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Top-down estimate of black carbon emissions for city clusters using ground observations: a case study in southern Jiangsu, China

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Number of tables: 10 Number of figures: 16

Table list

Figure list

Figure S2. Observed BC concentrations at NJU (a) and PAES (b) in January, April, July, and October of 2015 (unit: ug/m^3). The box plot indicates the median of observed concentration (square symbols), and the maximum, 95th, 75th, 50th, 25th, 5th percentiles and the minimum.

Figure S3. Spatial distributions of BC emissions by sector (unit: Mg) in JS-prior (a) and JS-posterior (b).

Figure S4. The simulated concentrations contributed by industry, power generation, residential sources and transportation at NJU for January (a), April (b), July (c) and October (d) in 2015 (unit: ug/m^3).

Figure S5. The same as Figure S4 but at PAES.

Figure S6. The transport pathways of air masses sampled at NJU based on cluster analysis of back trajectories in HYSPLIT model in January (a), April (b), July (c) and October (d).

Figure S7. BC emissions by sector from the bottom-up method for Nanjing in 2012 and 2015 (unit: Gg).

Figure S8. The seasonal variation of BC emissions by source (a) and total emissions (b) in JS-prior, JS-posterior and MEIC-prior.

Figure S9. The simulated daily average PBL heights in January in 2015 at PAES (unit: m).

Figure S10. The contributions of emissions from Nanjing (a) and Suzhou–Wuxi–Changzhou-Zhenjiang city cluster (b) to ambient BC levels at NJU and PAES.

Figure S11. The correlation between the simulated BC concentrations with JS-prior and those with doubled (a and c) or halved emissions (b and d) in JS-prior in July (a and b) and October (c and d) at NJU. F_{emis}. and F_{conc}. indicate respectively the fraction of changed emissions and that of changed simulated monthly average concentrations between sensitivity and base simulation (JS-prior). ⊿E and ⊿C indicate the change in emissions and that in simulated monthly average concentrations, respectively.

Figure S12. The same as Figure S11 but at PAES. As can be seen in all the panels in Figures S11 and S12, the fraction of change in simulated monthly average concentration ($F_{conc.}$) was close to that of emission change ($F_{emis.}$), i.e., the ratio of $F_{emis.}$ to $F_{conc.}$ was around 1.0, within a range of ±10%. Similar ratio of change in emissions ($\triangle E$) to that in simulated average concentration ($\triangle C$) was obtained for each month and site as well.

Figure S13. The observed and simulated hourly precipitation at Lukou (a), Liyang (b) and Shanghai (c) for January of 2015 (unit: mm/hr).

Figure S14. The same as Figure S13 but for April of 2015.

Figure S15. The same as Figure S13 but for July of 2015.

Figure S16. The same as Figure S13 but for October of 2015.

Tables

Table S1. Data sources of activity levels and scaling factors for BC emissions from 2012 to 2015 by source category in southern Jiangsu.

Sector	Subsector	Main sources of activity level	Scaling factor
Power generation		Jiangsu Statistical Yearbook	1.108
Industry	Iron and steel	China and Jiangsu Statistical Yearbook; China Energy and Industry Statistical Yearbook	1.302
	Nonmetal mineral production		1.074
	Nonferrous metal smelting		0.690
	Oil refinery		1.089
	Chemical industry		1.107
	Glass		0.716
	Other industry		1.020
Residential sources	Fossil fuel combustion	Jiangsu Energy Statistical Yearbook; Jiangsu Statistical Yearbook	1.106
	Biofuel		1.043
Transportation	On-road	Jiangsu Energy Statistical Yearbook; Jiangsu Statistical Yearbook	1.112
	Off-road		1.182

Table S2. Reduction rates in monthly emissions from 2012 to 2015 in MEIC for southern Jiangsu and other regions within the third modeling domain (unit: %).

Region	Jan.	Apr.	Jul.	Oct.
Southern Jiangsu (%)	18	18	26	21
Outside southern Jiangsu (%)	12	16	21	15

Table S3. Reduction rates in annual $PM_{2.5}$ concentration for cities within the third modeling domain from 2013 to 2015 (unit: %).

Province	City	Reduction rate (%)
Anhui	Hefei	15.26
Jiangsu	Nantong	15.90
	Taizhou	11.76
	Yangzhou	16.84
	Nanjing	15.58
	Suzhou	12.76
	Wuxi	10.45
	Changzhou	12.31
	Zhenjiang	12.80
Shanghai	Shanghai	10.88

Table S4. Statistic indicators of meteorological parameters at three stations in the third modeling domain for January (a), April (b), July (c) and October (d) in 2015.

Variable	Parameter	Lukou	Hongqiao	Liyang
	Average OBS (°C)	4.63	6.81	5.40
	Average SIM (°C)	5.28	5.89	5.70
	Bias (°C)	0.64	-0.92	0.30
T2	NMB (%)	13.85	-13.52	5.49
	NME (%)	30.23	20.13	22.34
	RMSE (°C)	1.78	1.80	1.61
	IOA	0.95	0.95	0.96
	Average OBS (%)	74.14	66.99	70.97
	Average SIM (%)	73.24	75.52	71.63
	Bias (%)	-0.90	8.63	0.66
RH2	NMB (%)	-1.21	12.90	0.92
	NME (%)	17.11	18.65	18.85
	RMSE (%)	16.89	15.78	17.49
	IOA	0.84	0.85	0.82
	Average OBS (m/s)	2.34	3.90	1.98
	Average SIM (m/s)	3.20	3.68	3.47
	Bias (m/s)	0.86	-0.22	1.49
WS10	NMB (%)	36.94	-5.62	75.50
	NME (%)	52.02	31.40	83.33
	RMSE (m/s)	1.50	1.52	2.02
	IOA	0.76	0.77	0.51
	Average OBS (deg)	159.39	201.94	175.17
	Average SIM (deg)	162.71	190.50	172.29
	Bias (deg)	3.32	-11.44	-2.89
WD10	NMB(%)	2.09	-5.66	-1.65
	NME(%)	27.73	27.94	36.27
	RMSE (deg)	85.02	116.00	116.03
	IOA	0.85	0.78	0.76

(a)

Variable	Parameter	Lukou	Hongqiao	Liyang
T2	Average OBS (°C)	15.54	16.51	16.05
	Average SIM (°C)	15.05	14.99	15.44
	Bias (°C)	-0.49	-1.53	-0.59
	NMB (%)	-3.19	-9.30	-3.68
	NME (%)	9.21	11.70	8.39
	RMSE (°C)	1.86	2.42	1.76
	IOA	0.97	0.95	0.98
RH2	Average OBS (%)	70.84	65.91	68.85
	Average SIM (%)	77.27	80.28	75.31
	Bias (%)	6.43	14.40	6.38
	NMB (%)	9.08	21.85	9.26
	NME (%)	16.66	23.07	19.07
	RMSE (%)	16.29	18.97	17.49
	IOA	0.85	0.79	0.82
WS10	Average OBS (m/s)	2.88	4.13	2.46
	Average SIM (m/s)	3.57	4.08	3.56
	Bias (m/s)	0.69	-0.05	1.31
	NMB (%)	24.10	-1.26	53.35
	NME (%)	42.71	23.93	65.83
	RMSE (m/s)	1.57	1.30	2.01
	IOA	0.81	0.87	0.68
WD10	Average OBS (deg)	159.28	182.74	145.96
	Average SIM (deg)	146.63	155.97	151.14
	Bias (deg)	-12.66	-26.77	5.18
	NMB(%)	-7.95	-14.65	3.55
	NME(%)	34.68	27.75	36.30
	RMSE (deg)	102.58	105.95	95.15
	IOA	0.74	0.75	0.77

(b)

Variable	Parameter	Lukou	Hongqiao	Liyang
T2	Average OBS (ºC)	26.51	27.31	26.74
	Average SIM (ºC)	25.20	25.28	25.22
	Bias (ºC)	-1.23	-1.88	-1.41
	NMB (%)	-4.62	-6.90	-5.26
	NME (%)	6.02	8.13	6.52
	RMSE (ºC)	1.97	2.72	2.19
	IOA	0.92	0.89	0.92
RH2	Average OBS (%)	83.92	77.01	79.34
	Average SIM (%)	86.57	85.49	85.50
	Bias (%)	2.34	7.78	5.63
	NMB (%)	2.79	10.10	7.10
	NME (%)	7.01	14.05	9.55
	RMSE (%)	8.04	13.28	9.64
	IOA	0.90	0.77	0.86
WS10	Average OBS (m/s)	2.76	3.91	1.97
	Average SIM (m/s)	2.89	3.24	2.95
	Bias (m/s)	0.13	-0.62	0.97
	NMB (%)	4.58	-15.88	49.50
	NME (%)	38.09	28.71	64.82
	RMSE (m/s)	1.34	1.42	1.65
	IOA	0.76	0.88	0.65
WD10	Average OBS (deg)	144.66	143.00	142.43
	Average SIM (deg)	131.51	127.30	134.01
	Bias (deg)	-12.67	-15.50	-8.36
	NMB(%)	-8.76	-10.86	-5.87
	NME(%)	27.75	27.22	28.38
	RMSE (deg)	73.74	77.58	74.94
	IOA	0.79	0.76	0.79

(c)

Variable	Parameter	Lukou	Hongqiao	Liyang
T2	Average OBS (^oC)	17.97	20.13	18.46
	Average SIM (^oC)	18.69	18.72	18.80
	Bias (^oC)	0.70	-1.42	0.32
	NMB (%)	3.87	-7.03	1.72
	NME (%)	7.52	8.25	5.76
	RMSE (^oC)	1.72	2.10	1.36
	IOA	0.95	0.90	0.96
RH2	Average OBS (%)	77.67	68.84	75.70
	Average SIM (%)	67.74	76.94	70.72
	Bias (%)	-9.58	8.00	-4.62
	NMB (%)	-12.34	11.62	-6.10
	NME (%)	16.85	14.97	12.52
	RMSE (%)	18.35	12.71	13.53
	IOA	0.82	0.87	0.88
WS10	Average OBS (m/s)	2.43	3.24	1.81
	Average SIM (m/s)	2.92	2.84	3.11
	Bias (m/s)	0.51	-0.37	1.27
	NMB (%)	20.98	-11.31	70.27
	NME (%)	44.50	34.11	82.49
	RMSE (m/s)	1.40	1.44	1.90
	IOA	0.74	0.74	0.55
WD10	Average OBS (deg)	149.11	152.48	131.42
	Average SIM (deg)	134.04	134.22	138.19
	Bias (deg)	-15.43	-14.32	8.64
	NMB(%)	-10.34	-9.39	6.58
	NME(%)	30.36	27.30	28.26
	RMSE (deg)	83.86	80.38	63.01
	IOA	0.80	0.83	0.85

(d)

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

$$Bias = \frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)\,;$$

$$NMB = \frac{\sum_{i=1}^{n} (P_i - O_i)}{\sum_{i=1}^{n} O_i} \times 100\%;$$

$$NME = \frac{\sum_{i=1}^{n} | P_i - O_i |}{\sum_{i=1}^{n} O_i} \times 100\%;$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (P_i - O_i)^2};$$

$$IOA = 1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (| P_i - \overline{O} | + | \mathrm{O}_i - \overline{O} |)^2}$$

Table S5. The monthly and annual contributions of industry, power generation, residential resources and transportation to ambient BC concentrations at NJU and PAES (unit: %).

Period	Site	Industry (%)	Power generation (%)	Residential resources (%)	Transportation (%)	Sum (%)
January	NJU	11.48	0.53	11.72	11.27	35.00
	PAES	12.78	0.25	13.17	13.31	39.51
April	NJU	25.22	0.53	16.97	21.33	64.05
	PAES	25.26	0.21	19.54	24.23	69.24
July	NJU	29.73	0.62	20.16	32.27	82.78
	PAES	27.05	0.35	23.61	35.43	86.44
October	NJU	24.31	0.99	13.55	19.96	58.81
	PAES	23.58	0.57	16.14	23.32	63.61
Annual	NJU	21.01	0.68	14.71	19.21	55.61
	PAES	21.91	0.34	17.84	23.53	63.62

Table S6. Statistical indicators for observed and simulated BC concentrations using JS-prior and JS-posterior in January excluding data from 16th to 26th at PAES.

Site	Parameter	JS-prior	JS-posterior
PAES	Average SIM (μg/m^3)	2.86	2.68
	Average OBS (μg/m^3)	2.15	2.15
	NMB (%)	32.95	24.65
	NME (%)	52.61	49.63
	R	0.72	0.74

Table S7. The simulated monthly average PBL heights and the range of hourly simulations at NJU and PAES in four months (unit: m).

Month	Site	Monthly average PBL (m)	Hourly average PBL (m)
January	NJU	370.25	27.59-1443.64
	PAES	384.56	27.20-1460.07
April	NJU	432.73	28.61-2157.87
	PAES	441.72	28.61-2157.87
July	NJU	381.14	30.70-1617.69
	PAES	431.02	30.02-1975.01
October	NJU	462.57	29.70-2065.97
	PAES	488.30	29.78-2073.46

Table S8. Statistical indicators for observed and simulated BC concentrations for all periods, those included in the multiple regression model, and those excluded from the model in JS-prior and Case 2 for April 2015 at NJU.

Site	Parameter	JS-prior: All period	JS-prior: Included	JS-prior: Excluded	Case 2: All period	Case 2: Included	Case 2: Excluded
NJU	Average SIM (μg/m^3)	2.38	2.71	2.08	2.27	2.42	2.08
	Average OBS (μg/m^3)	2.69	2.56	2.99	2.69	2.56	2.99
	NMB (%)	-16.02	5.90	-56.48	-21.59	-5.32	-56.63
	NME (%)	42.31	34.01	57.62	32.47	21.09	57.61

Table S9. BC emissions from Nanjing and Suzhou–Wuxi–Changzhou-Zhenjiang city cluster in different cases in April 2015 (unit: Gg).

Case	Sector	Nanjing	Suzhou–Wuxi–Changzhou -Zhenjiang	Southern Jiangsu
Scenario B	Power	0	0.01	0.01
	Industry	0.21	1.13	1.34
	Residential	0.08	0.24	0.32
	Transportation	0.12	0.30	0.42
	Total	0.41	1.68	2.09
Case 1	Power	0	0.01	0.01
	Industry	0.05	0.25	0.30
	Residential	0.04	0.14	0.19
	Transportation	0.08	0.20	0.28
	Total	0.17	0.60	0.78
Case 2	Power	0	0.01	0.01
	Industry	0.09	0.47	0.56
	Residential	0.07	0.23	0.30
	Transportation	0.08	0.20	0.27
	Total	0.24	0.91	1.14
Case 3	Power	0	0.01	0.01
	Industry	0.04	0.47	0.51
	Residential	0.03	0.23	0.26
	Transportation	0.08	0.20	0.27
	Total	0.15	0.90	1.05

Table S10. The monthly emissions, simulated wet depositions and the ratios of wet deposition to emissions at NJU (a), PAES (b) and southern Jiangsu (c) using JS-prior and JS-posterior, respectively.

	January		April		July		October	
	JS-prior	JS-posterior	JS-prior	JS-posterior	JS-prior	JS-posterior	JS-prior	JS-posterior
Emission (kg)	410.84	383.01	379.81	225.56	417.61	203.25	368.48	347.25
Wet deposition (kg)	100.97	93.81	172.97	169.79	254.33	194.64	91.62	85.88
Wet deposition/emissions (%)	24.58	24.49	45.54	75.27	60.90	95.77	24.86	24.73

(a)

	January		April		July		October	
	JS-prior	JS-posterior	JS-prior	JS-posterior	JS-prior	JS-posterior	JS-prior	JS-posterior
Emission (kg)	1221.70	1286.89	1145.83	698.33	1130.99	528.42	1103.29	1219.42
Wet deposition (kg)	109.27	105.10	186.10	183.60	189.71	146.10	51.03	50.00
Wet deposition/emissions (%)	8.94	8.17	16.24	26.29	16.77	27.65	4.63	4.10

(b)

	January		April		July		October	
	JS-prior	JS-posterior	JS-prior	JS-posterior	JS-prior	JS-posterior	JS-prior	JS-posterior
Emission (Gg)	2.26	1.45	2.10	0.78	2.26	0.90	2.38	1.33
Wet deposition (Gg)	0.54	0.48	0.59	0.53	0.71	0.58	0.41	0.37
Wet deposition/emissions (%)	24.06	33.36	27.96	67.58	31.26	64.26	17.24	27.85

(c)

Figures

Figure S1.

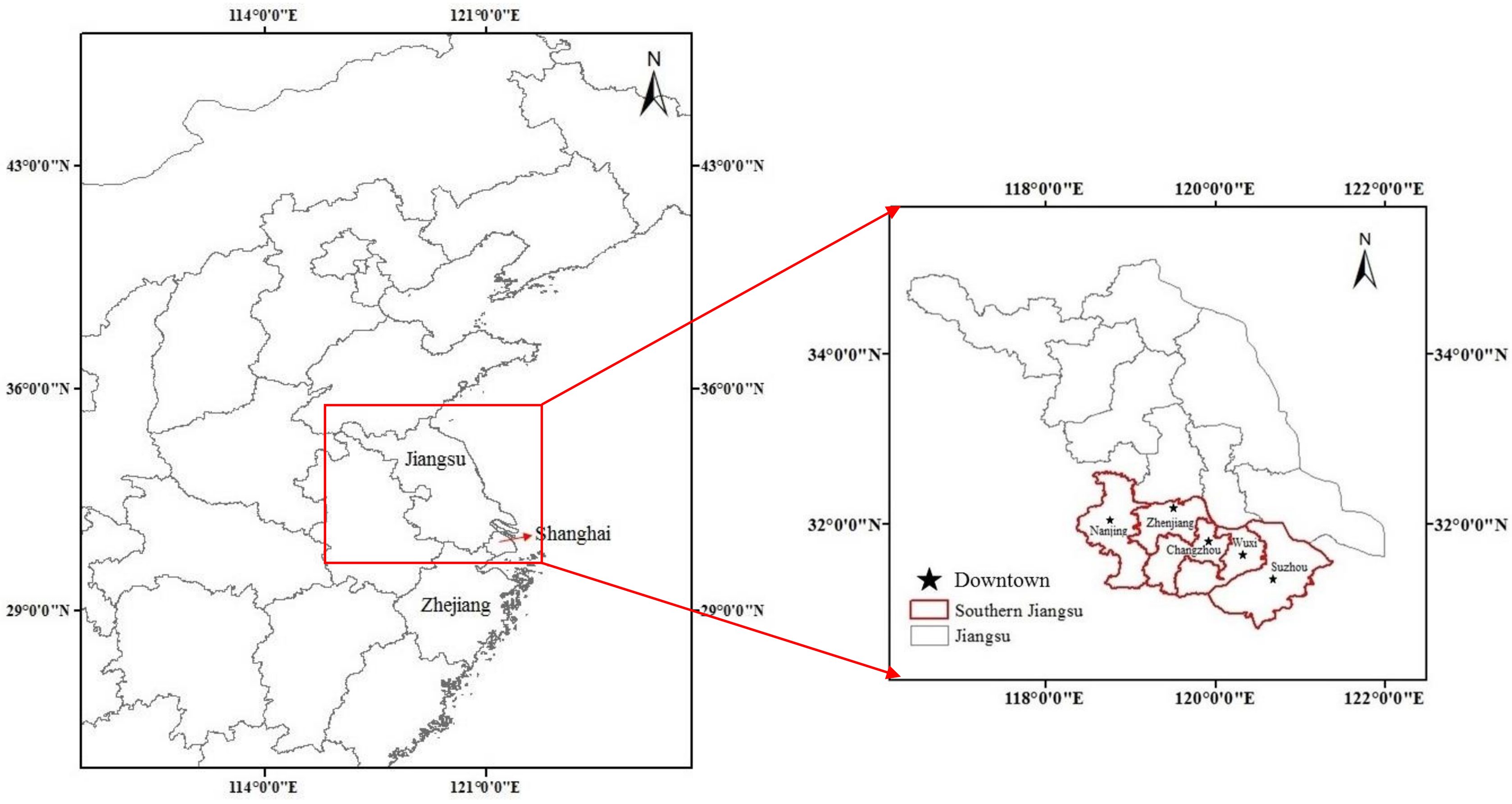
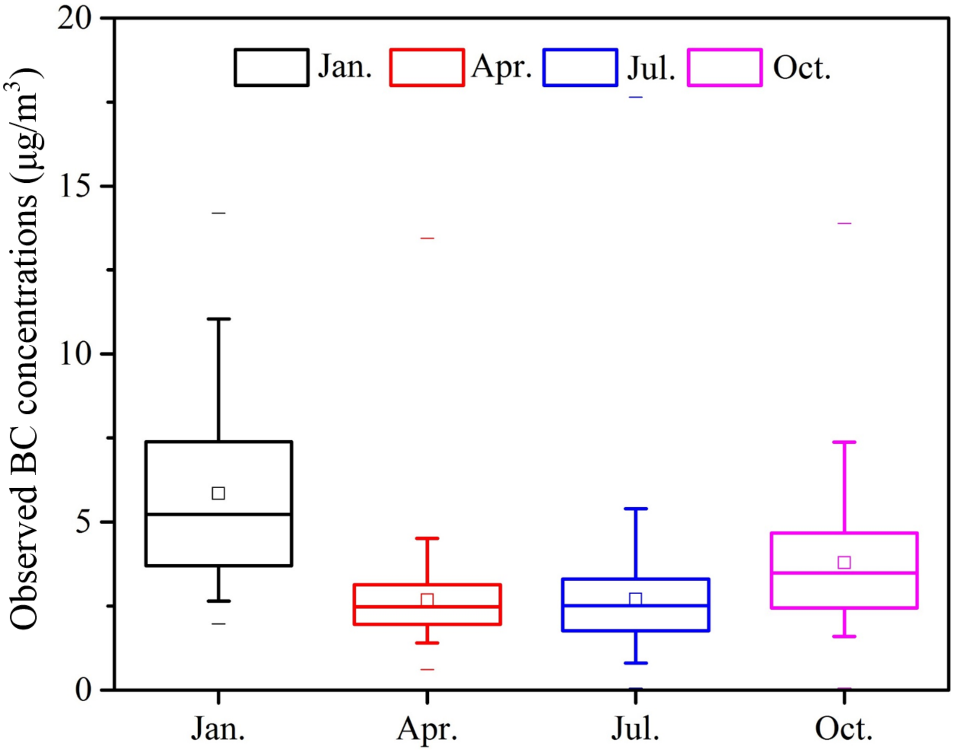
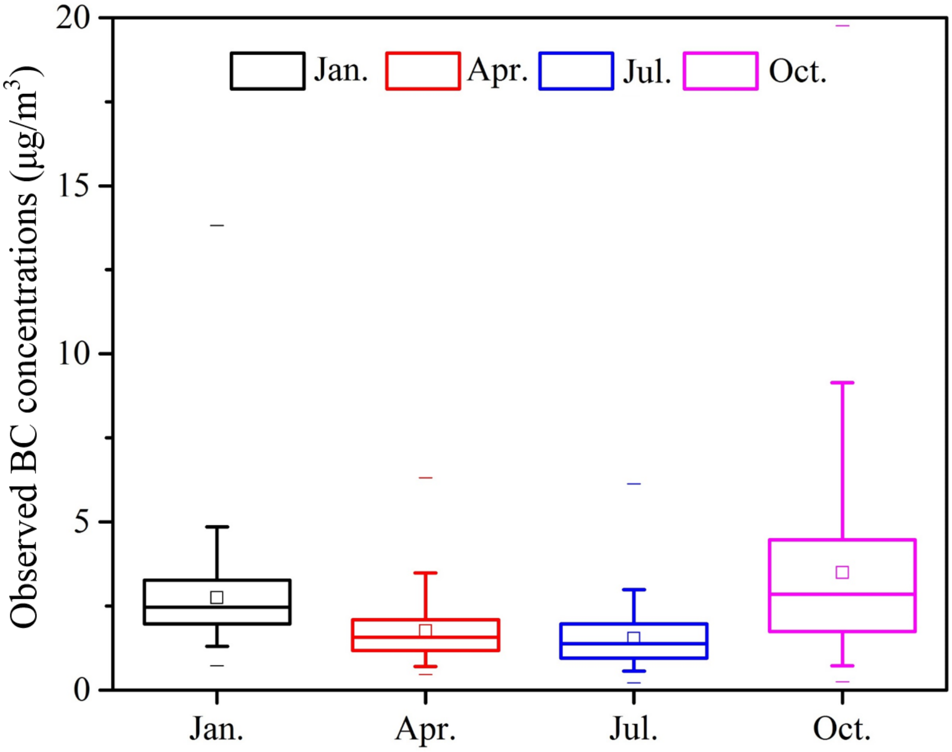


Figure S2.



Observed BC concentrations (μg/m³)
20
15
10
5
0
Jan.
Apr.
Jul.
Oct.
Jan.
Apr.
Jul.
Oct.

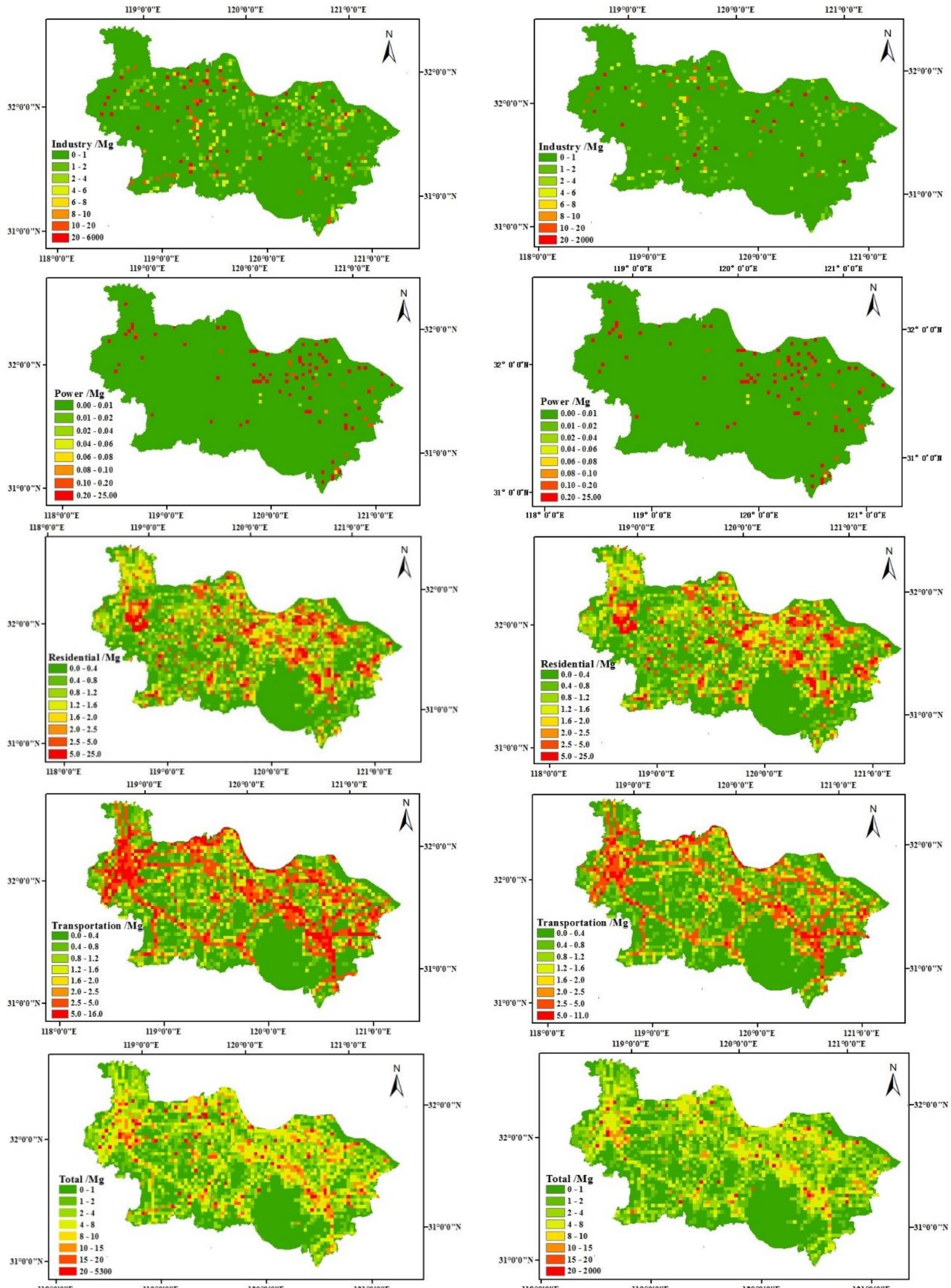
(a)



Observed BC concentrations (μg/m³)
20
15
10
5
0
Jan.
Apr.
Jul.
Oct.
Jan.
Apr.
Jul.
Oct.

(b)

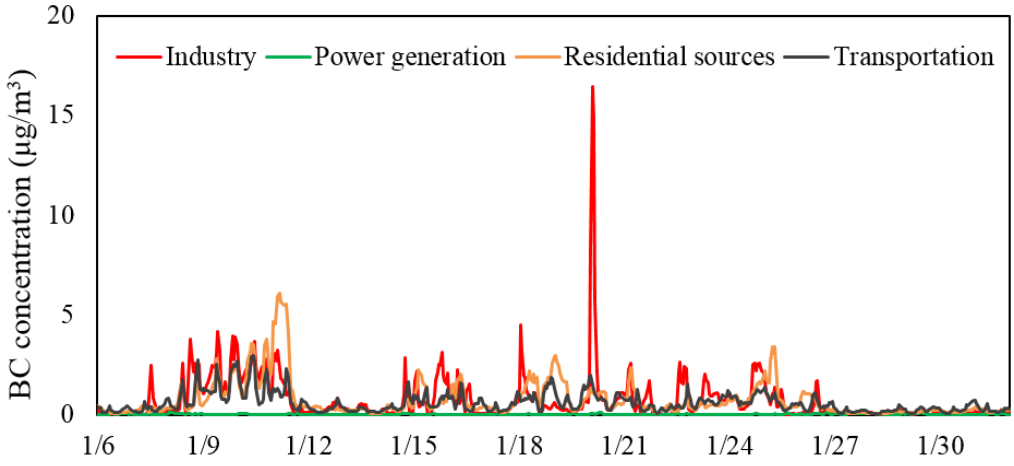
Figure S3.



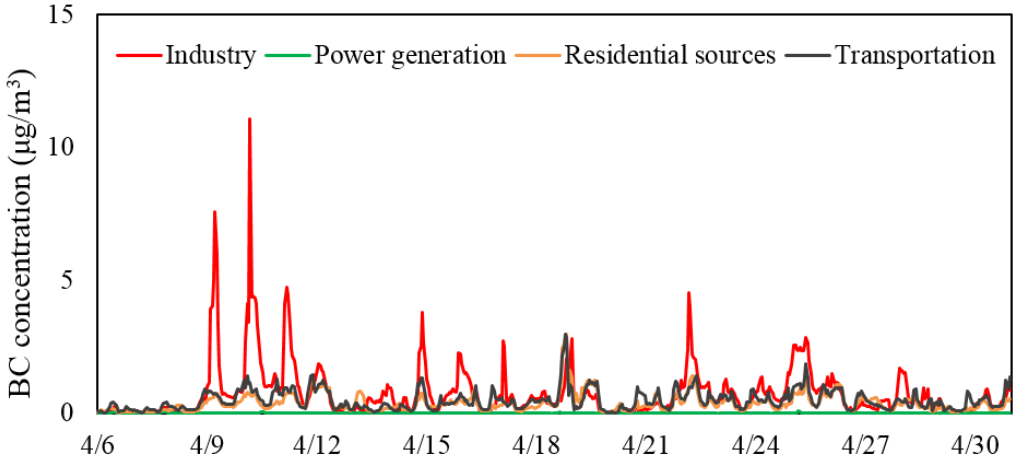
Industry /Mg
0 - 1
1 - 2
2 - 4
4 - 6
6 - 8
8 - 10
10 - 20
20 - 6000
20 - 2000
Power /Mg
0.00 - 0.01
0.01 - 0.02
0.02 - 0.04
0.04 - 0.06
0.06 - 0.08
0.08 - 0.10
0.10 - 0.20
0.20 - 25.00
Residential /Mg
0.0 - 0.4
0.4 - 0.8
0.8 - 1.2
1.2 - 1.6
1.6 - 2.0
2.0 - 2.5
2.5 - 5.0
5.0 - 25.0
Transportation /Mg
0.0 - 0.4
0.4 - 0.8
0.8 - 1.2
1.2 - 1.6
1.6 - 2.0
2.0 - 2.5
2.5 - 5.0
5.0 - 16.0
5.0 - 11.0
Total /Mg
0 - 1
1 - 2
2 - 4
4 - 8
8 - 10
10 - 15
15 - 20
20 - 5300
20 - 2000
N
118°0'0"E
119°0'0"E
120°0'0"E
121°0'0"E
31°0'0"N
32°0'0"N

(a) (b)

Figure S4.



(a)



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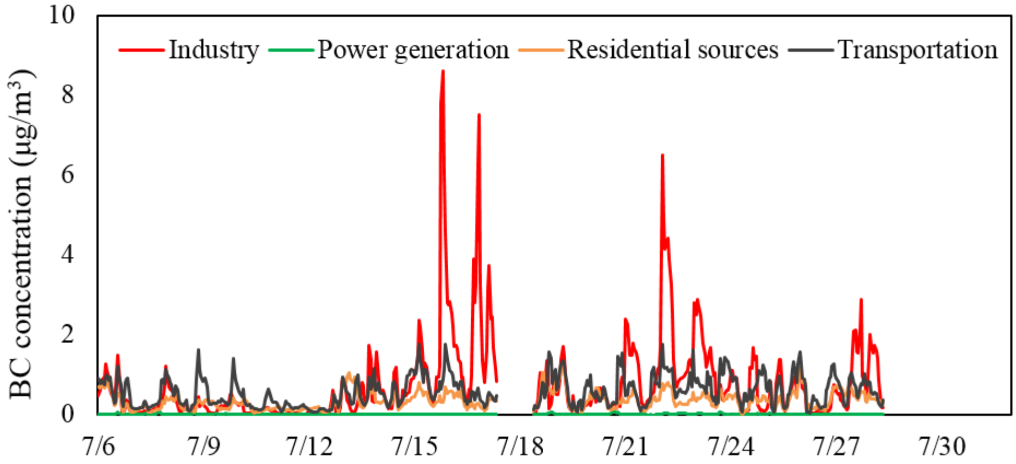

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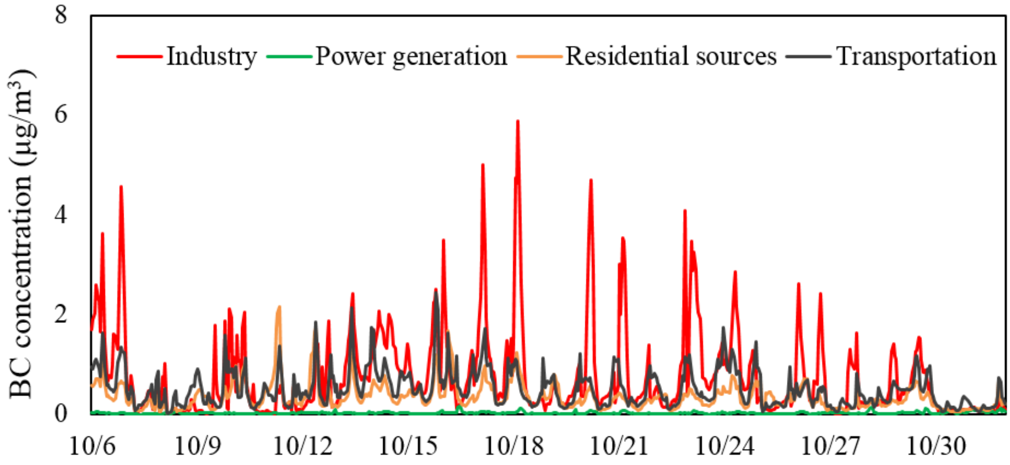
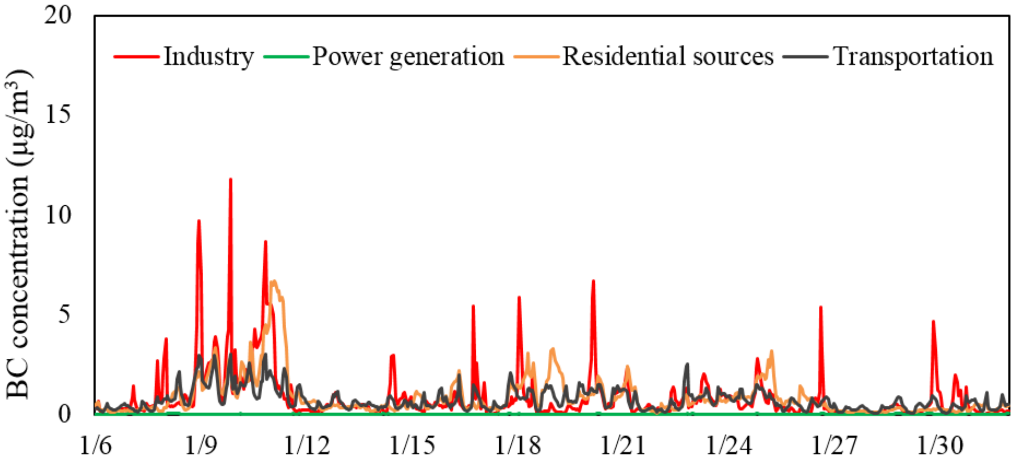


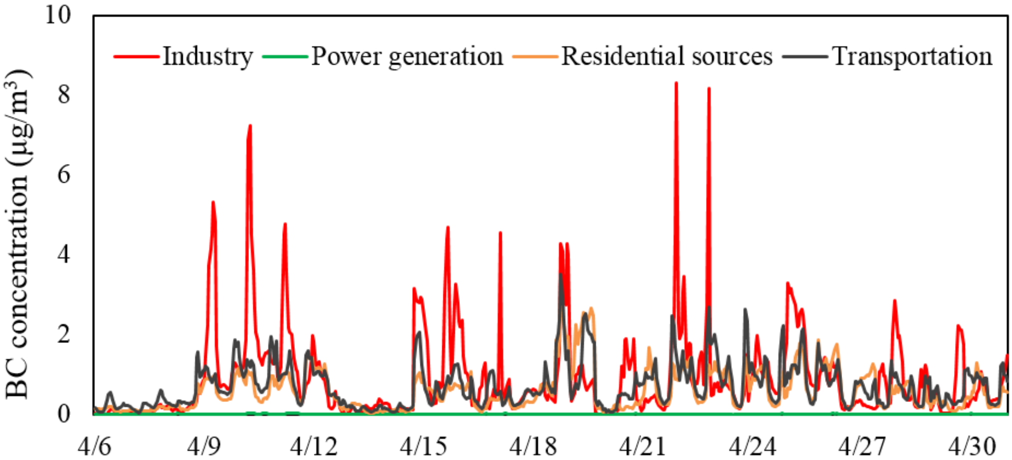
Industry
Power generation
Residential sources
Transportation
BC concentration (μg/m3)
0
2
4
6
8
10/6
10/9
10/12
10/15
10/18
10/21
10/24
10/27
10/30

(d)

Figure S5.



(a)



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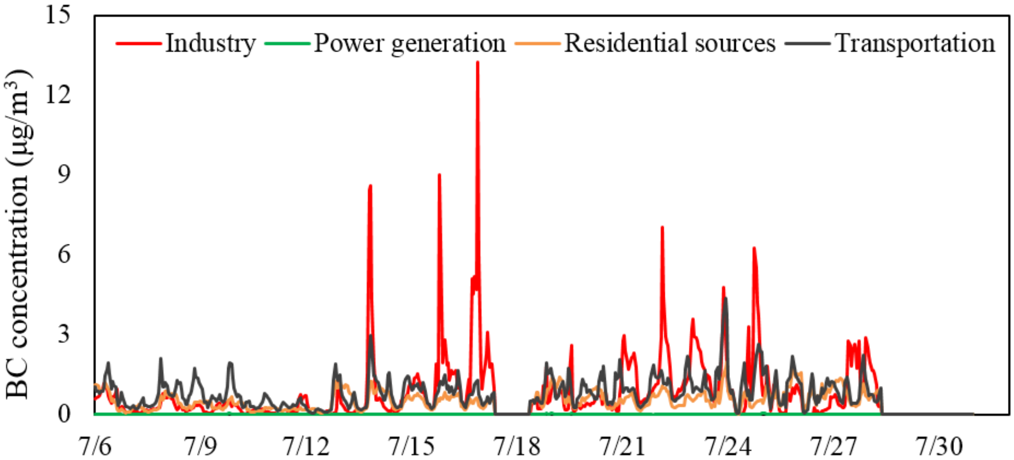

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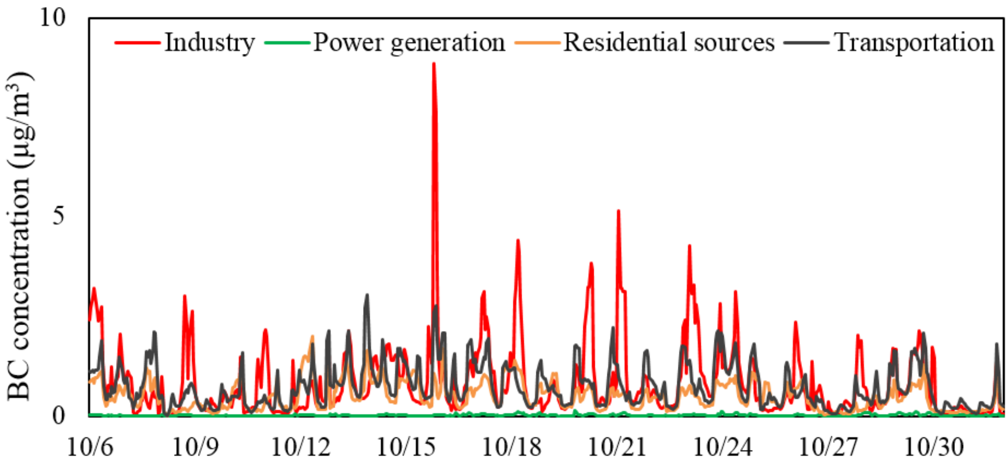
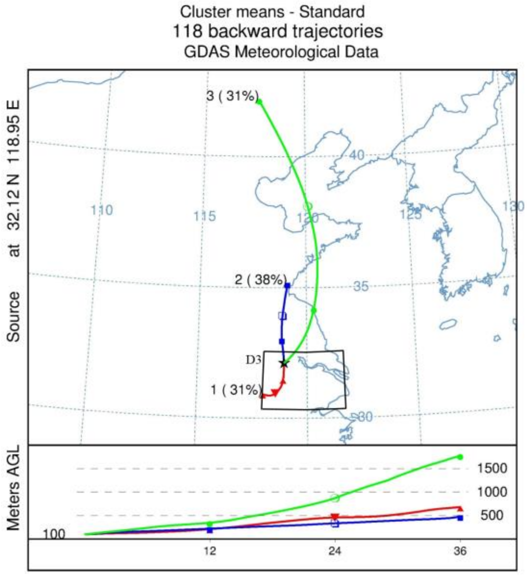


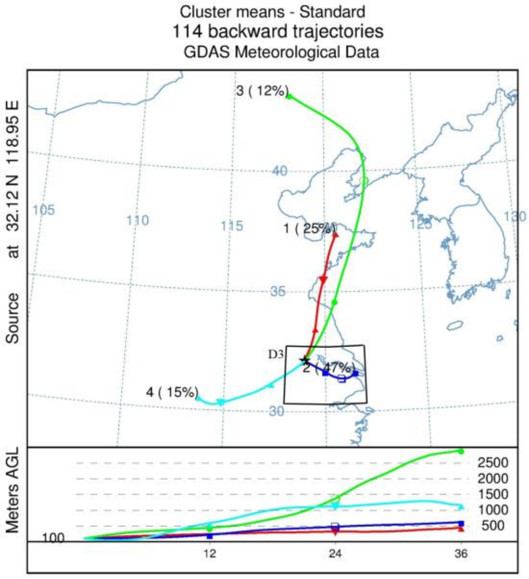
BC concentration (μg/m³)
10
5
0
Industry
Power generation
Residential sources
Transportation
10/6
10/9
10/12
10/15
10/18
10/21
10/24
10/27
10/30

(d)

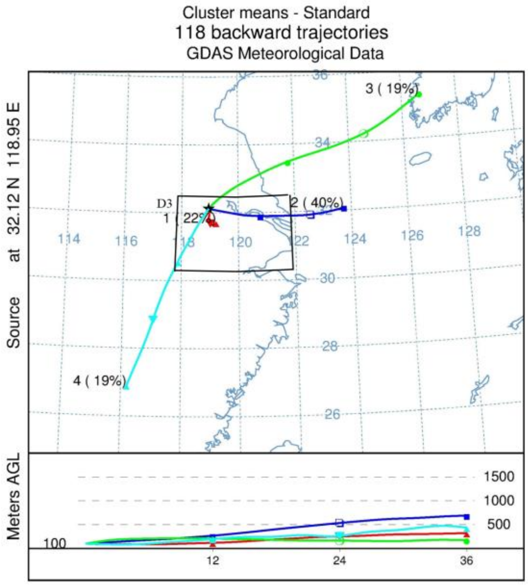
Figure S6.



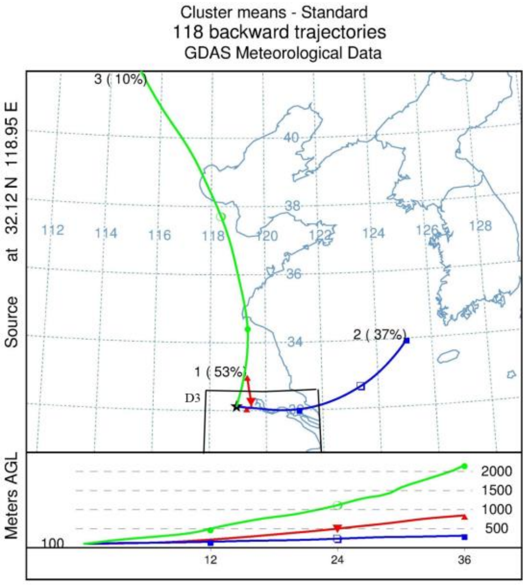
(a)



(b)

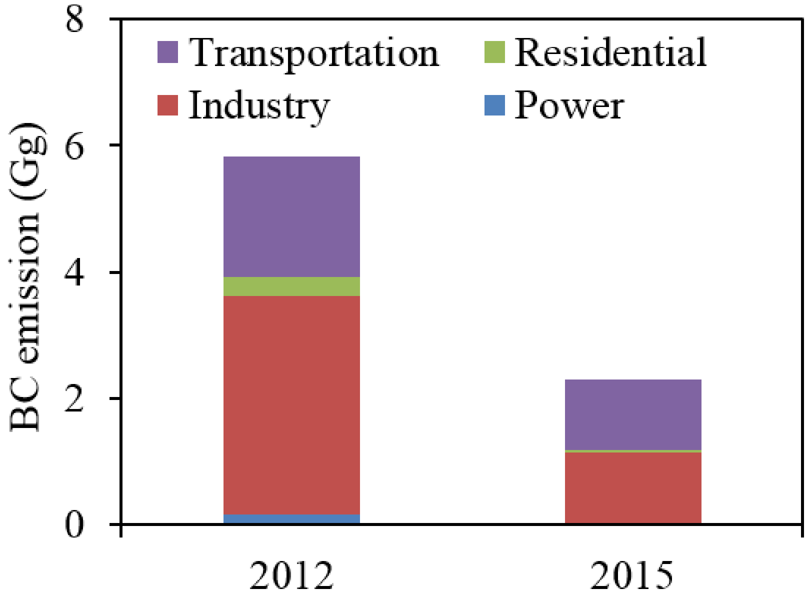


(c)



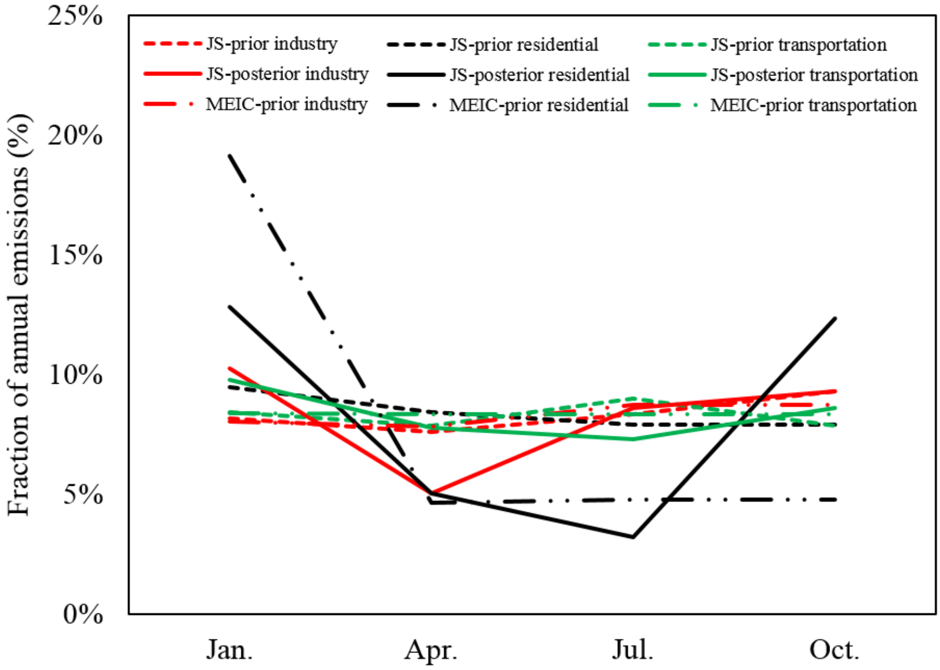
(d)

Figure S7.

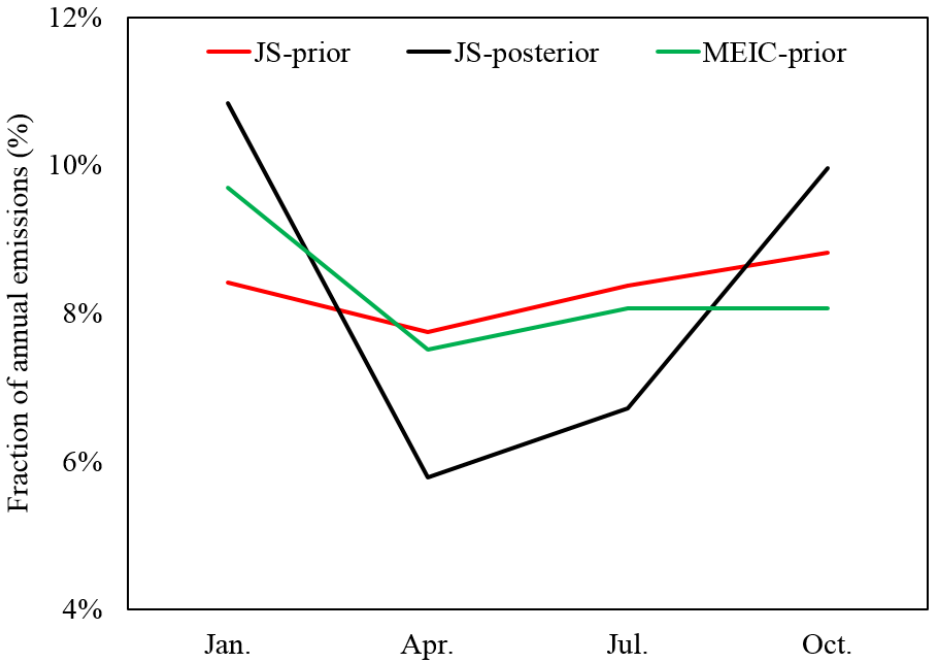


8
6
4
2
0
BC emission (Gg)
Transportation
Residential
Industry
Power
2012
2015

Figure S8.

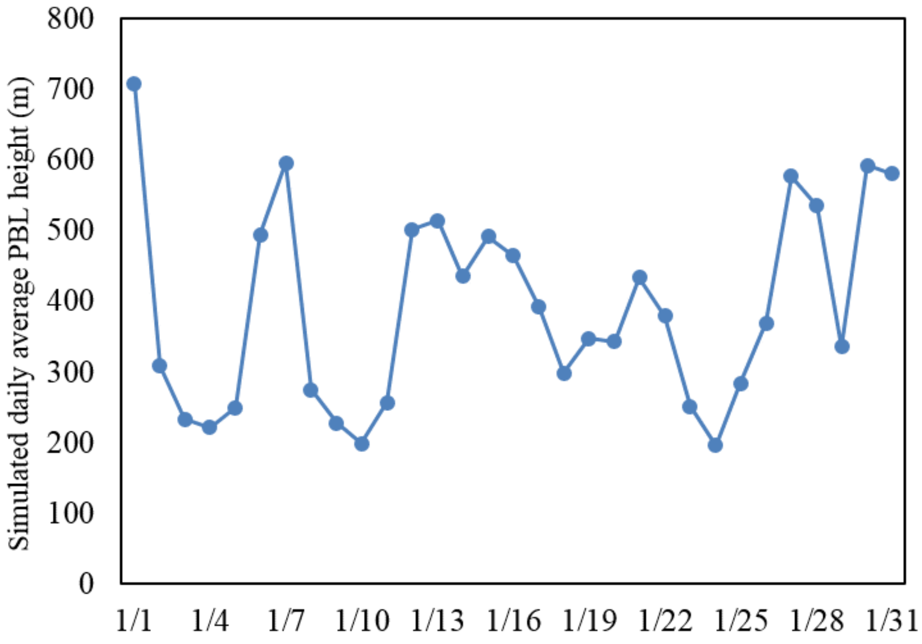

25%
20%
15%
10%
5%
0%
Fraction of annual emissions (%)
JS-prior industry
JS-prior residential
JS-prior transportation
JS-posterior industry
JS-posterior residential
JS-posterior transportation
MEIC-prior industry
MEIC-prior residential
MEIC-prior transportation
Jan.
Apr.
Jul.
Oct.

(a)


12%
10%
8%
6%
4%
Fraction of annual emissions (%)
JS-prior
JS-posterior
MEIC-prior
Jan.
Apr.
Jul.
Oct.

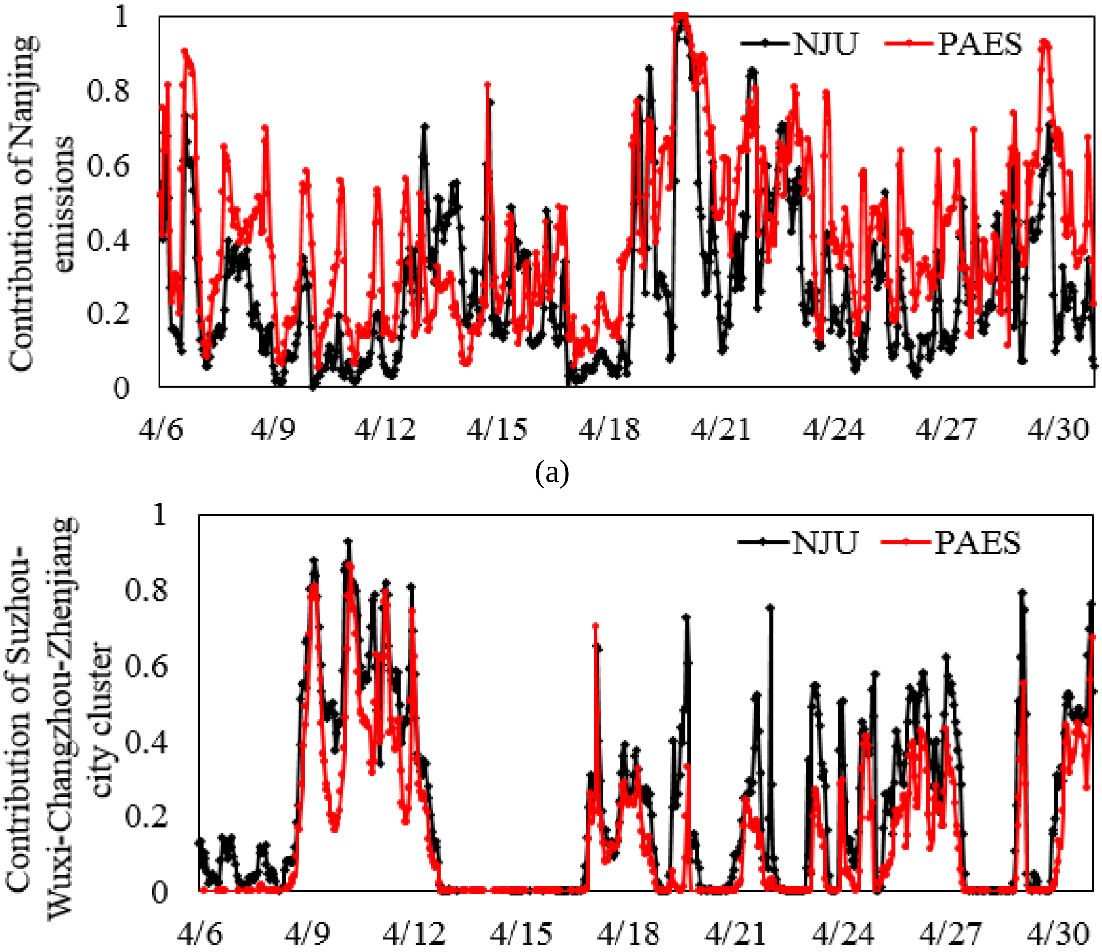
(b)

Figure S9.



800
700
600
500
400
300
200
100
0
Simulated daily average PBL height (m)
1/1
1/4
1/7
1/10
1/13
1/16
1/19
1/22
1/25
1/28
1/31

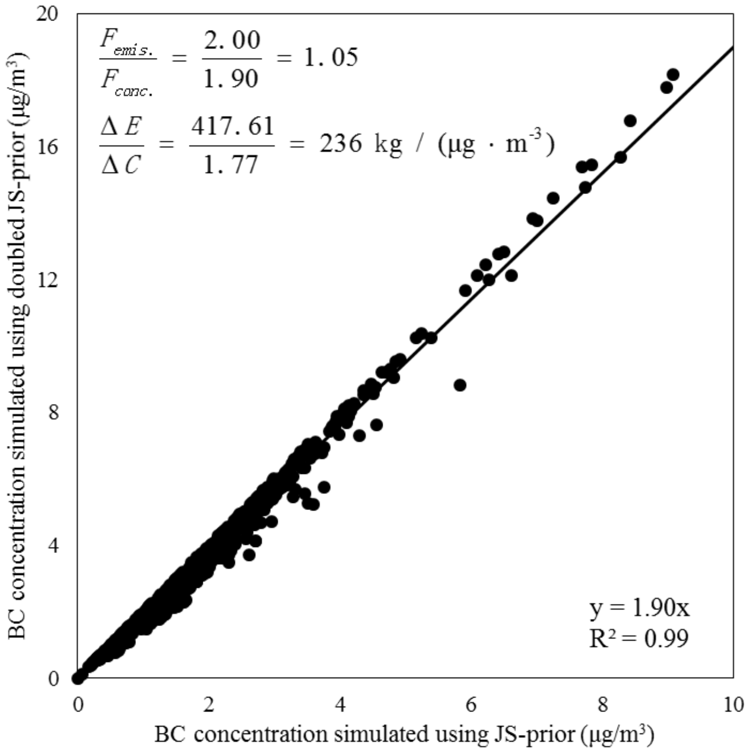
Figure S10.



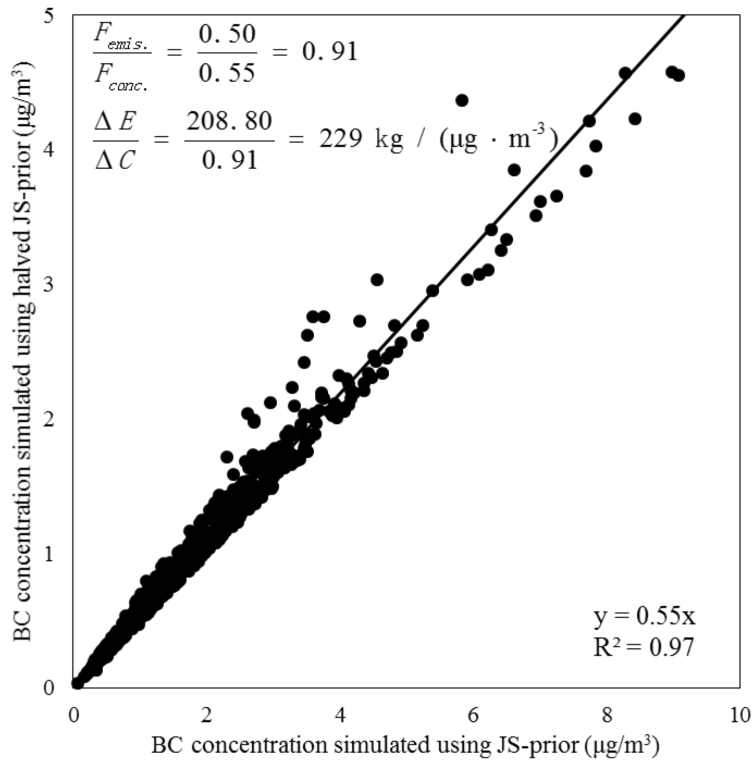
(a)

(b)

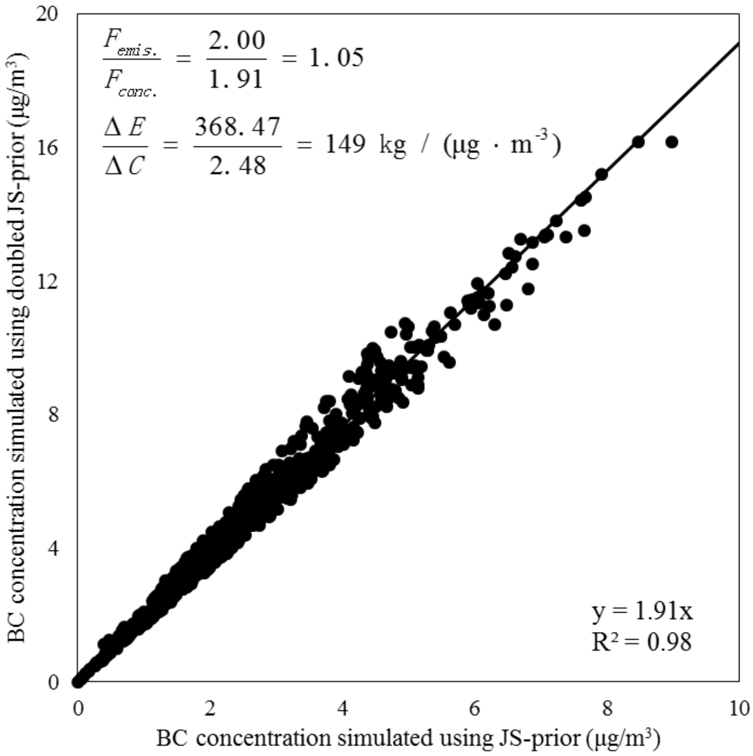
Figure S11.



(a)

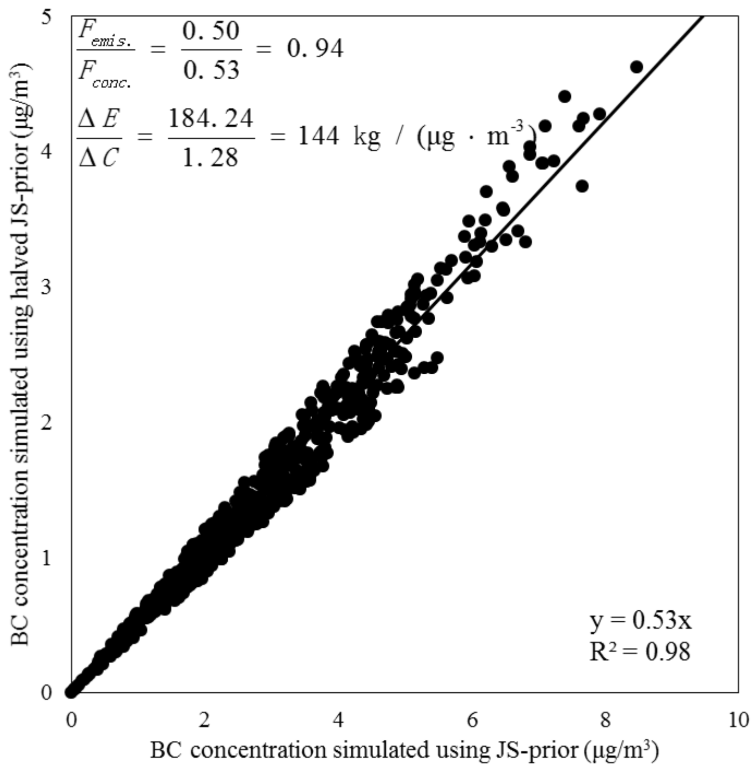


(b)



$\frac{F_{emis.}}{F_{conc.}} = \frac{2.00}{1.91} = 1.05$
$\frac{\Delta E}{\Delta C} = \frac{368.47}{2.48} = 149$ kg / (μg · m^{-3})
y = 1.91x
R² = 0.98
BC concentration simulated using doubled JS-prior (μg/m³)
BC concentration simulated using JS-prior (μg/m³)

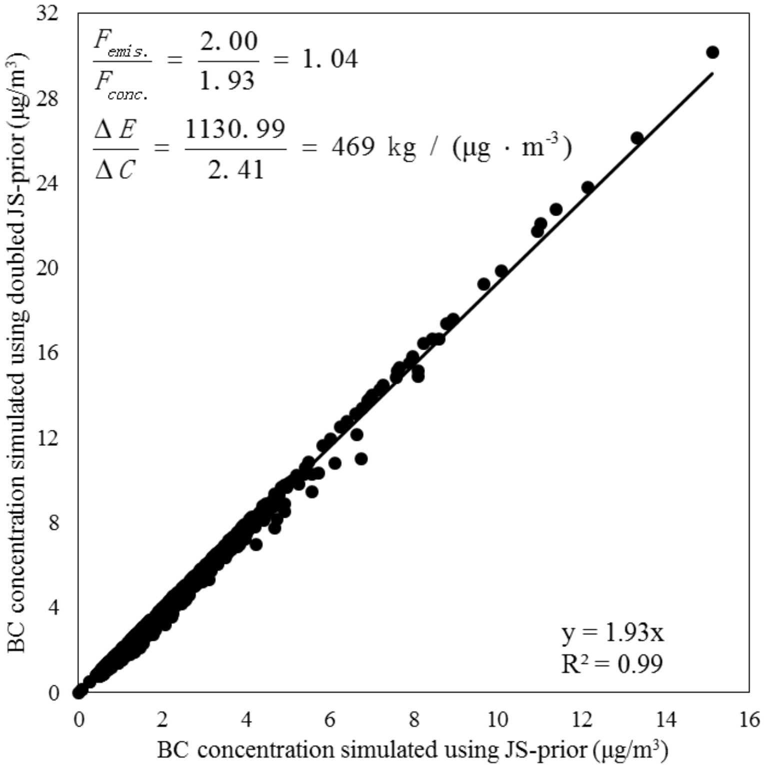
(c)



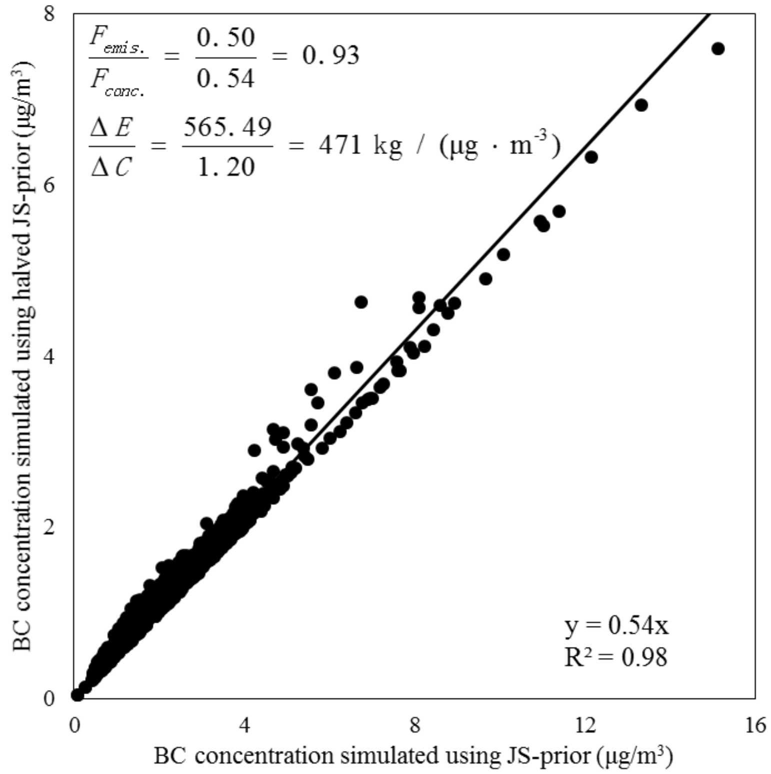
$\frac{F_{emis.}}{F_{conc.}} = \frac{0.50}{0.53} = 0.94$
$\frac{\Delta E}{\Delta C} = \frac{184.24}{1.28} = 144$ kg / (μg · m^{-3})
y = 0.53x
R² = 0.98
BC concentration simulated using halved JS-prior (μg/m³)
BC concentration simulated using JS-prior (μg/m³)

(d)

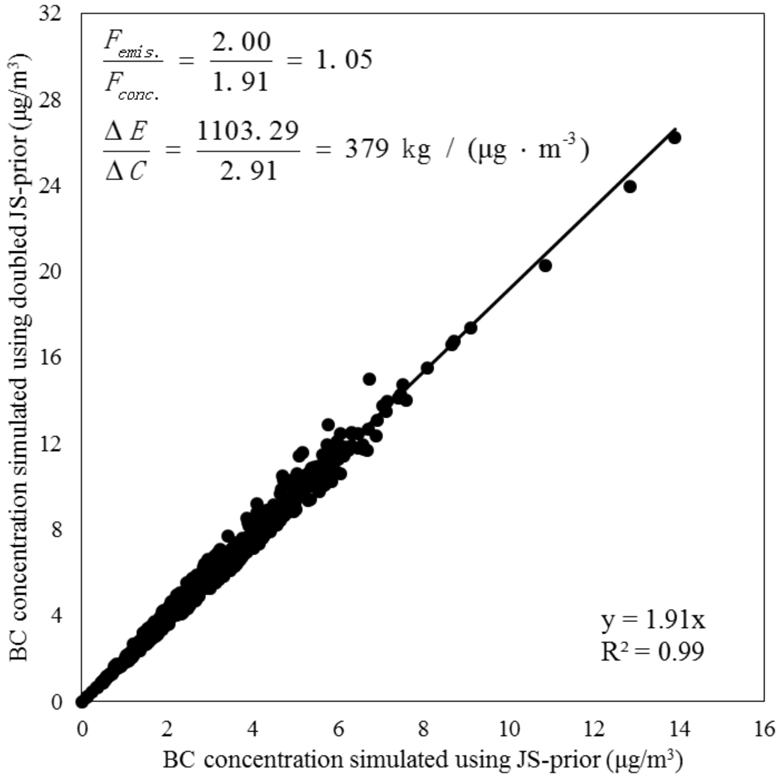
Figure S12.



(a)

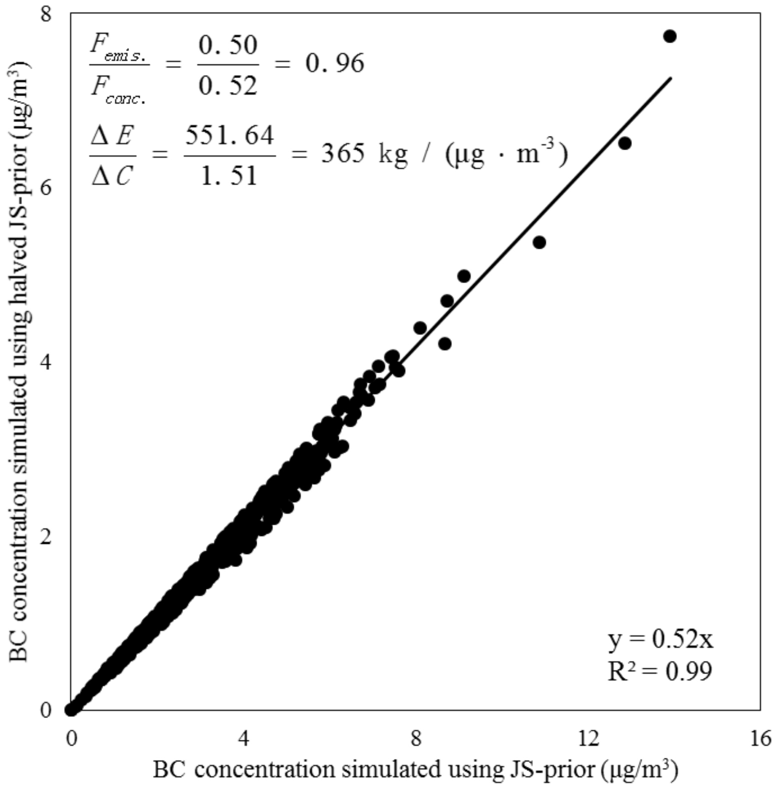


(b)



$\frac{F_{emis.}}{F_{conc.}} = \frac{2.00}{1.91} = 1.05$
$\frac{\Delta E}{\Delta C} = \frac{1103.29}{2.91} = 379$ kg / (µg · m^{-3})
y = 1.91x
$R^2 = 0.99$
BC concentration simulated using doubled JS-prior (µg/m^3)
BC concentration simulated using JS-prior (µg/m^3)

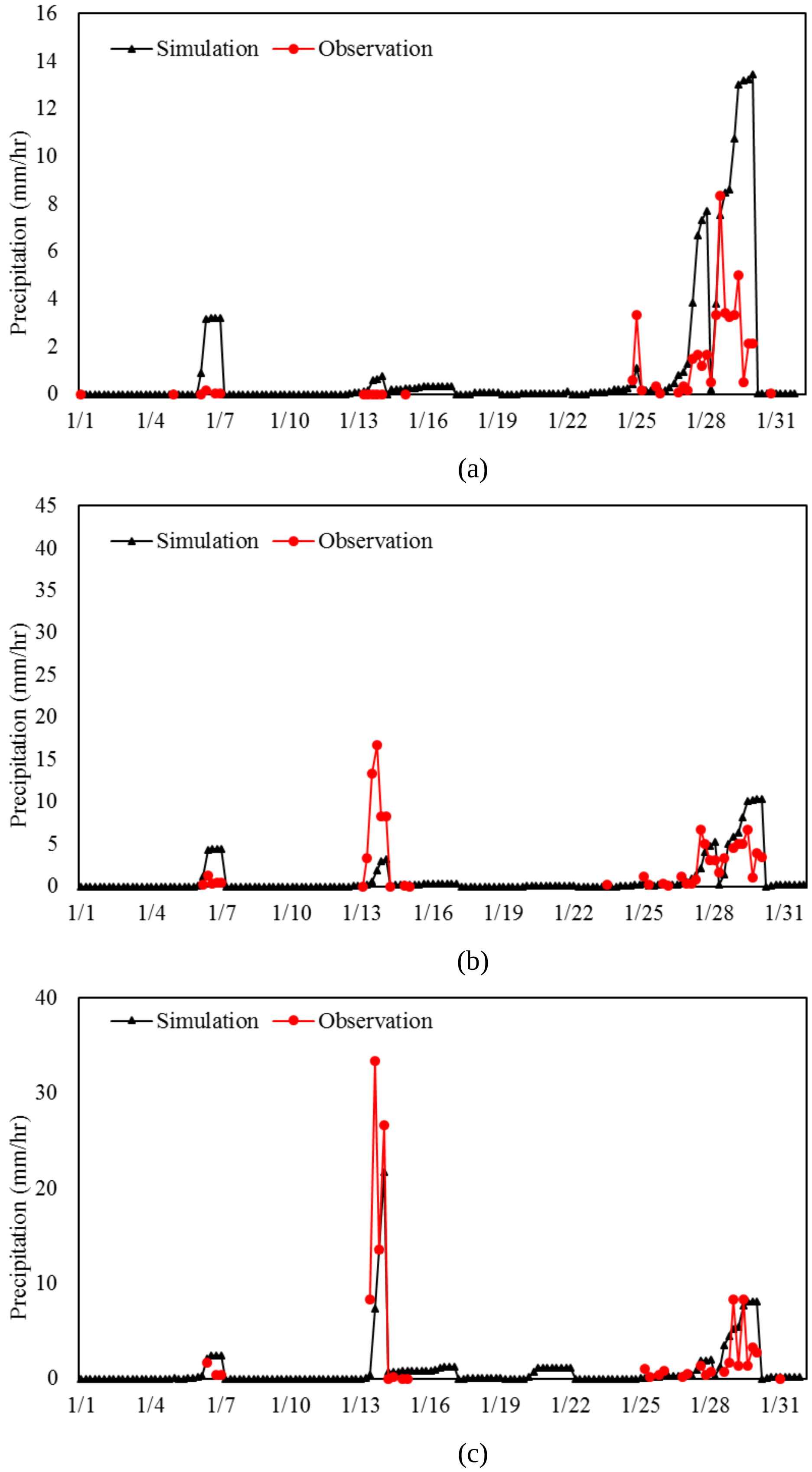
(c)



$\frac{F_{emis.}}{F_{conc.}} = \frac{0.50}{0.52} = 0.96$
$\frac{\Delta E}{\Delta C} = \frac{551.64}{1.51} = 365$ kg / (µg · m^{-3})
y = 0.52x
$R^2 = 0.99$
BC concentration simulated using halved JS-prior (µg/m^3)
BC concentration simulated using JS-prior (µg/m^3)

(d)

Figure S13.

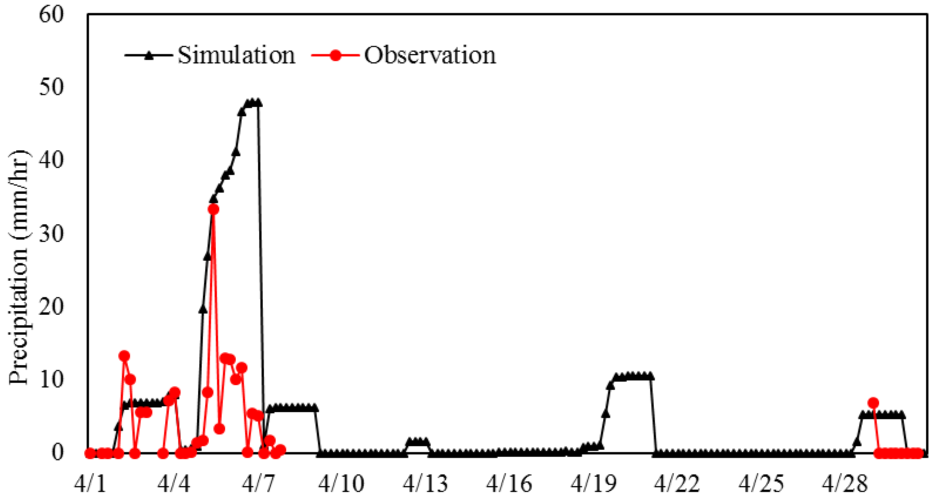


(a)

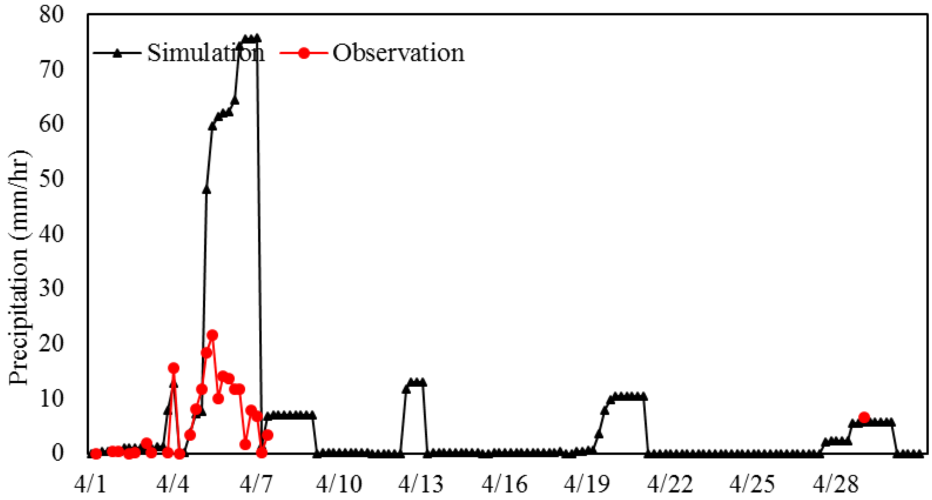
(b)

(c)

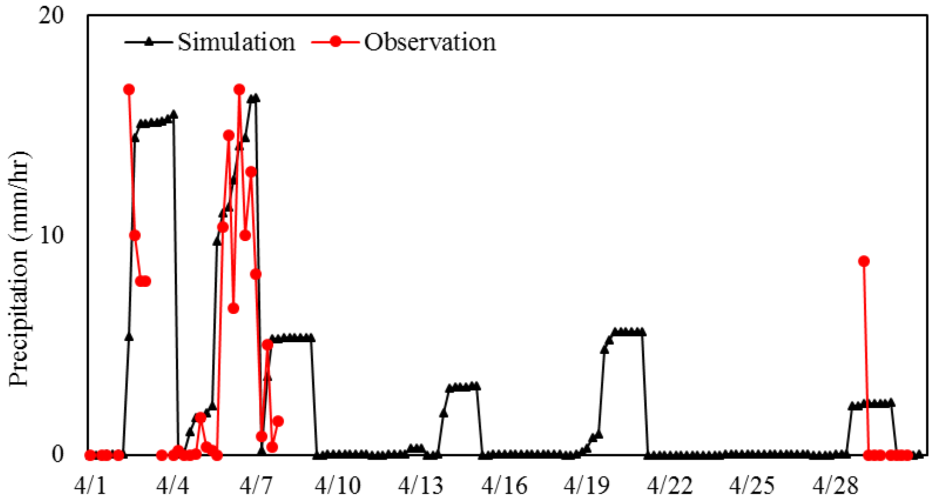
Figure S14.



(a)

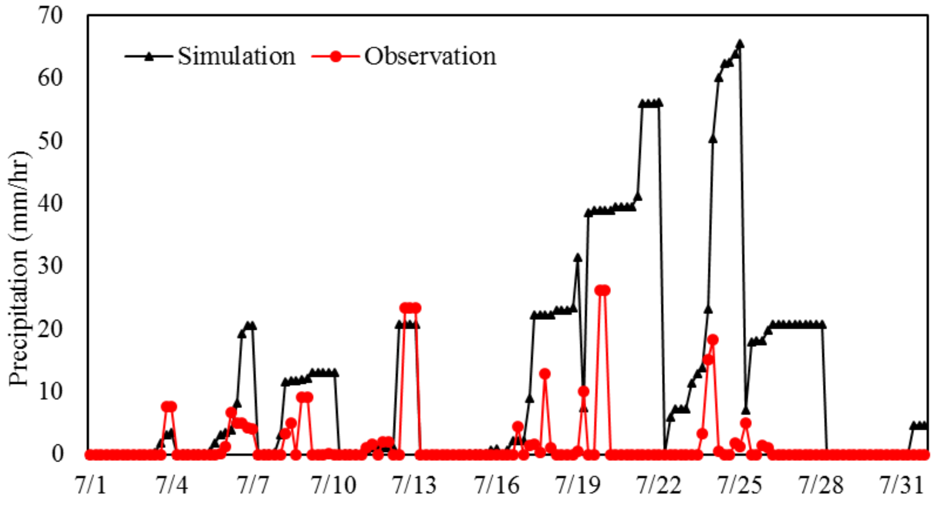


(b)

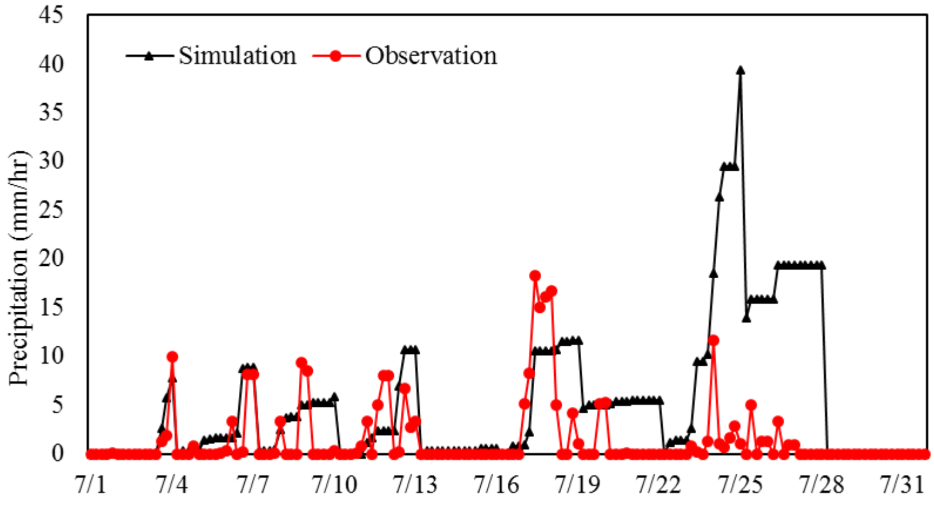


(c)

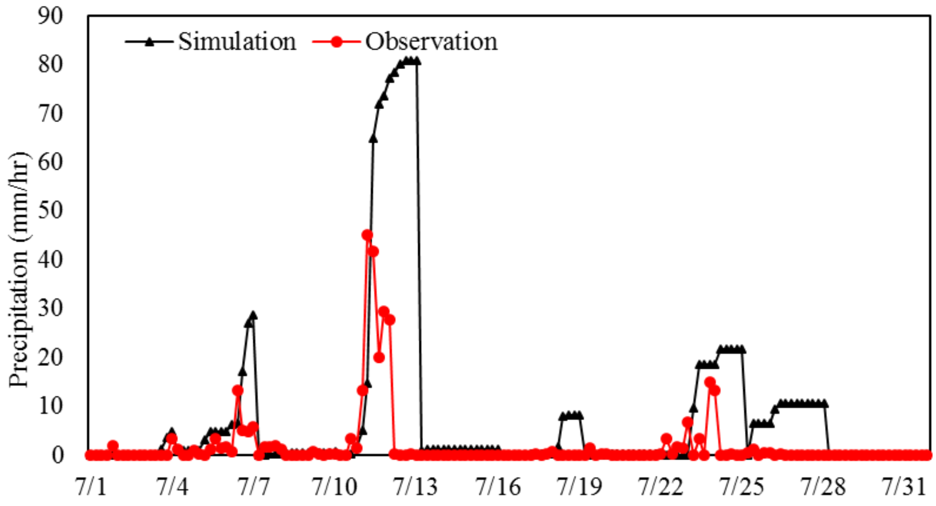
Figure S15.



(a)

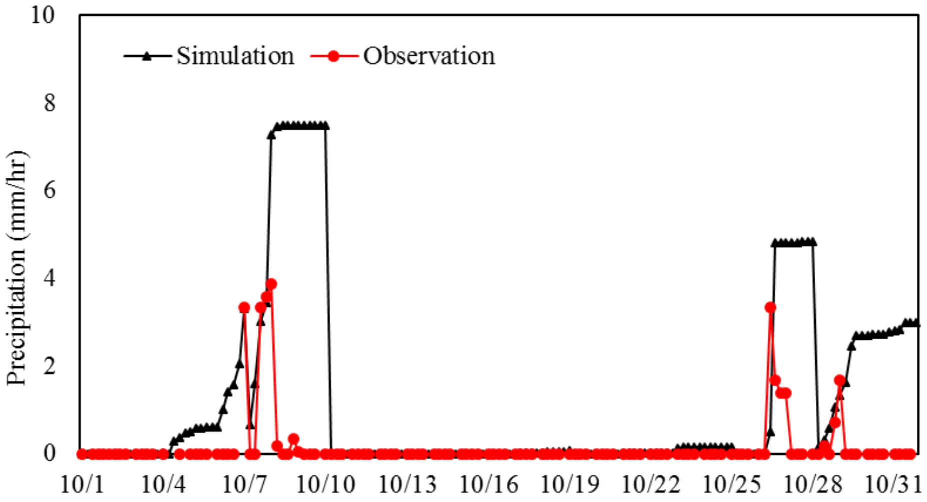


(b)

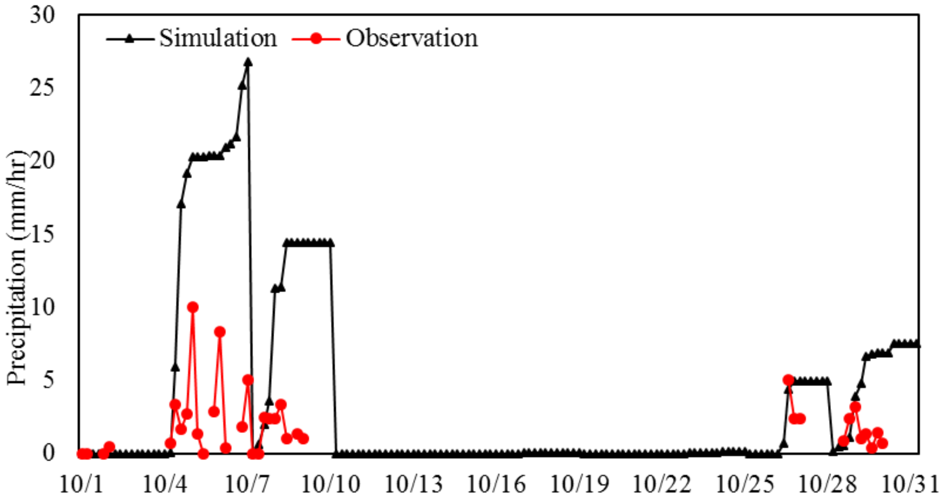


(c)

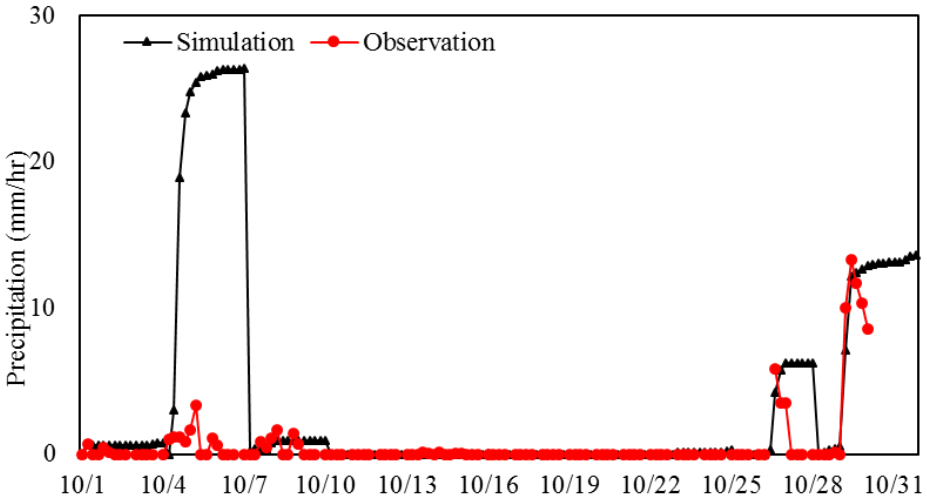
Figure S16.



(a)



(b)



(c)