SUPPORTING INFORMATION FOR

A quantitative decoupling analysis (QDA v1.0) method for assessing the contributions of meteorology, emissions, and chemistry to fine particulate pollution

Text S1 Model Performance Evaluation

To assess the accuracy of the model, simulated meteorological parameters and air pollutant concentrations were compared with observed values. We use several evaluation indicators to quantitatively assess model performance, including Simulated average (MM), Observed average (OM), correlation coefficient (R), mean fractional bias (MFB), mean deviation (MB), standard mean deviation (NMB), standard mean error (NME), root-mean-square error (RMSE), and index of agreement (IOA), which are defined in Table S1.

Tables

Table S1. Equations of model evaluation metrics

Metrics	Mathematical Expression	Range
Simulated mean (MM)	$MM = \frac{\sum_{i=1}^{N} M_i}{N}$	$[-\infty,+\infty]$
Observed mean (OM)	$OM = \frac{\sum_{i=1}^{N} O_i}{N}$	$[-\infty,+\infty]$
Correlation coefficient (R)	$R = \frac{\sum_{i=1}^{N}(M_i - MM)(O_i - OM)}{\sqrt{\sum_{i=1}^{N}(M_i - MM)^2}\sqrt{\sum_{i=1}^{N}(O_i - OM)^2}}$	$[-1,1]$
Mean Bias (MB)	$MB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{N}$	$[-\infty,+\infty]$
Mean Error (MEr)	$MEr = \frac{\sum_{i=1}^{N}\lvert M_i - O_i\rvert}{N}$	$[0,+\infty]$
Normalized Mean Bias (NMB)	$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i}$	$[-1,+\infty]$
Normalized Mean Error (NME)	$NME = \frac{\sum_{i=1}^{N}\lvert M_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$	$[0,+\infty]$
Mean Fractional Bias (MFB)	$MFB = \frac{1}{N}\sum \frac{M_i - O_i}{(M_i + O_i)/2} \times 100\%$	$[-200\%,200\%]$
Mean Fractional Error (MFE)	$MFE = \frac{1}{N}\sum \frac{\lvert M_i - O_i\rvert}{(M_i + O_i)/2} \times 100\%$	$[0,200\%]$
Root Mean Square Error (RMSE)	$RMSE = \sqrt{\frac{\sum(M_i - O_i)^2}{N}}$	$[0,+\infty]$
Index of Agreement (IOA)	$IOA = \begin{cases} 1 - \frac{\sum\lvert M_i - O_i\rvert}{2\sum\lvert O_i - OM\rvert} & ,\sum\lvert M_i - O_i\rvert \le 2\sum\lvert O_i - OM\rvert \\ \frac{2\sum\lvert O_i - OM\rvert}{\sum\lvert M_i - O_i\rvert} - 1 & ,\sum\lvert M_i - O_i\rvert > 2\sum\lvert O_i - OM\rvert \end{cases}$	$[-1,1]$

N: the number of modeled and observed data pairs; M_i: modeled concentration at time i; O_i: observed concentration at time i;

Table S2. Evaluation results for simulated meteorological elements, precursor gas concentration and chemical components against observations in Beijing

Meteorological Elements	**OM**	**SD OBS**	**MM**	**SD MOD**	**R**	**MB**	**NMB**	**NME**	**MEr**	**MFB(%)**	**MFE(%)**	**RSME**	**IOA**
Ideal value	-	-	-	-	1	0	0	0	0	0	0	0	1
Temp(°C)	0.45	3.86	-0.83	3.88	0.93**	-1.25	-2.86	3.22	1.44	-14.21	8.00	1.81	0.77
WS(m/s)	1.74	0.99	2.39	1.33	0.47**	0.65	0.37	0.62	1.08	26.10	54.97	1.40	0.26
WD(°)	121.84	86.74	170.71	94.17	0.24**	49.12	0.40	0.70	84.73	27.25	64.84	123.93	0.42
RH(%)	65.04	17.54	62.09	15.03	0.85**	-1.10	-0.02	0.11	6.34	-0.08	11.80	8.27	0.78
Pressure(hPa)	1025	3.59	1025	3.05	0.93**	-0.07	-7e-05	0.001	1.07	-0.01	0.10	1.30	0.81
Precursor Gases													
NO_2(μg/m^3)	81.66	30.96	70.54	29.81	0.71**	-12.43	-0.15	0.23	19.04	-18.67	27.80	26.33	0.61
SO_2(μg/m^3)	68.55	42.19	46.58	20.86	0.76**	-23.21	-0.34	0.38	26.08	-23.78	10.20	33.64	0.63
$PM_{2.5}$ and its Chemical Component													
$PM_{2.5}$(μg/m^3)	168.93	105.96	171.62	107.40	0.83**	-13.01	-0.08	0.23	39.17	-4.35	25.76	60.38	0.79
NH_4^+(μg/m^3)	32.15	17.13	43.72	27.42	0.89**	18.14	0.56	0.63	20.22	30.03	39.11	27.82	0.29
SO_4^{2-}(μg/m^3)	43.19	24.00	17.91	12.90	0.82**	-23.28	-0.54	0.54	22.29	-59.42	59.42	27.46	0.41
NO_3^-(μg/m^3)	54.65	32.31	63.77	38.94	0.92**	19.17	0.35	0.42	22.95	22.45	33.74	32.15	0.58
OC(μg/m^3)	36.83	17.69	31.53	15.85	0.90**	-4.02	-0.10	0.16	6.06	-11.17	18.16	8.36	0.77

Note: MM: averaged model results; OM: averaged observations; SD: standard deviation; R is the Spearman correlation coefficient, ** denotes significant correlation at the 0.01 level, * denotes significant correlation at the 0.05 level

Figures

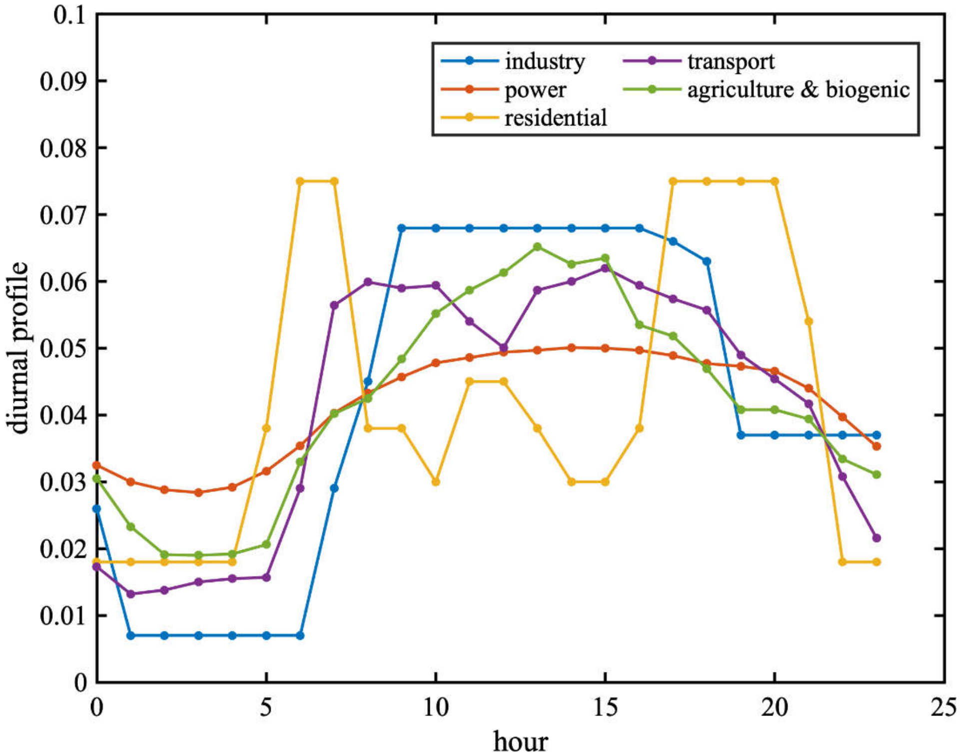

Figure S1. The diurnal profile of emissions from different sectors obtained from the MIX inventory used in MICS-Asia III (Li et al., 2017), which generally shows higher emissions during the daytime than the nighttime. The transport and residential emission also show a double-peak pattern in their diurnal profile.

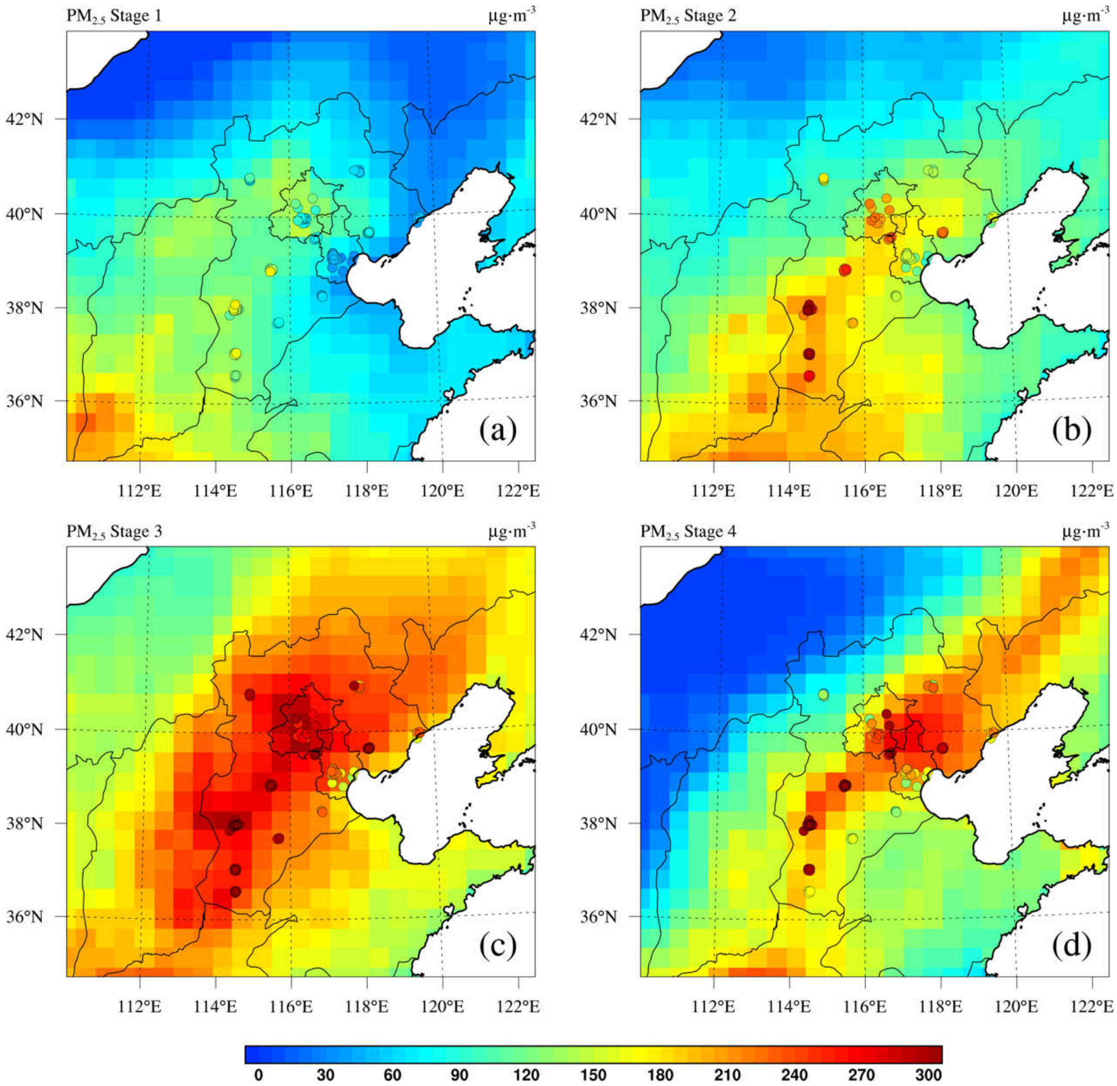

Figure S2. Evaluation of simulated $PM_{2.5}$ concentrations against ground-based observations over Beijing-Tianjin-Hebei Region during (a) precontamination, (b) accumulation, (c) maintenance and (d) removal stages.

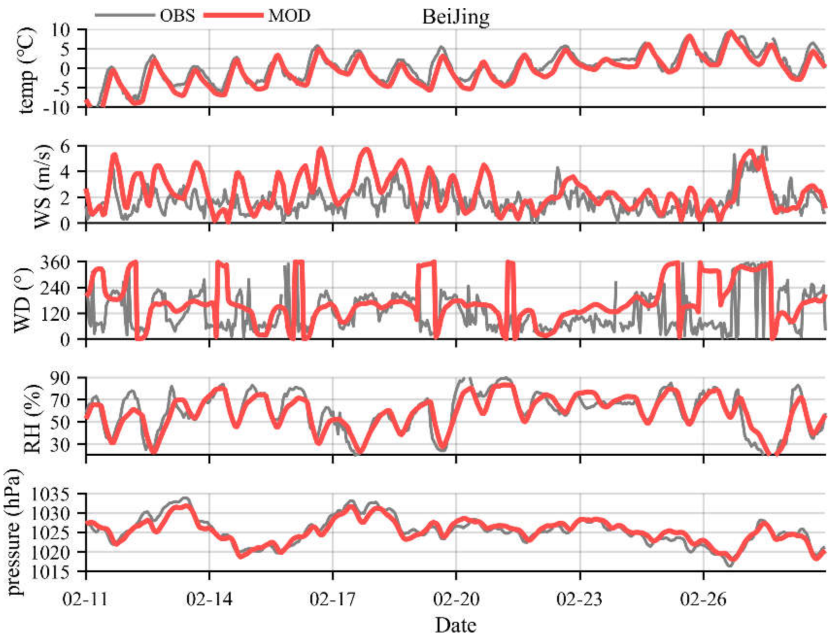

Figure S3. Comparisons of observed (grey lines) and simulated (red lines) values of different meteorology elements in Beijing from 11th Feb to 28th Feb 2014.

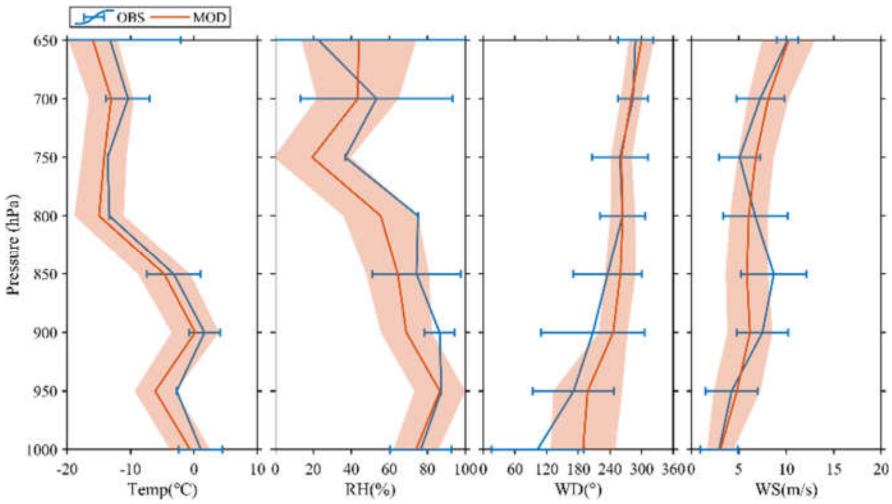

Figure S4. Comparisons of simulated and observed values of meteorological elements in Beijing in February 2014.

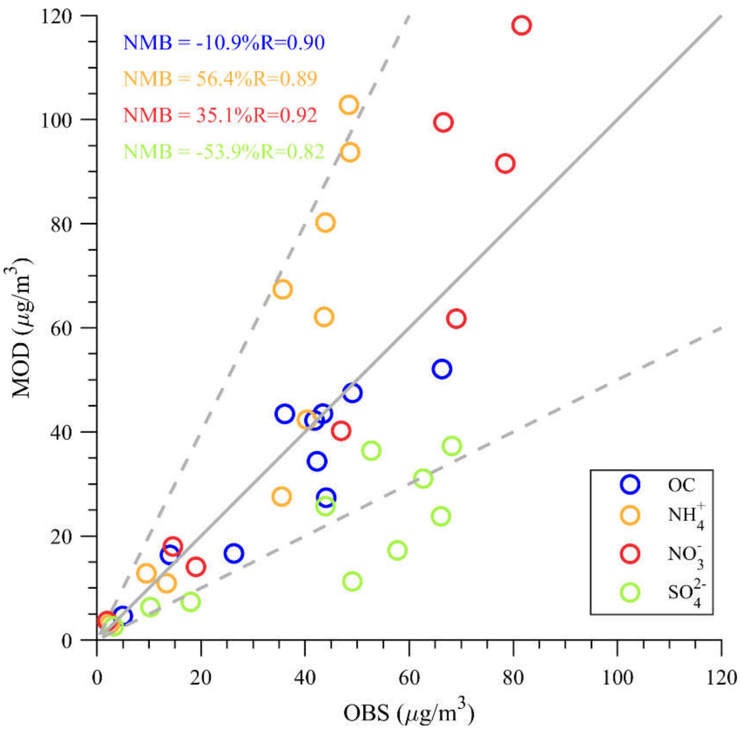

Figure S5. Evaluation of simulated $PM_{2.5}$ chemical composition concentrations against ground-based observations. The solid line corresponds to the 1:1 line, and the dashed lines correspond to the 1:2 and 2:1 line.

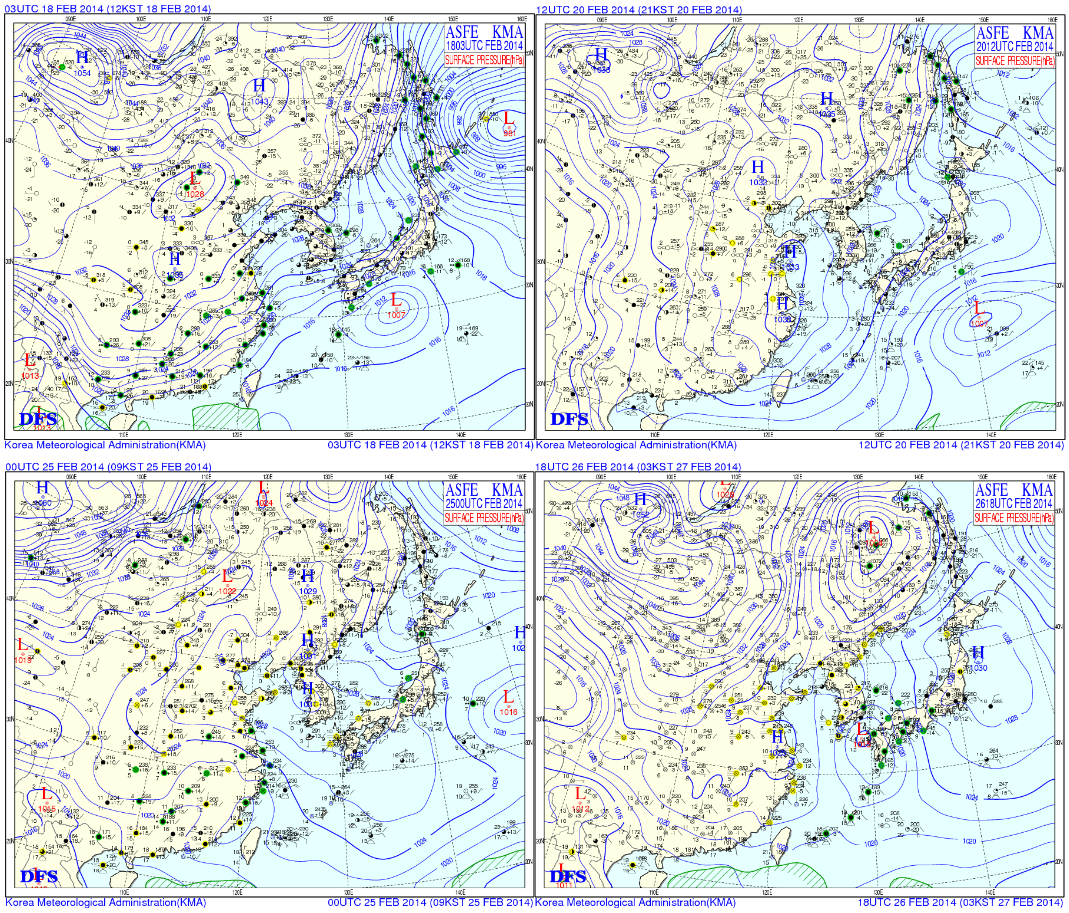

Figure S6. Surface weather chart at different stages of pollution（February 18th 03:00 UTC stands for the stage 1, February 20th 12:00 UTC stands for the stage 2, February 25th 00:00 UTC stands for the stage 3, and February 26th 18:00 UTC stands for the stage 4.）

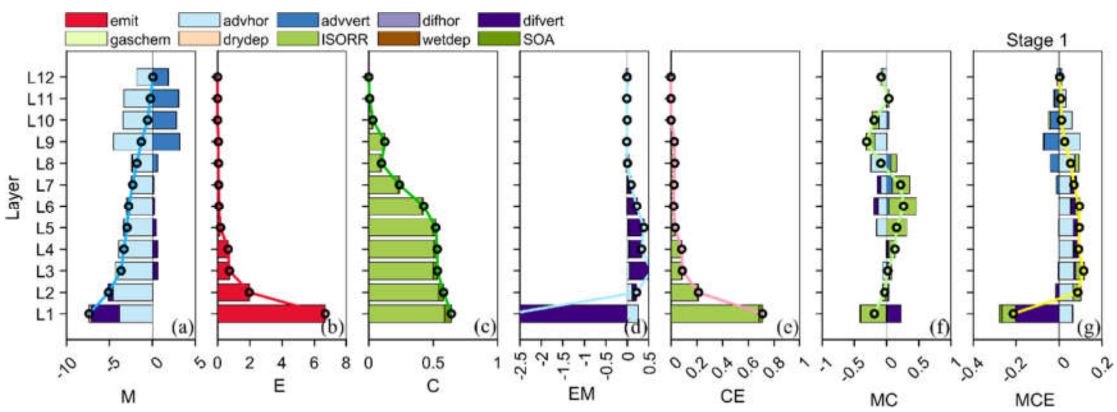

Figure S7. QDA results as well as process analysis results at different vertical layers of model in stage 1.

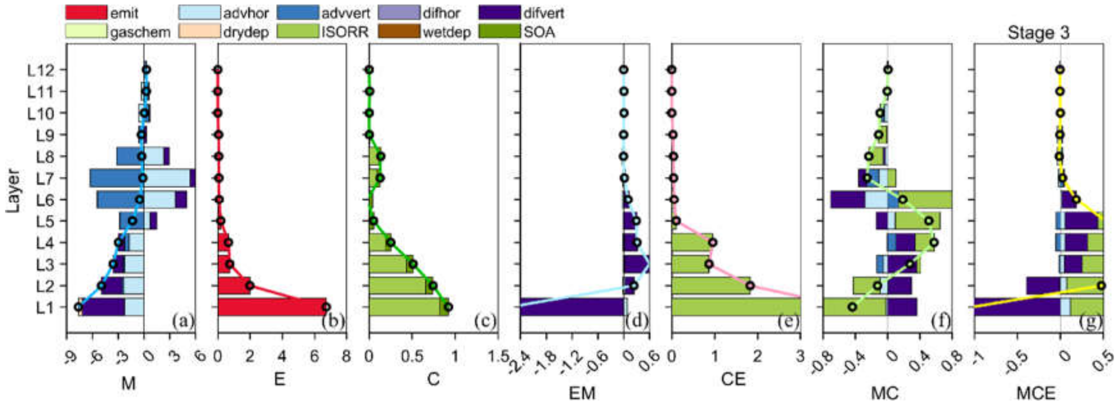

Figure S8. Same as Fig.S8 but for stage 3.

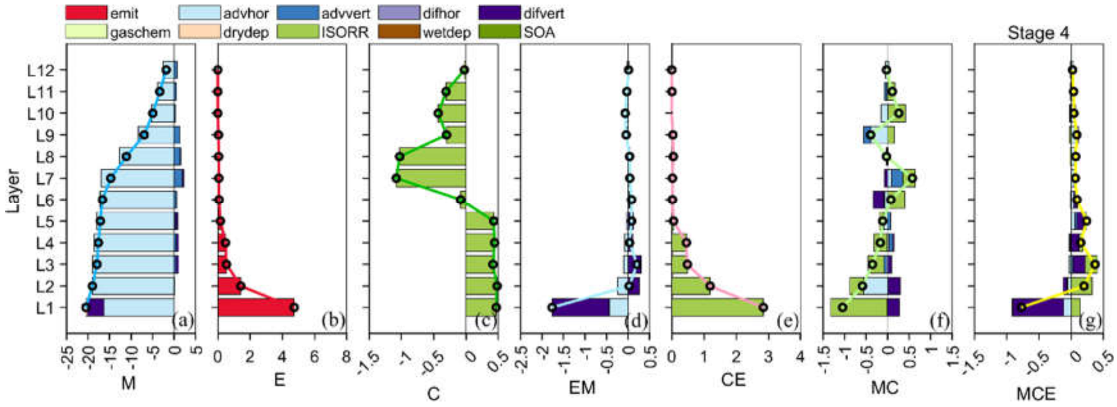

Figure S9. Same as Fig.S8 but for stage 4.

Reference

Li, M., Zhang, Q., Kurokawa, J. I., Woo, J. H., He, K., Lu, Z., Ohara, T., Song, Y., Streets, D. G., Carmichael, G. R., Cheng, Y., Hong, C., Huo, H., Jiang, X., Kang, S., Liu, F., Su, H., and Zheng, B.: MIX: a mosaic Asian anthropogenic emission inventory under the international collaboration framework of the MICS-Asia and HTAP, Atmos. Chem. Phys., 17, 935-963, 10.5194/acp-17-935-2017, 2017.