Atmospheric
Chemistry
and Physics

Supplement of

Ensemble prediction of air quality using the WRF/CMAQ model system for health effect studies in China

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Table S1. Total Emissions of major pollutants within China in a typical workday of each season. Unit for CO is billion moles/day. Unit for NOx, VOCs, SO_2, and NH_3 is Mmoles/day. Unit for EC, OC, and $PM_{2.5}$ is kton/day. SD is the standard deviation between the four inventories. Based on the weekly profiles used, the weekend day has ~30% emissions compared to workday of each season, and the relative differences among different inventories do not change.

	CO	NOx	VOCs	SO_2	NH_3	EC	OC	$PM_{2.5}$
Winter								
MEIC	21.0	1292.5	899.2	1050.8	1255.1	6.7	15.9	37.5
SOE	/	866.4	491.4	621.3	5249.7	5.3	16.1	26.6
EDGAR	10.7	1042.4	899.3	1343.3	2996.0	2.5	14.6	45.1
REAS2	18.5	1133.5	1354.3	1071.5	2560.1	4.5	10.3	30.4
SD	4.4	154.1	305.3	258.4	1440.4	1.5	2.3	7.1
Spring								
MEIC	10.2	1274.0	575.8	814.7	1733.9	3.1	5.6	20.4
SOE	/	933.6	395.1	576.0	2815.9	2.9	8.4	19.6
EDGAR	6.9	972.9	490.2	1343.2	872.6	1.4	5.1	27.5
REAS2	14.7	1125.1	1029.4	1059.3	2479.9	3.1	5.4	26.3
SD	3.2	134.6	243.4	284.9	747.6	0.7	1.3	3.5
Summer								
MEIC	9.7	1281.5	585.1	826.0	2145.5	2.9	5.2	19.8
SOE	/	906.3	341.9	560.8	6406.4	2.6	6.7	16.3
EDGAR	6.3	983.8	459.2	1376.3	712.5	1.3	4.4	26.8
REAS2	13.9	1148.0	1004.0	1068.6	2478.0	3.0	5.2	25.8
SD	3.1	145.5	249.9	301.0	2110.8	0.7	0.8	4.3
Fall								
MEIC	10.1	1251.2	597.9	817.9	1367.7	3.1	5.6	20.5
SOE	/	934.9	390.5	582.4	3641.6	2.9	5.2	19.4
EDGAR	6.9	970.8	485.8	1351.3	845.1	1.4	5.0	27.4
REAS2	13.9	1066.5	1028.5	991.5	2481.5	2.9	5.3	24.8
SD	2.9	122.6	243.9	280.4	1076.1	0.7	0.2	3.2

Table S2. Predicted annual average PM$_{2.5}$ concentrations at 60 cities using different anthropogenic emission inventory, and weighted ensemble based on linear combination of the four simulations, along with observed concentrations. Units are μg m^{-3}.

City	MEIC	SOE	EDGAR	REAS2	ENSEMBLE	Observation
Shijiazhuang	86.3	94.2	73.3	104.2	102.1	148.5
Baoding	113.4	79.5	78.1	115.1	111.9	127.9
Handan	97.9	89.7	89.7	135.2	119.0	127.8
Hengshui	103.2	87.9	88.5	113.3	112.3	120.6
Tangshan	84.8	90.6	52.8	80.7	88.2	114.2
Jinan	96.3	95.0	86.6	119.0	113.5	114.0
Langfang	93.5	72.6	70.6	82.2	90.7	113.8
Xi'an	70.9	87.5	69.6	66.1	81.4	104.2
Zhengzhou	107.5	90.5	92.9	105.4	112.3	102.4
Tianjin	84.0	73.8	84.4	95.9	95.7	95.6
Cangzhou	90.6	73.2	67.8	87.4	91.3	93.6
Beijing	62.2	59.2	77.3	71.6	75.2	90.1
Wuhan	94.4	98.5	102.9	89.9	106.7	94.0
Chengdu	52.9	67.8	50.0	52.6	62.0	86.3
Wulumuqi	22.0	39.1	20.1	32.4	32.1	85.2
Hefei	86.6	84.4	74.9	88.5	94.5	84.9
Huai'an	72.4	65.7	66.1	75.8	79.3	80.8
Changsha	87.9	109.8	70.7	82.2	98.0	79.1
Wuxi	64.6	65.6	63.6	74.3	75.7	75.8
Harbin	59.4	150.6	58.6	47.2	84.1	75.7
Nanjing	79.1	79.5	88.9	94.8	96.1	75.3
Xuzhou	100.6	85.8	101.3	102.3	109.6	74.9
Taiyuan	64.5	67.8	61.0	78.1	77.0	74.2
Huzhou	52.8	57.8	63.5	68.2	67.9	73.5
Shenyang	97.3	101.5	75.0	111.6	110.3	72.7
Yangzhou	74.7	67.2	71.5	78.9	82.5	71.1
Suqian	78.1	66.0	69.1	81.9	83.9	70.7
Nantong	77.1	58.8	60.9	70.0	75.9	70.2
Changchun	60.5	55.2	44.3	49.7	59.2	69.2
Nanchang	53.6	82.6	61.6	114.9	90.4	69.1
Jinhua	34.2	39.5	45.2	45.6	45.8	69.0
Lianyungang	66.5	55.0	56.6	66.7	69.6	68.0
Lanzhou	22.9	18.0	28.6	24.1	26.0	67.1
Suzhou	58.2	74.1	69.6	86.0	81.2	67.1
Jiaxing	60.2	59.9	66.4	70.0	71.9	66.9
Quzhou	31.0	34.3	39.5	38.4	39.8	66.5
Shaoxing	47.1	54.0	58.3	59.9	61.2	66.4
Hangzhou	47.2	58.8	63.0	64.6	65.0	66.1
Qinhuangdao	65.5	50.4	39.6	53.9	60.2	65.2
Chongqing	89.2	90.5	80.5	88.5	98.0	63.9
Xining	11.2	11.2	16.3	13.6	14.4	63.2
Qingdao	66.0	62.8	59.5	66.6	71.9	61.7

Shanghai	51.4	50.0	65.2	61.8	63.6	60.7
Huhehaote	27.5	20.1	18.6	21.5	25.0	59.1
Wenzhou	26.1	33.2	45.3	47.0	42.3	56.5
Nanning	37.0	43.4	45.0	43.8	47.0	54.7
Taizhou	71.3	62.3	66.7	72.1	76.8	53.0
Guangzhou	31.2	46.2	58.1	35.3	45.4	52.2
Chengde	40.0	35.1	35.0	49.7	46.0	51.5
Dalian	41.5	46.1	34.4	52.9	50.1	50.7
Guiyang	48.9	60.9	46.2	50.8	57.7	49.4
Lishui	26.2	30.7	37.4	36.9	36.5	47.9
Yinchuan	18.7	27.0	18.6	19.9	23.3	43.7
Shenzhen	23.0	32.8	45.2	24.4	33.1	39.7
Zhuhai	24.0	32.2	47.9	31.4	36.3	37.9
Kunming	29.4	32.8	28.0	31.8	34.3	35.5
Fuzhou	22.6	30.8	44.0	27.1	33.2	33.2
Zhoushan	24.4	24.1	26.8	29.3	29.4	32.1
Lasa	3.0	3.4	3.8	3.6	3.9	26.0
Haikou	21.2	28.2	29.9	24.8	28.4	25.6

Table S3. Comparison of the data-withholding ensemble prediction of PM$_{2.5}$ and O$_3$-1h at each city with predictions of individual inventories. The ensemble predictions at each city are calculated by using the data in the other 59 cities (i.e., withholding the data at that city) to determine the ensemble weighting factors. Symbol '×' indicates the ensemble prediction performance is better than the performance of a specific inventory (i.e., both MFB (MNB) and MFE (MNE) values are smaller for PM$_{2.5}$ (O$_3$-1h)); otherwise symbol '-' indicates the ensemble prediction performance is worse.

City	PM$_{2.5}$				O$_3$-1h			
	MEIC	SOE	EDGAR	REAS2	MEIC	SOE	EDGAR	REAS2
Shijiazhuang	×	×	×	-	×	×	×	×
Baoding	-	×	×	-	-	-	-	×
Handan	×	×	×	-	×	×	×	×
Hengshui	×	×	×	-	-	-	-	-
Tangshan	-	-	×	×	-	×	-	-
Jinan	×	×	×	×	-	-	-	-
Langfang	-	×	×	×	×	×	×	×
Xi'an	×	-	×	×	×	×	×	×
Zhenzhou	-	×	-	-	×	-	×	×
Tianjing	×	×	×	×	-	×	-	-
Wuhan	-	-	-	-	×	×	×	×
Cangzhou	×	×	×	×	-	×	-	-
Beijing	×	×	-	×	×	×	×	×
Chendu	×	-	×	×	-	-	-	-
Wulumuqi	×	-	×	-	×	-	×	×
Hefei	-	-	×	-	×	-	×	×
Huai'an	×	×	×	×	-	-	-	-
Changsha	-	×	-	-	×	×	×	×
Wuxi	×	×	×	×	-	-	-	-
Harbin	-	×	-	×	×	×	×	×
Nanjing	-	-	-	-	×	×	×	×
Xuzhou	-	-	-	-	-	-	-	-
Taiyuan	×	×	×	×	-	-	-	×
Huzhou	×	×	×	-	×	×	×	×
Shenyang	-	-	-	-	×	×	×	×
Yangzhou	-	-	-	-	×	×	×	×
Suqian	-	-	-	-	×	×	×	×
Nantong	×	×	×	-	×	×	×	×
Changchun	-	×	×	×	-	-	-	-

Nanchang	-	-	-	×	×	×	×	×
Jinghua	×	×	×	-	×	×	×	×
Lianyungang	-	×	×	-	×	-	×	×
Lanzhou	×	×	-	×	×	×	×	×
Suzhou	-	-	-	×	-	×	-	×
Jiaxing	×	×	-	-	×	-	×	×
Quzhou	×	×	-	×	×	×	×	×
Shaoxing	×	×	×	×	-	-	-	-
Hangzhou	×	×	×	×	×	×	×	×
Qinghuangdao	-	×	×	×	×	×	×	×
Chongqing	-	-	-	-	×	×	×	×
Xining	×	×	-	×	-	-	-	-
Qingdao	-	-	-	-	×	×	×	×
Shanghai	×	×	×	-	×	×	×	×
Huhehaote	-	×	×	×	×	×	×	×
Wenzhou	×	×	-	-	×	×	×	×
Nanning	×	×	×	×	-	-	-	-
Taizhou	-	-	-	-	-	×	-	×
Guangzhou	×	-	-	×	×	-	×	×
Chende	×	×	×	-	-	-	-	-
Dalian	×	×	×	×	-	-	-	-
Guiyang	-	×	-	-	-	-	-	-
Lishui	×	×	-	-	×	×	×	×
Yinchuan	×	-	×	×	×	×	×	×
Shenzhen	×	-	-	×	×	×	×	×
Zhuhai	×	×	×	×	×	×	×	×
Kunming	×	×	×	×	-	-	-	-
Fuzhou	×	×	×	×	×	×	×	×
Zhoushan	×	×	×	×	×	×	×	×
Lasa	×	×	×	×	×	×	×	×
Haikou	×	-	×	-	×	×	×	×

Table S4. MNB and MNE of the ensemble predictions in different regions of China using the monthly average predictions and observations of $PM_{2.5}$ and O_3-1h; and MNB, MNE and the weighting factors (w) of each set of predictions using different inventories. The best performance is indicated by the bold numbers.

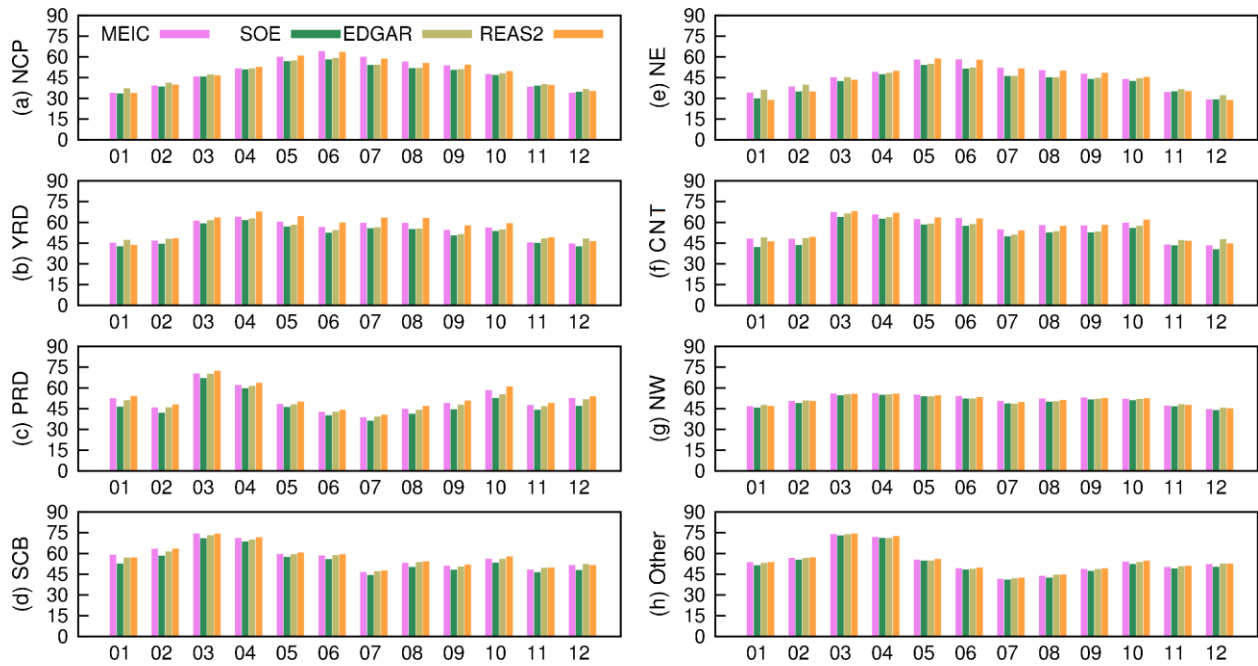|		MEIC			SOE			EDGAR			REAS2			ENSEMBLE	
		w	MFB	MFE	w	MFB	MFE	w	MFB	MFE	w	MFB	MFE	MNB	MNE
$PM_{2.5}$	NE	0.12	-0.22	0.32	0.40	0.25	0.44	0.00	-0.32	0.35	0.41	-0.14	0.32	**-0.05**	**0.31**
	NCP	0.00	-0.28	0.34	0.26	-0.33	0.36	0.00	-0.41	0.43	0.98	-0.21	0.27	**-0.05**	**0.23**
	NW	0.00	-0.87	0.87	0.53	-0.81	0.82	0.30	-0.85	0.85	1.00	-0.82	0.82	**-0.47**	**0.56**
	YRD	0.08	-0.25	0.31	0.01	-0.23	0.29	0.54	-0.20	0.27	0.48	-0.09	0.24	**-0.06**	**0.23**
	CNT	0.50	-0.09	0.27	0.11	**-0.04**	0.24	0.00	-0.25	0.28	0.35	0.09	0.28	-0.06	**0.20**
	SCB	0.00	0.11	0.28	0.66	0.25	0.30	0.00	-0.10	0.26	0.08	**0.08**	0.29	-0.11	**0.24**
	SOUTH	0.00	-0.29	0.36	0.00	-0.14	0.24	0.47	-0.02	0.28	0.65	-0.21	0.27	**-0.02**	**0.21**
	CHINA	0.13	-0.32	0.39	0.16	-0.25	0.37	0.23	-0.32	0.39	0.63	-0.21	0.33	**-0.12**	**0.31**
		w	MNB	MNE	w	MNB	MNE	w	MNB	MNE	w	MNB	MNE	MNB	MNE
O_3-1h	NE	0.08	0.35	0.35	0.00	0.11	0.20	0.56	0.31	0.32	0.17	0.32	0.34	**0.06**	**0.18**
	NCP	0.73	0.16	0.21	0.00	0.09	0.19	0.02	0.22	0.27	0.15	0.25	0.28	**0.06**	**0.16**
	NW	0.00	0.50	0.53	0.81	0.41	0.45	0.00	0.53	0.57	0.00	0.51	0.54	**0.14**	**0.29**
	YRD	0.11	0.08	0.21	0.92	**0.02**	**0.19**	0.00	0.09	0.23	0.00	0.15	0.24	0.06	0.20
	CNT	0.42	0.19	0.33	0.00	0.10	0.30	0.00	0.23	0.38	0.48	0.24	0.37	**0.10**	**0.29**
	SCB	0.82	0.44	0.49	0.00	0.29	0.39	0.00	0.44	0.50	0.00	0.43	0.51	**0.19**	**0.33**
	SOUTH	0.83	0.24	0.31	0.00	0.15	0.29	0.00	0.21	0.32	0.00	0.26	0.34	**0.03**	**0.21**
	CHINA	0.27	0.20	0.28	0.06	0.11	0.25	0.00	0.22	0.32	0.55	0.26	0.32	**0.09**	**0.23**

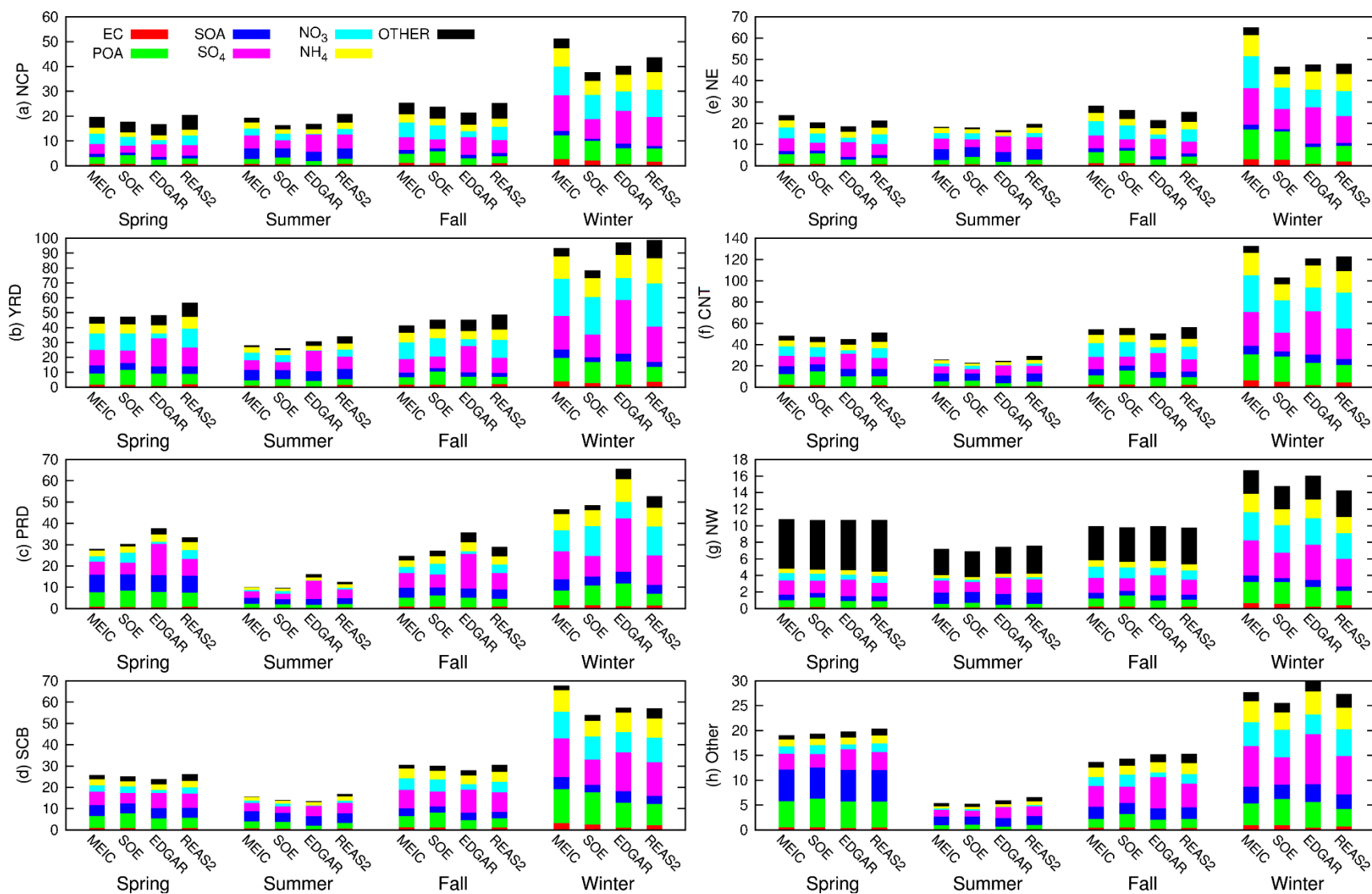Figure S1. Comparison of predicted O$_3$-1h concentration in different months in different regions.

Figure S2. Comparison of predicted PM$_{2.5}$ component concentrations in different seasons in different regions.
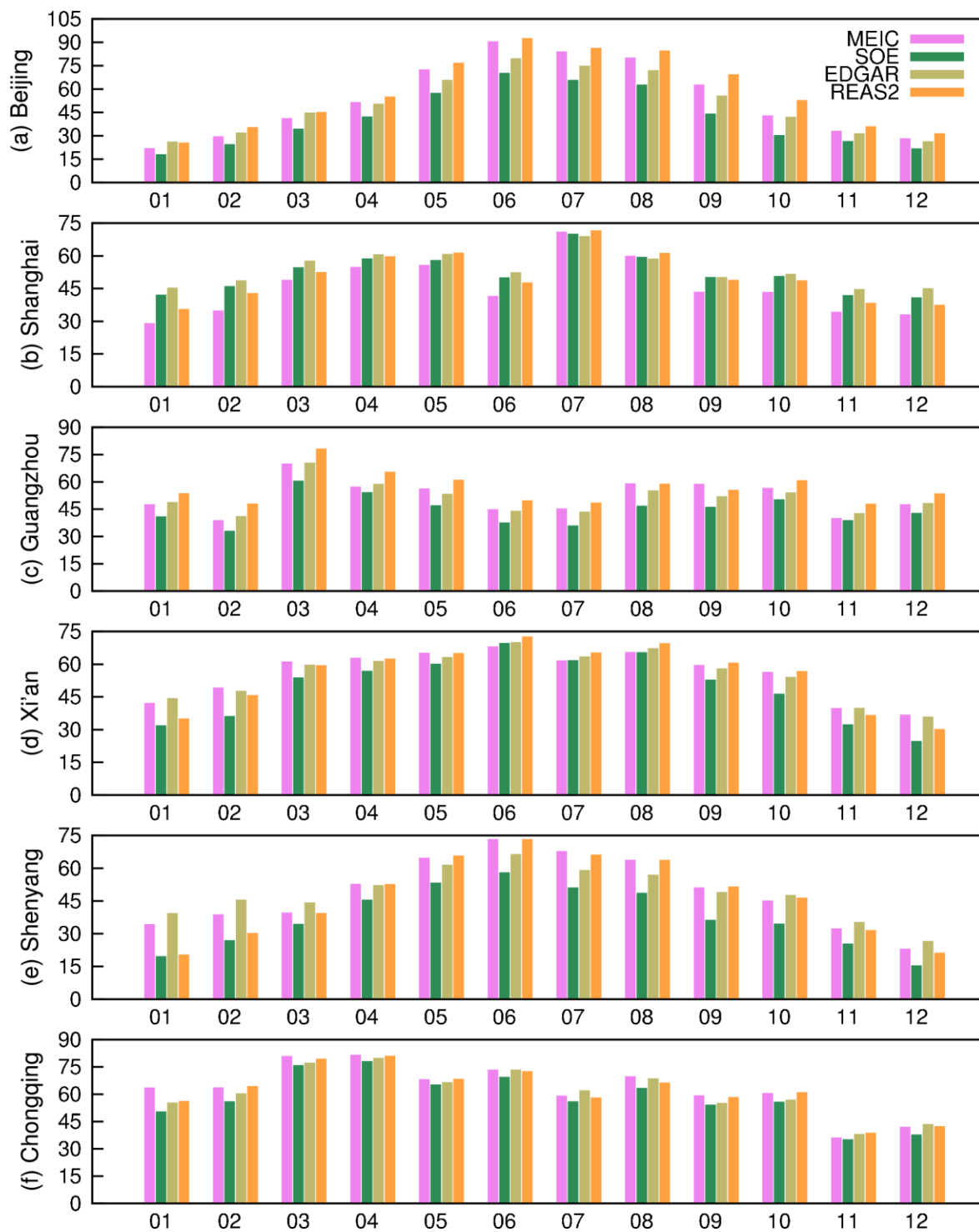
Figure S3. Comparison of predicted O$_3$-1h concentration in different months in 6 major cities: Beijing in NCP, Shanghai in YRD, Guangzhou in PRD, Xi'an in NW, Chongqing in SCB, and Shenyang in NE.
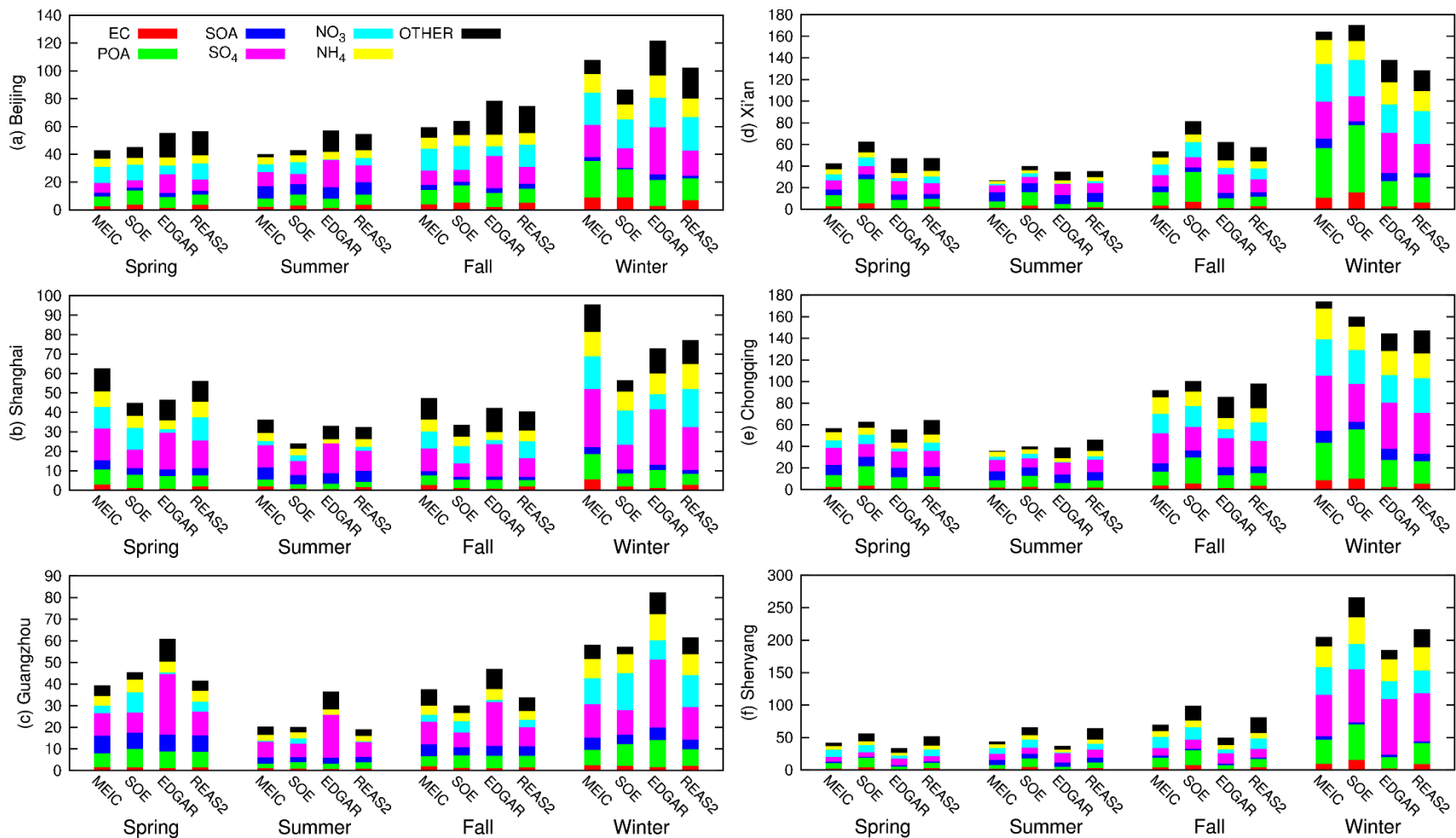
Figure S4. Comparison of predicted PM$_{2.5}$ component concentrations in different seasons in 6 major cities: Beijing in NCP, Shanghai in YRD, Guangzhou in PRD, Xi'an in NW, Chongqing in SCB, and Shenyang in NE.