}\sum_{i=1}^{n}(P_i - O_i); \quad IOA = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(\left|P_i - \overline{O}\right| + \left|O_i - \overline{O}\right|)^2}; \quad RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}$$

Figures

Figure S1.

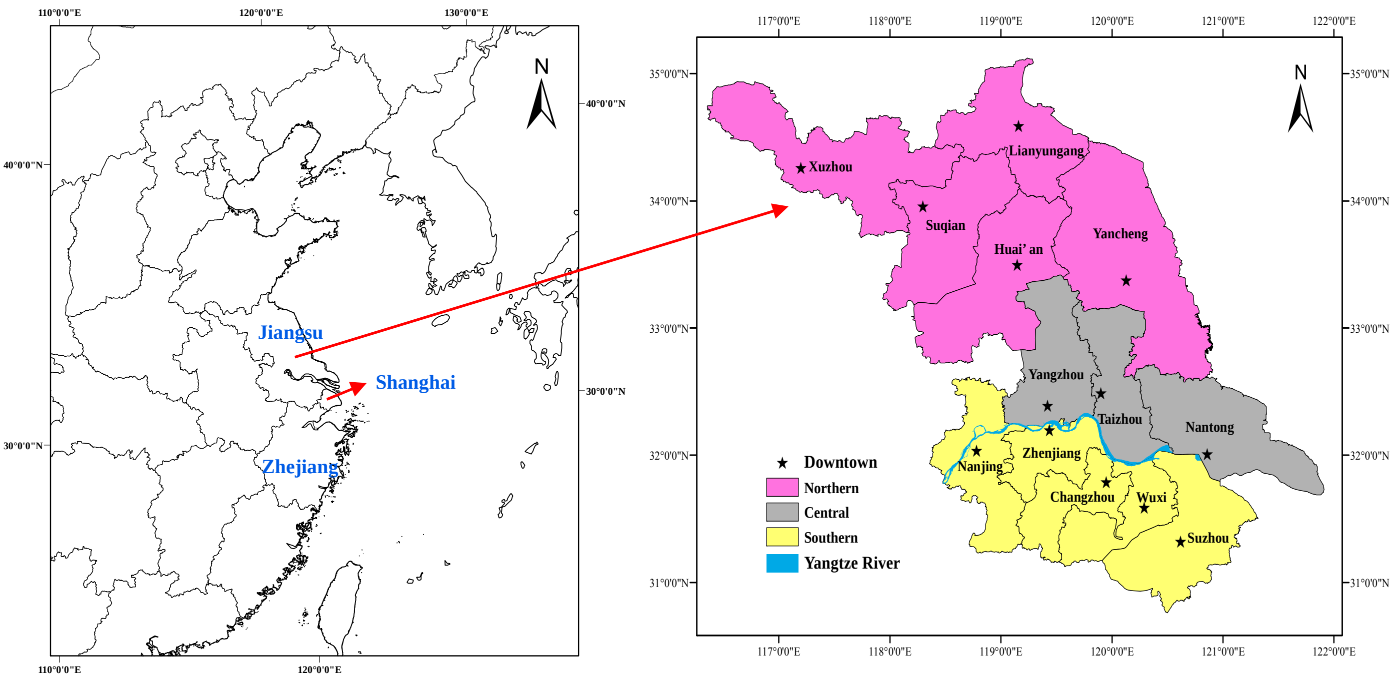
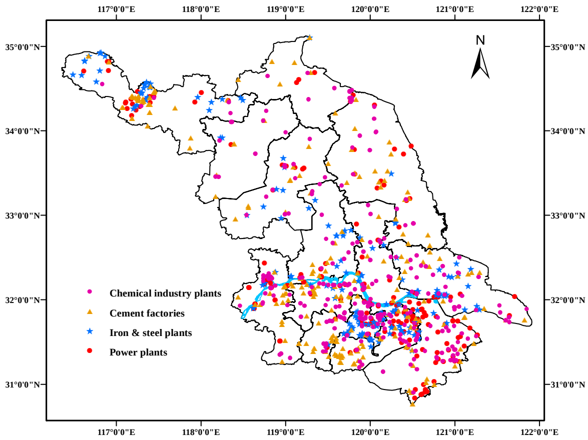
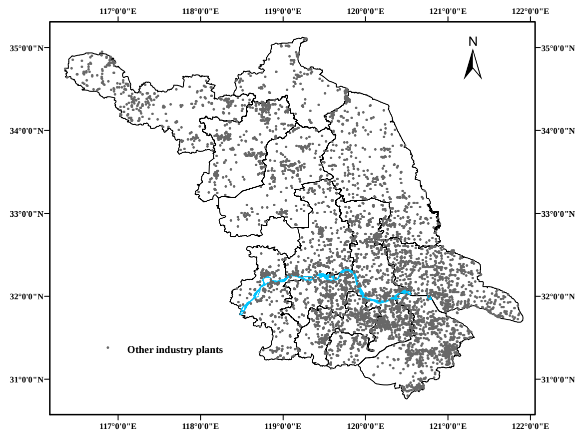


Figure S2.

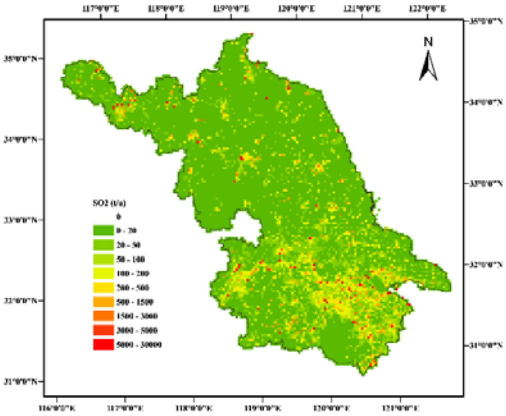

117°0'0"E
118°0'0"E
119°0'0"E
120°0'0"E
121°0'0"E
122°0'0"E
35°0'0"N
34°0'0"N
33°0'0"N
32°0'0"N
31°0'0"N
N
Chemical industry plants
Cement factories
Iron & steel plants
Power plants

(a)

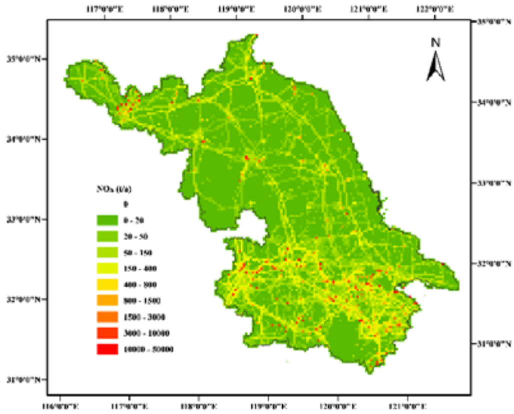

117°0'0"E
118°0'0"E
119°0'0"E
120°0'0"E
121°0'0"E
122°0'0"E
35°0'0"N
34°0'0"N
33°0'0"N
32°0'0"N
31°0'0"N
N
Other industry plants

(b)

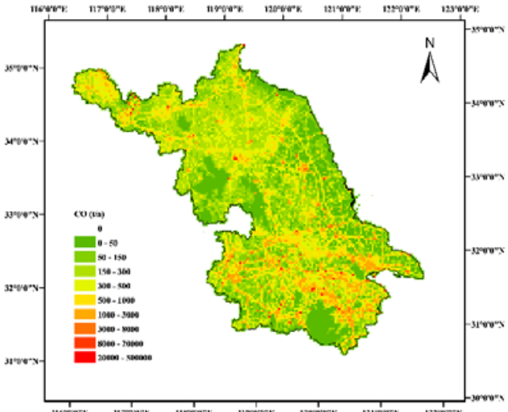
Figure S3.



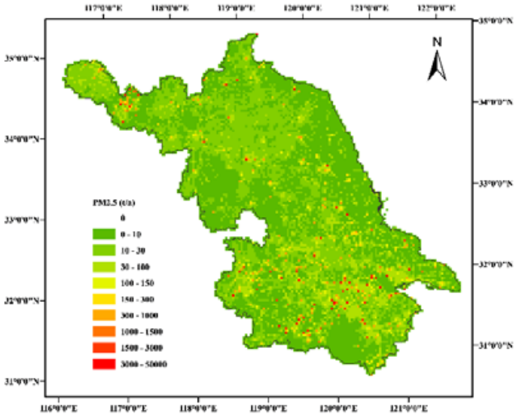
(a) SO_2



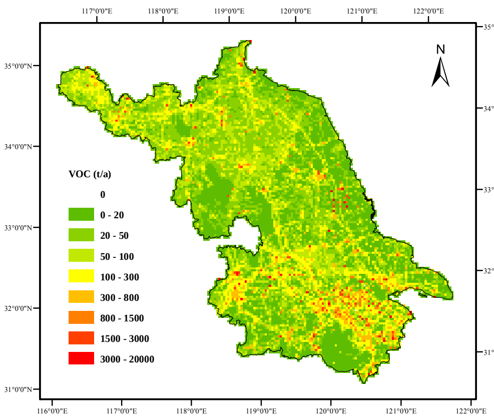
(b) NOx



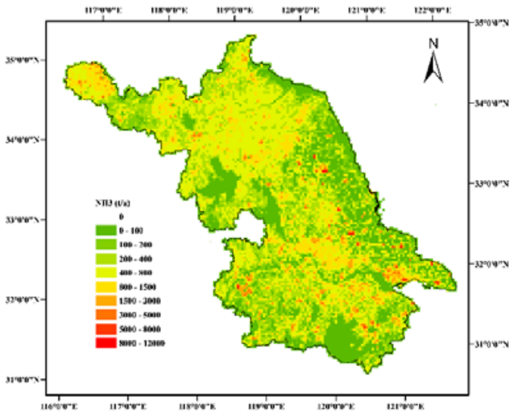
(c) CO



(d) $PM_{2.5}$



(e) VOC



(f) NH_3

Figure S4.

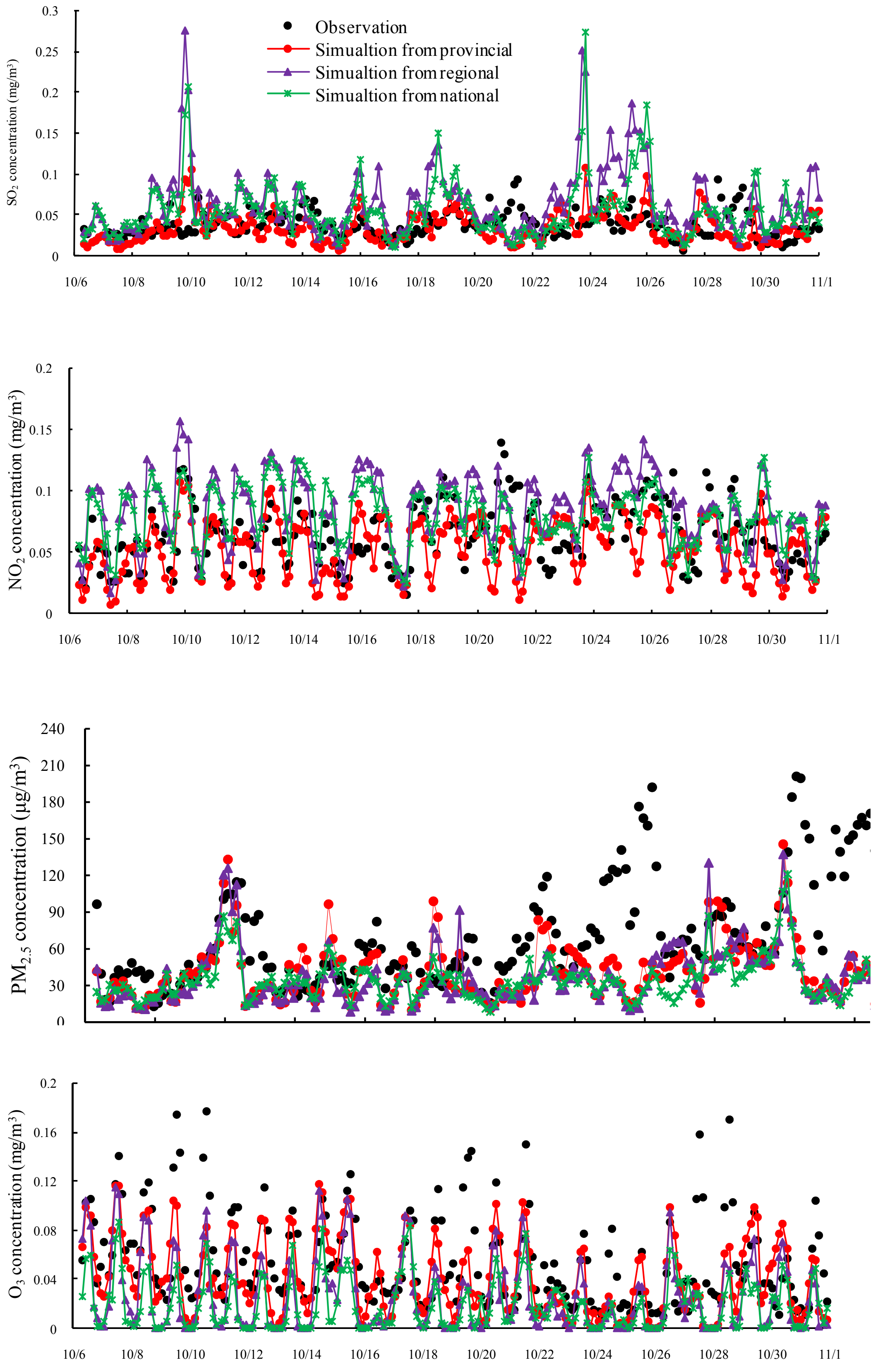
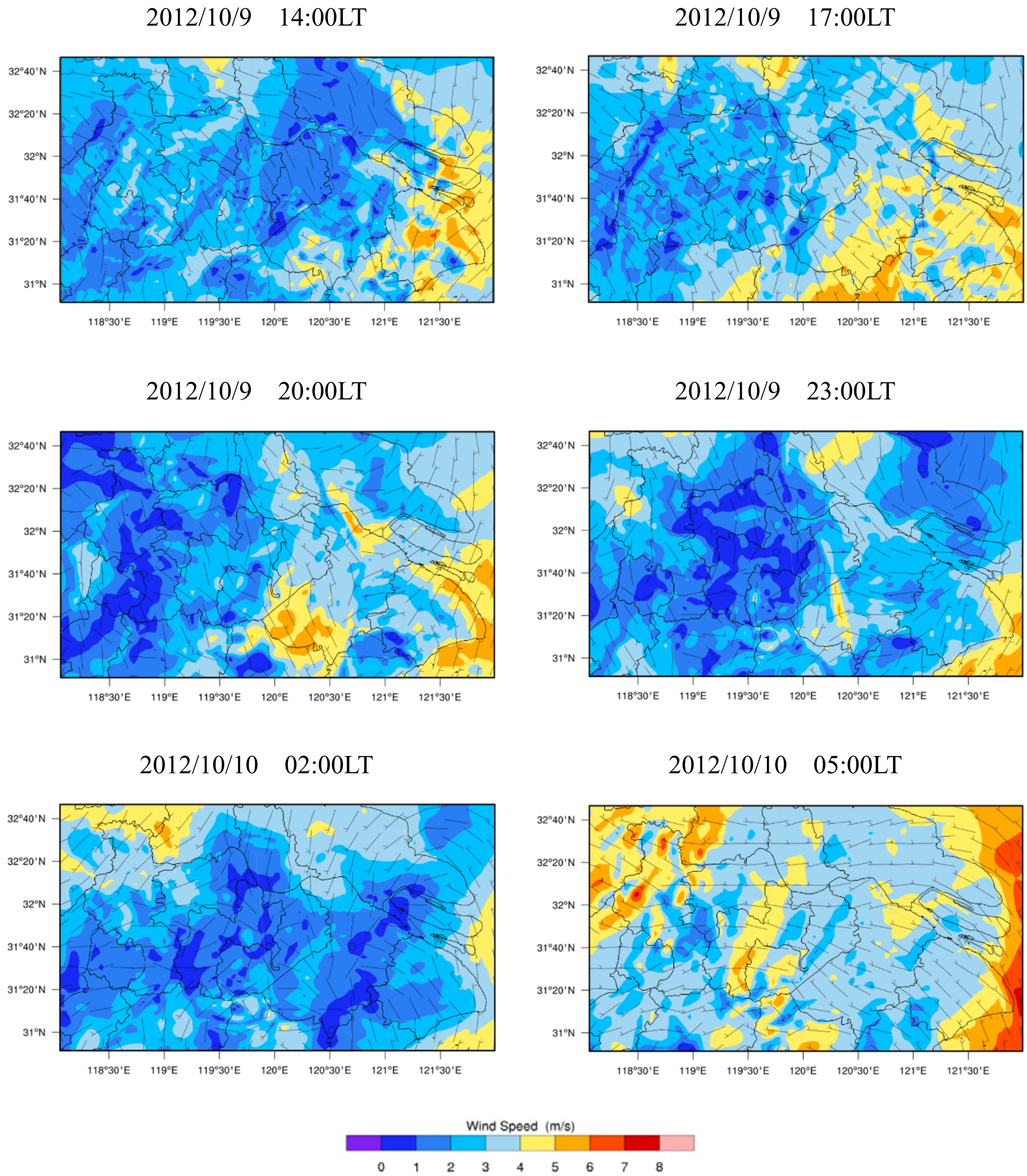
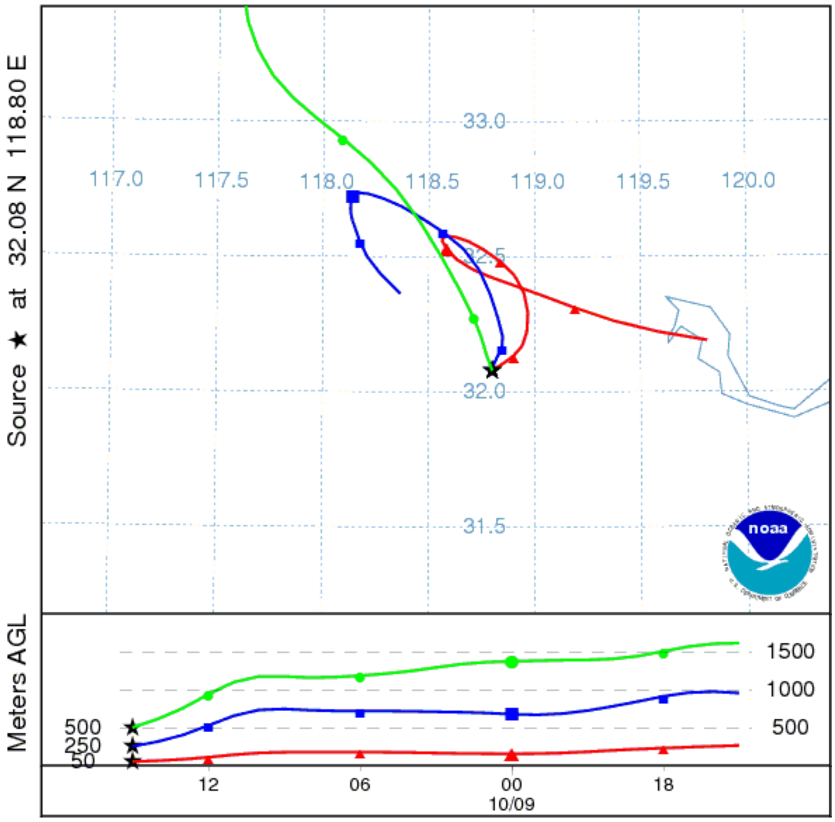

Observation
Simualtion from provincial
Simualtion from regional
Simualtion from national
SO2 concentration (mg/m3)
0.3
0.25
0.2
0.15
0.1
0.05
0
10/6
10/8
10/10
10/12
10/14
10/16
10/18
10/20
10/22
10/24
10/26
10/28
10/30
11/1
NO2 concentration (mg/m3)
0.2
0.15
0.1
0.05
0
PM2.5 concentration (μg/m3)
240
210
180
150
120
90
60
30
0
O3 concentration (mg/m3)
0.2
0.16
0.12
0.08
0.04

Figure S5.



2012/10/9 14:00LT
2012/10/9 17:00LT
2012/10/9 20:00LT
2012/10/9 23:00LT
2012/10/10 02:00LT
2012/10/10 05:00LT
32°40'N
32°20'N
32°N
31°40'N
31°20'N
31°N
118°30'E
119°E
119°30'E
120°E
120°30'E
121°E
121°30'E
Wind Speed (m/s)
0 1 2 3 4 5 6 7 8

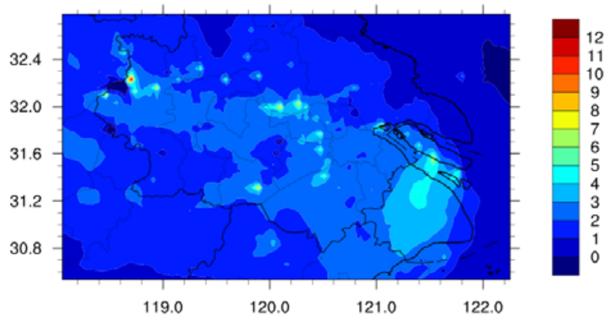
Figure S6.



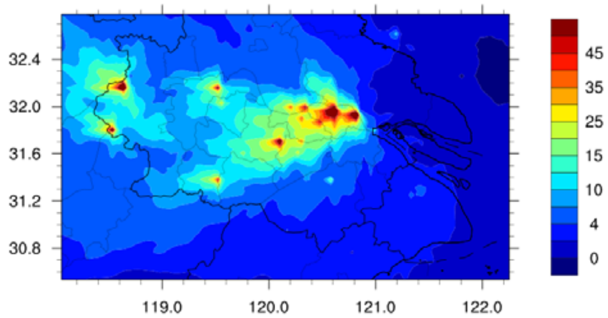
Source ★ at 32.08 N 118.80 E
33.0
117.0
117.5
118.0
118.5
119.0
119.5
120.0
32.5
32.0
31.5
Meters AGL
1500
1000
500
500
250
50
12
06
00
10/09
18

Figure S7.

(a)



(b)



(c)

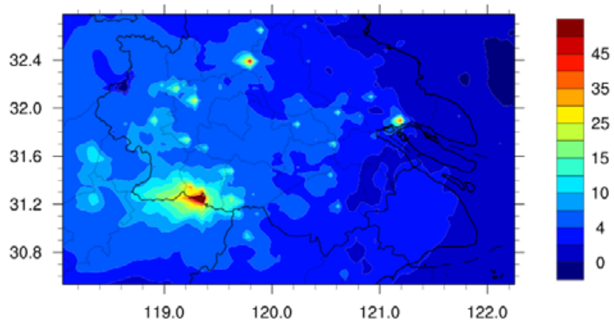
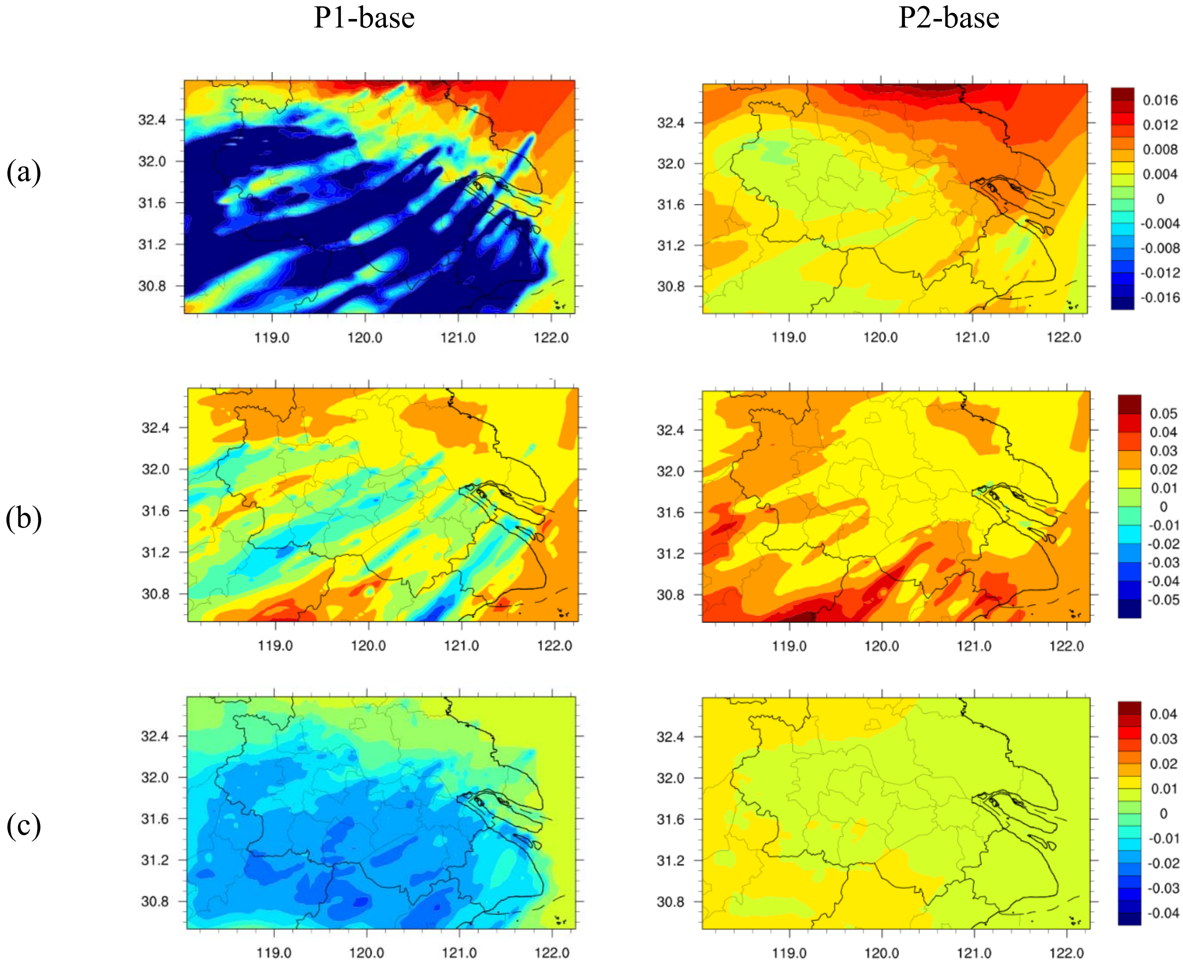


Figure S8.



P1-base
P2-base
(a)
(b)
(c)
0.016
0.012
0.008
0.004
0
-0.004
-0.008
-0.012
-0.016
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
32.4
32.0
31.6
31.2
30.8
119.0
120.0
121.0
122.0

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