*Supplement of*

# Sources of organic aerosols in east China: A modeling study with high-resolution intermediate-volatility and semi-volatile organic compound emissions

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**Table S1.** Gas-phase I/SVOCs-to-VOCs ratios for specific sources and emission profiles used in CMAQ simulations.

| Source | | I/SVOCs-G to VOCs | Volatility (C* at 298 K, μg·m$^{-3}$) | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | IVOCP6 | IVOCP5 | IVOCP4 | IVOCP3 | SVOCP2 | SVOCP1 | SVOCP0 | SVOCN1 | IVOCP6ARO | IVOCP5ARO |
| | | | $10^6$ | $10^5$ | $10^4$ | $10^3$ | $10^2$ | 10 | 1 | $10^{-1}$ | $10^6$ | $10^5$ |
| Industrial process | Oil refinery | 0.039 | 0.759 | 0.123 | 0.004 | 0.110 | 0.003 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Chemical production | 0.282 | 0.430 | 0.230 | 0.025 | 0.116 | 0.199 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Pulp and paper | 0.140 | 0.571 | 0.393 | 0.028 | 0.006 | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 |
| Industrial solvent-use | Textile | 2.473 | 0.041 | 0.448 | 0.182 | 0.268 | 0.040 | 0.002 | 0.019 | 0.000 | 0.000 | 0.000 |
| | Leather tanning | 0.231 | 1.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Timber processing | 0.119 | 0.584 | 0.416 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Furniture coating | 0.021 | 0.888 | 0.112 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Solvent-based coating | 0.177 | 0.948 | 0.044 | 0.008 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Water-based coating | 0.504 | 0.096 | 0.893 | 0.011 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Dry cleaning | 0.004 | 0.885 | 0.115 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Paint remover | 0.072 | 0.987 | 0.010 | 0.004 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| Mobile sources | Gasoline vehicle | 0.106 | 0.206 | 0.056 | 0.113 | 0.098 | 0.000 | 0.000 | 0.000 | 0.000 | 0.406 | 0.121 |
| | Diesel vehicle | 1.358 | 0.331 | 0.318 | 0.244 | 0.095 | 0.000 | 0.000 | 0.000 | 0.000 | 0.004 | 0.007 |
| | Fuel evaporation | 0.002 | 0.841 | 0.159 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Diesel machinery[a] | 0.400 | 0.282 | 0.279 | 0.264 | 0.102 | 0.057 | 0.012 | 0.003 | 0.000 | 0.000 | 0.000 |
| | Marine vessel[b] | 0.300 | 0.230 | 0.375 | 0.193 | 0.097 | 0.029 | 0.000 | 0.000 | 0.000 | 0.077 | 0.000 |
| | Aircraft | 0.482 | 0.761 | 0.148 | 0.063 | 0.028 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| Residential sources | Coal combustion[c] | 0.180 | 0.439 | 0.439 | 0.088 | 0.035 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | Residential solvent-use | 0.240 | 0.938 | 0.047 | 0.003 | 0.007 | 0.000 | 0.003 | 0.000 | 0.001 | 0.000 | 0.000 |
| | Cooking | 0.036 | 0.554 | 0.374 | 0.052 | 0.015 | 0.003 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 |
| Agriculture sources | Biomass burning | 0.006 | 1.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |

[a] Qi et al. (2019); [b] Huang et al. (2018); [c] Cai et al. (2019)

**Table S2.** Particle-phase I/SVOCs-to-POA ratios for specific sources and emission profiles used in CMAQ simulations.

| Source | | I/SVOCs-P to POA | Volatility (C* at 298 K, μg·m$^{-3}$) | | | | |
|---|---|---|---|---|---|---|---|
| | | | IVOCP3 | SVOCP2 | SVOCP1 | SVOCP0 | SVOCN1 |
| | | | $10^3$ | $10^2$ | 10 | 1 | $10^{-1}$ |
| Mobile sources | Gasoline vehicle | 0.901 | 0.000 | 0.323 | 0.406 | 0.073 | 0.197 |
| | Diesel vehicle | 0.867 | 0.000 | 0.419 | 0.420 | 0.099 | 0.063 |
| | Diesel machinery[a] | 0.420 | 0.455 | 0.204 | 0.123 | 0.131 | 0.087 |
| | Marine vessel[b] | 0.570 | 0.636 | 0.156 | 0.083 | 0.074 | 0.052 |
| Residential sources | Cooking | 0.830 | 0.670 | 0.157 | 0.003 | 0.000 | 0.000 |
| Agriculture sources | Biomass burning | 0.155 | 0.283 | 0.140 | 0.069 | 0.045 | 0.305 |

[a] Qi et al. (2019); [b] Huang et al. (2018)

**Table S3.** Source-specific emissions of VOCs and POA for the year 2017 in the Yangtze River Delta region.

| Source | | VOCs | | POA | |
|---|---|---|---|---|---|
| | | kt | % | kt | % |
| Industrial process | Oil refinery | 146.07 | 3.50 | 1.49 | 0.74 |
| | Chemical production | 864.99 | 20.70 | 1.65 | 0.82 |
| | Pulp and paper | 0.80 | 0.02 | 0.01 | 0.00 |
| Industrial solvent-use | Textile | 92.90 | 2.22 | 0.11 | 0.06 |
| | Leather tanning | 16.56 | 0.40 | 0.02 | 0.01 |
| | Timber processing | 262.17 | 6.27 | 0.10 | 0.05 |
| | Furniture coating | 62.98 | 1.51 | 0.00 | 0.00 |
| | Solvent-based coating | 978.81 | 23.42 | 1.80 | 0.89 |
| | Water-based coating | 99.80 | 2.39 | 0.00 | 0.00 |
| | Dry cleaning | 5.49 | 0.13 | 0.00 | 0.00 |
| | Paint remover | 0.07 | 0.00 | 0.00 | 0.00 |
| Mobile source | Gasoline vehicle | 575.15 | 13.76 | 9.37 | 4.64 |
| | Diesel vehicles | 87.96 | 2.10 | 28.03 | 13.90 |
| | Fuel evaporation | 356.44 | 8.53 | 0.00 | 0.00 |
| | Diesel machinery | 111.80 | 2.68 | 11.66 | 5.78 |
| | Marine vessel | 7.77 | 0.19 | 10.23 | 5.07 |
| | Aircraft | 1.32 | 0.03 | 0.00 | 0.00 |
| Residential source | Coal combustion | 15.14 | 0.36 | 6.42 | 3.18 |
| | Residential solvent-use | 146.77 | 3.51 | 0.00 | 0.00 |
| | Cooking | 223.59 | 5.35 | 82.85 | 41.07 |
| Agriculture source | Biomass burning | 122.13 | 2.92 | 47.96 | 23.78 |
| Total anthropogenic emissions | | 4178.70 | 100.00 | 201.70 | 100.00 |
| Total biogenic emissions | | 2004.7 | / | / | / |

**Table S4.** Parameterization scheme and inputs for the WRF model.

| Option | Configuration/Data source |
|---|---|
| Version | WRF-v3.9.1 |
| IC/BC condition | NCEP FNL1°×1° |
| Microphysical Process | Purdue Lin Scheme |
| Cumulus Convective Scheme | Grell-3 Scheme |
| Road Process Scheme | Noah Scheme |
| Boundary Layer Scheme | Yonsei University (YSU) Scheme |
| Long-wave and Short-wave radiation scheme | RRTM and Goddard radiation Scheme |

**Table S5.** The statistical results of model performance for the meteorological parameters in each season (MB: mean bias; MGE: mean gross error; RMSE: root-mean-square error; IOA: index of agreement).

| Parameters* | Seasons | MB | Criteria | MGE | Criteria | RMSE | Criteria | IOA (-) | Criteria |
|---|---|---|---|---|---|---|---|---|---|
| Temperature (K) | Spr | 0.2 | ≤ +0.5 | 1.46 | ≤ 2 | 2.0 | - | 0.96 | ≥ 0.8 |
| | Sum | -1.5 | | 2.26 | | 2.9 | | 0.80 | |
| | Aut | 0.5 | | 1.49 | | 2.4 | | 0.89 | |
| | Win | 1.4 | | 1.87 | | 2.5 | | 0.94 | |
| Humidity (%) | Spr | -8.0 | - | 11.03 | - | 15.7 | - | 0.85 | ≥ 0.6 |
| | Sum | -2.8 | | 7.82 | | 13.2 | | 0.80 | |
| | Aut | -10.9 | | 11.79 | | 16.9 | | 0.82 | |
| | Win | -12.2 | | 13.71 | | 19.6 | | 0.73 | |
| Wind speed ($m \cdot s^{-1}$) | Spr | 0.5 | ≤ +0.5 | 1.28 | - | 1.7 | ≤ 2 | 0.77 | ≥ 0.6 |
| | Sum | 0.2 | | 1.15 | | 1.5 | | 0.75 | |
| | Aut | 0.6 | | 1.14 | | 1.5 | | 0.75 | |
| | Win | 0.9 | | 1.50 | | 1.9 | | 0.75 | |
| Wind direction (°) | Spr | 2.6 | ≤ +10 | 31.52 | ≤ 30 | 46.7 | - | 0.93 | - |
| | Sum | 1.6 | | 31.31 | | 46.0 | | 0.91 | |
| | Aut | 10.3 | | 28.29 | | 42.9 | | 0.96 | |
| | Win | 8.1 | | 26.65 | | 41.2 | | 0.97 | |

*The units in the brackets are only for MB, MGE and RMSE. IOA is unitless.

**Table S6.** The statistical results of model performance for major air pollutants in each season. (MB: mean bias; MGE: mean gross error; RMSE: root-mean-square error; MFB: mean fractional bias; MFE: mean fractional error; IOA: index of agreement)

| Species | Scenario | Seasons | MB ($\mu g \cdot m^{-3}$) | MGE ($\mu g \cdot m^{-3}$) | RMSE ($\mu g \cdot m^{-3}$) | MFB (%) | MFE (%) |
|---|---|---|---|---|---|---|---|
| $SO_2$ | IMPROVE | Spr | 8.0 | 11.0 | 21.9 | 33 | 70 |
| | | Sum | 5.9 | 9.6 | 20.5 | 15 | 80 |
| | | Aut | 9.9 | 12.5 | 23.2 | 43 | 73 |
| | | Win | 11.4 | 14.2 | 25.0 | 44 | 74 |
| $NO_2$ | IMPROVE | Spr | -8.3 | 18.4 | 26.2 | -37 | 61 |
| | | Sum | 5.1 | 13.7 | 21.9 | 7 | 57 |
| | | Aut | -7.1 | 17.0 | 23.1 | -29 | 53 |
| | | Win | -10.1 | 19.1 | 25.5 | -31 | 53 |
| $O_3$ | IMPROVE | Spr | 39.8 | 45.5 | 55.0 | 27 | 34 |
| | | Sum | 29.8 | 43.7 | 54.3 | 17 | 33 |
| | | Aut | 30.0 | 35.4 | 43.1 | 23 | 29 |
| | | Win | 19.1 | 32.5 | 43.4 | 14 | 31 |
| $PM_{2.5}$ | BASE | Spr | 2.3 | 19.6 | 27.4 | 5 | 46 |
| | | Sum | 6.1 | 13.6 | 20.2 | 18 | 52 |
| | | Aut | 9.7 | 21.3 | 31.2 | 19 | 49 |
| | | Win | 3.4 | 24.6 | 36.4 | 6 | 46 |
| | IMPROVE | Spr | 13.9 | 24.8 | 34.7 | 26 | 51 |
| | | Sum | 13.0 | 17.5 | 25.7 | 37 | 58 |
| | | Aut | 22.5 | 29.3 | 41.5 | 41 | 58 |
| | | Win | 14.1 | 29.3 | 43.7 | 21 | 49 |

**Table S6.** The statistical results of model performance for organic carbon (OC) in each season.

| Seasons | Sites | MB (μg·m$^{-3}$) | | MGE (μg·m$^{-3}$) | | RMSE (μg·m$^{-3}$) | | MFB (%) | | MFE (%) | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | BASE | IMPROVE | BASE | IMPROVE | BASE | IMPROVE | BASE | IMPROVE | BASE | IMPROVE |
| Spring | SAES | -5.0 | -3.2 | 5.0 | 3.2 | 28.8 | 14.0 | -80 | -48 | 80 | 48 |
| | Changzhou | -5.5 | -3.2 | 5.5 | 3.2 | 32.7 | 13.2 | -82 | -42 | 82 | 42 |
| | Dianshan Lake | -2.5 | -0.4 | 2.5 | 1.8 | 8.6 | 4.7 | -69 | -19 | 70 | 36 |
| | Chongming Dongtan | -2.5 | -1.2 | 2.5 | 1.3 | 7.1 | 2.7 | -88 | -44 | 88 | 45 |
| | Hefei | -4.2 | -3.1 | 4.2 | 3.1 | 20.2 | 13.4 | -79 | -52 | 79 | 52 |
| | Jinhua | -4.6 | -3.7 | 4.9 | 3.9 | 28.5 | 20.3 | -98 | -70 | 104 | 75 |
| | Qiandao Lake | -1.8 | -1.3 | 2.1 | 1.6 | 5.6 | 3.9 | -63 | -42 | 71 | 50 |
| | Jiaxing | -3.5 | -1.0 | 3.5 | 1.5 | 15.3 | 4.1 | -75 | -19 | 75 | 25 |
| Summer | SAES | -0.6 | 0.2 | 1.0 | 0.9 | 2.3 | 1.7 | -11 | 7 | 26 | 22 |
| | Changzhou | -4.6 | -3.3 | 4.6 | 3.3 | 24.8 | 14.7 | -81 | -53 | 81 | 54 |
| | Chongming Dongtan | -0.1 | 0.5 | 1.1 | 1.5 | 2.4 | 5.6 | -45 | -28 | 102 | 109 |
| | Jinhua | -2.2 | -1.5 | 2.2 | 2.0 | 6.6 | 5.4 | -67 | -46 | 68 | 56 |
| | Qiandao Lake | -1.0 | -0.5 | 1.5 | 1.6 | 3.3 | 3.6 | -48 | -27 | 63 | 57 |
| | Suzhou | -1.8 | -0.6 | 1.8 | 1.0 | 4.0 | 1.4 | -44 | -15 | 44 | 22 |
| | Jiaxing | -1.8 | -0.6 | 1.8 | 0.9 | 4.7 | 1.2 | -58 | -18 | 58 | 23 |
| Autumn | SAES | -1.6 | -0.3 | 2.0 | 1.8 | 4.9 | 4.8 | -45 | -18 | 50 | 38 |
| | Changzhou | -3.7 | -1.4 | 3.8 | 2.3 | 17.4 | 7.7 | -67 | -24 | 68 | 34 |
| | Dianshan Lake | -2.0 | -0.6 | 2.0 | 1.2 | 4.8 | 2.4 | -62 | -24 | 62 | 34 |
| | Chongming Dongtan | -1.6 | -1.0 | 1.6 | 1.1 | 2.8 | 1.7 | -104 | -66 | 104 | 69 |
| | Hefei | -3.2 | -0.9 | 3.2 | 1.6 | 12.4 | 3.8 | -71 | -23 | 71 | 34 |
| | Jinhua | -5.0 | -2.8 | 5.1 | 3.5 | 35.0 | 21.5 | -91 | -45 | 93 | 54 |
| | Nanjing | -0.4 | 1.6 | 0.9 | 1.8 | 1.3 | 7.0 | -11 | 23 | 20 | 28 |
| | Qiandao Lake | -0.9 | 1.0 | 1.3 | 2.1 | 2.6 | 7.2 | -36 | 10 | 50 | 54 |
| | Suzhou | -1.3 | 0.3 | 1.4 | 1.0 | 2.8 | 2.5 | -34 | 1 | 36 | 21 |
| | Jiaxing | -3.7 | -1.7 | 3.7 | 2.1 | 15.4 | 6.4 | -82 | -37 | 82 | 42 |
| Winter | SAES | -1.5 | -0.2 | 4.5 | 5.6 | 32.7 | 46.8 | -25 | -11 | 68 | 74 |
| | Changzhou | -4.3 | -1.9 | 4.3 | 2.5 | 25.4 | 10.5 | -63 | -25 | 63 | 31 |
| | Chongming | -2.7 | -2.0 | 2.7 | 2.1 | 10.3 | 5.6 | -125 | -101 | 125 | 103 |
| | Hefei | -3.9 | -1.8 | 3.9 | 1.9 | 18.5 | 5.9 | -69 | -31 | 69 | 33 |
| | Qiandao Lake | -2.6 | -1.2 | 2.6 | 1.7 | 9.6 | 5.1 | -91 | -48 | 91 | 57 |
| | Suzhou | -2.8 | -1.2 | 2.8 | 1.8 | 11.4 | 5.2 | -56 | -32 | 56 | 38 |
| | Jiaxing | -4.4 | -2.2 | 4.4 | 2.7 | 26.6 | 11.3 | -89 | -50 | 89 | 53 |

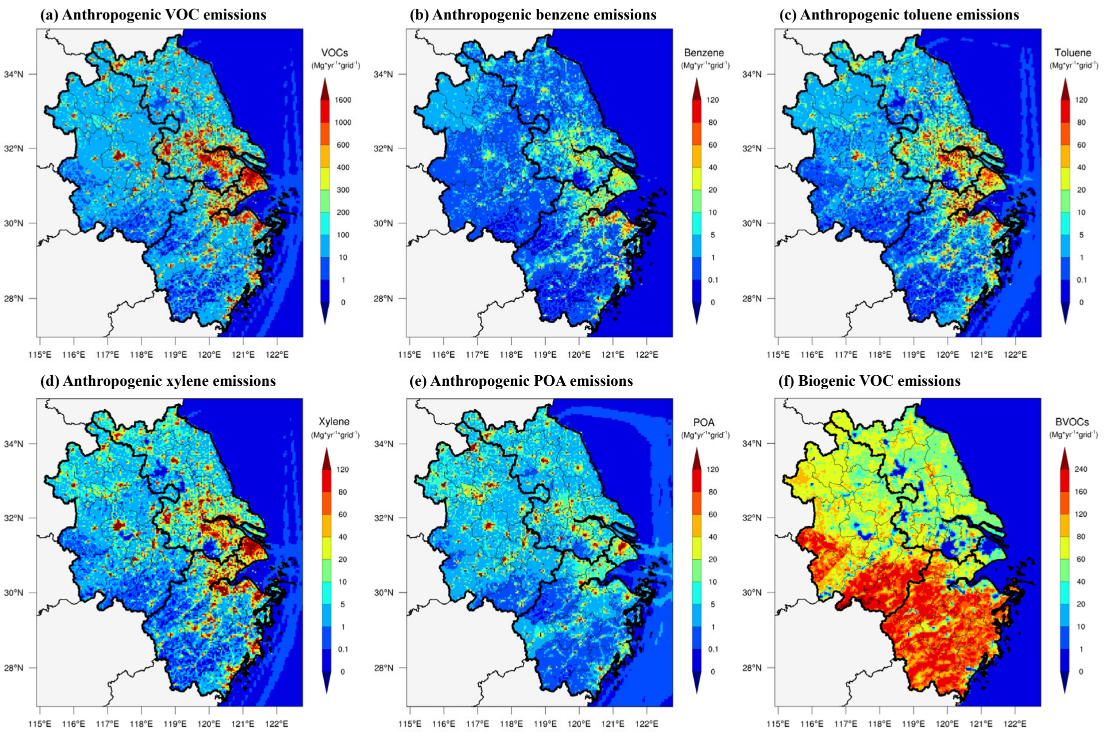


**Figure S1.** Spatial distribution of I/SVOC, POA, anthropogenic VOC (including benzene, toluene, and xylene), and biogenic VOC emissions in the YRD region for the year 2017.

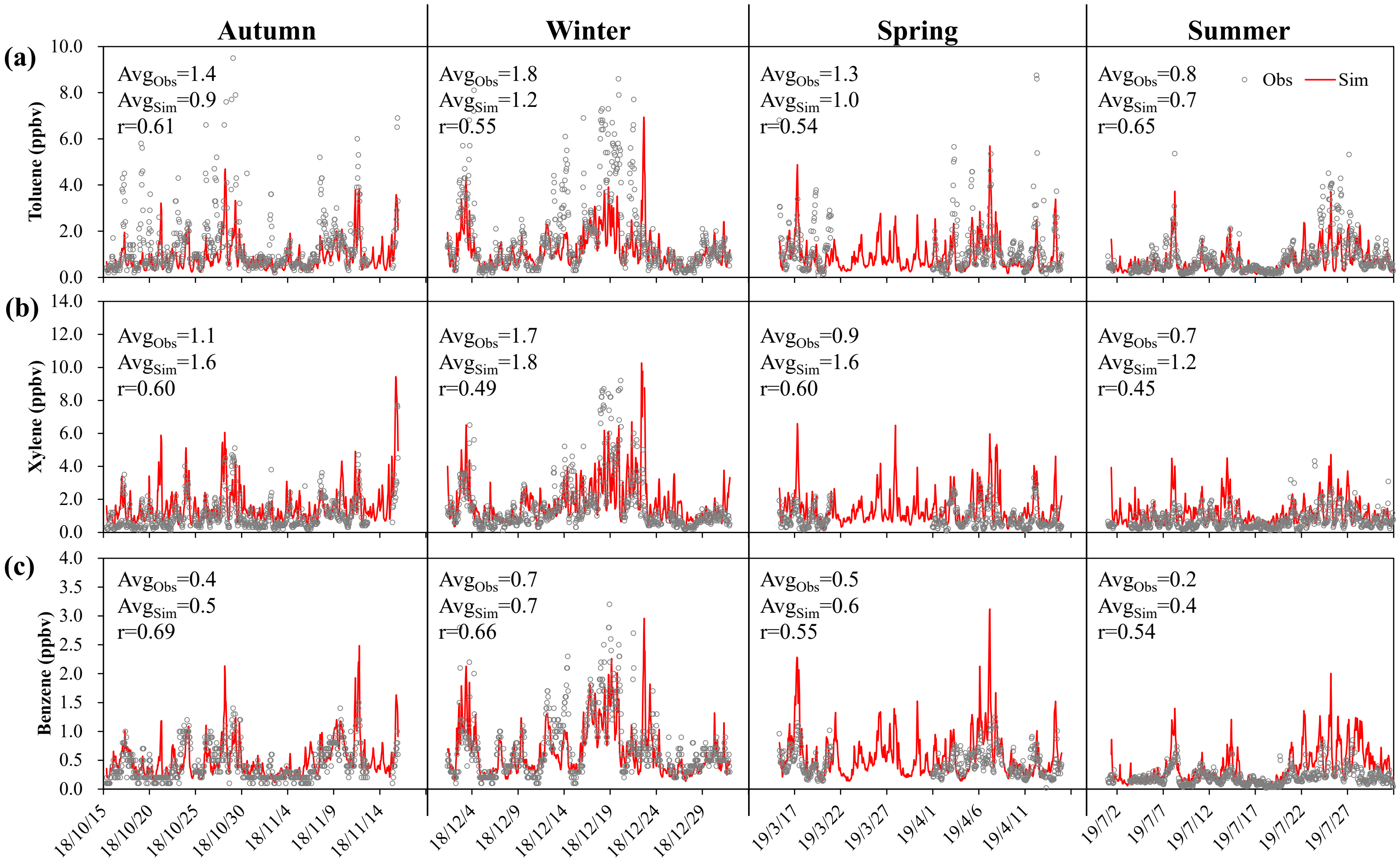


**Figure S2.** Comparisons of measured (black dots) and modeled (red lines) concentrations of (a) toluene, (b) xylene, and (c) benzene in different seasons at the SAES supersite in Shanghai.

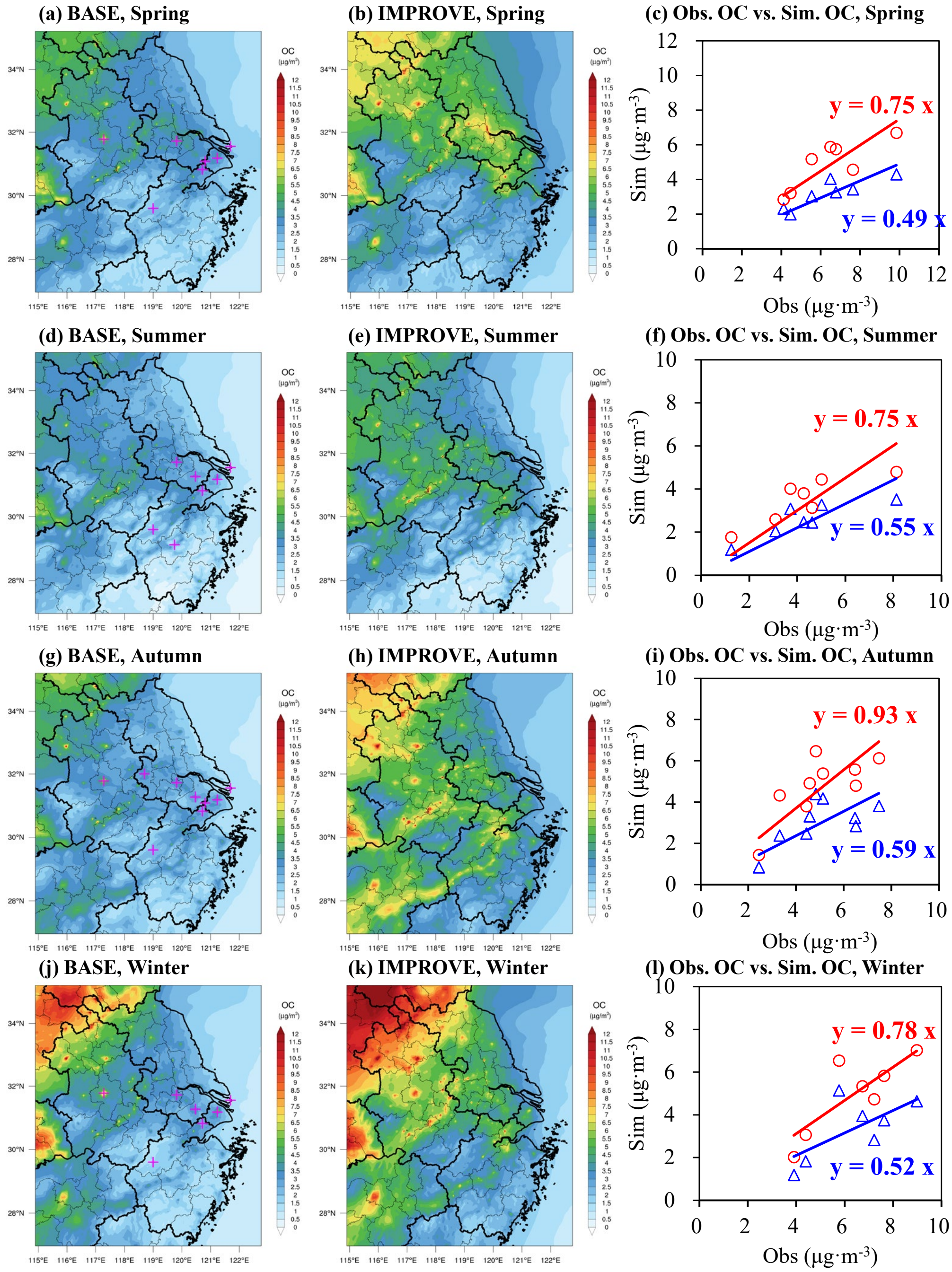


**Figure S3.** Spatial distributions of modeled OC concentrations in different seasons in BASE and IMPROVE simulations and their comparisons with OC observations. The blue triangle points represent the correlation between the modeled and observed OC in the BASE simulation, and the red dots represent the correlation between the modeled and observed OC in the IMPROVE simulation. The purple crosses in the left figures represent the observation sites of OC.

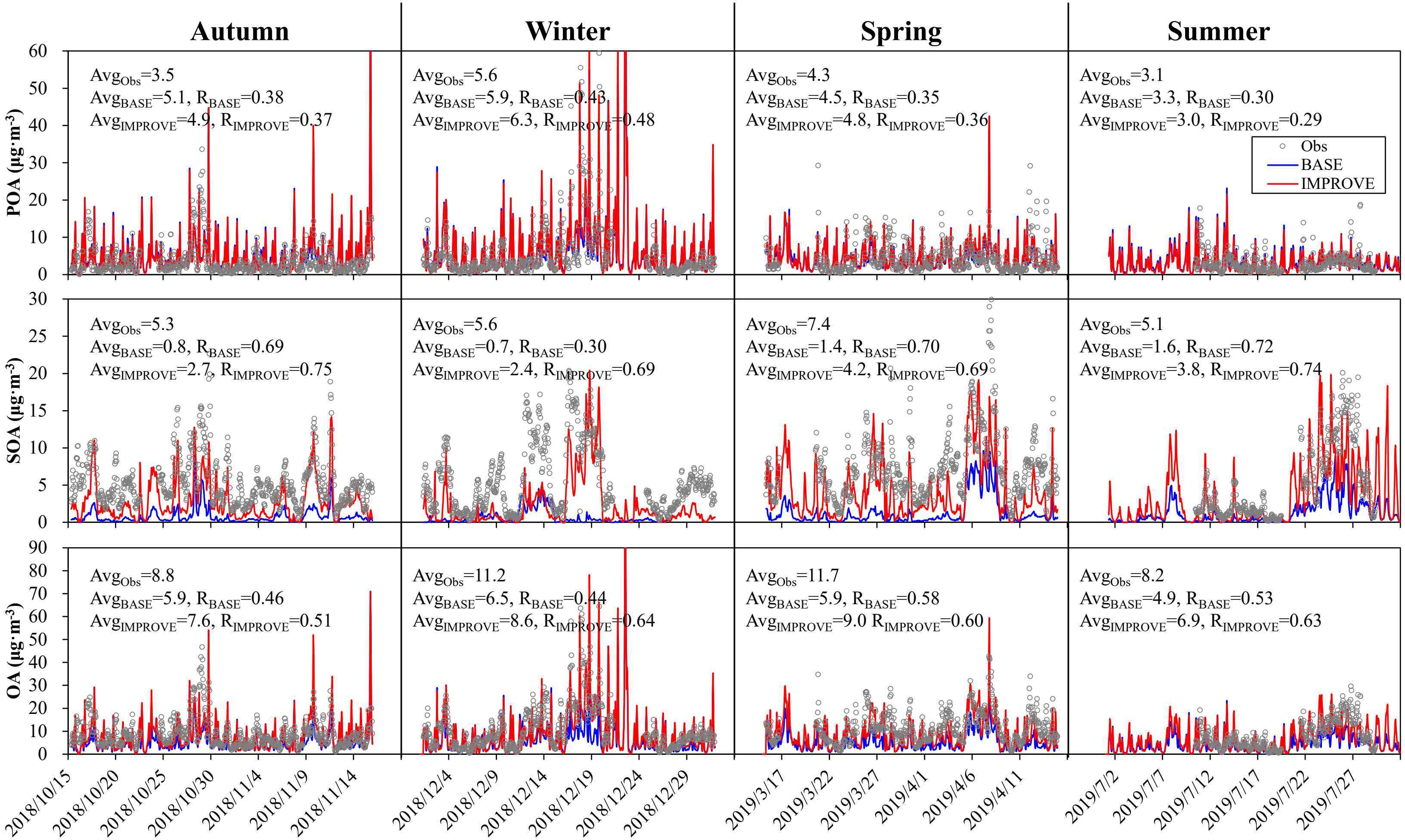


**Figure S4.** Comparisons of measured (grey dots) and modeled concentrations of (a) POA, (b) SOA, and (c) OA in different seasons in the BASE (bule lines) and IMPROVE (red lines) simulation cases at the SAES supersite in Shanghai.

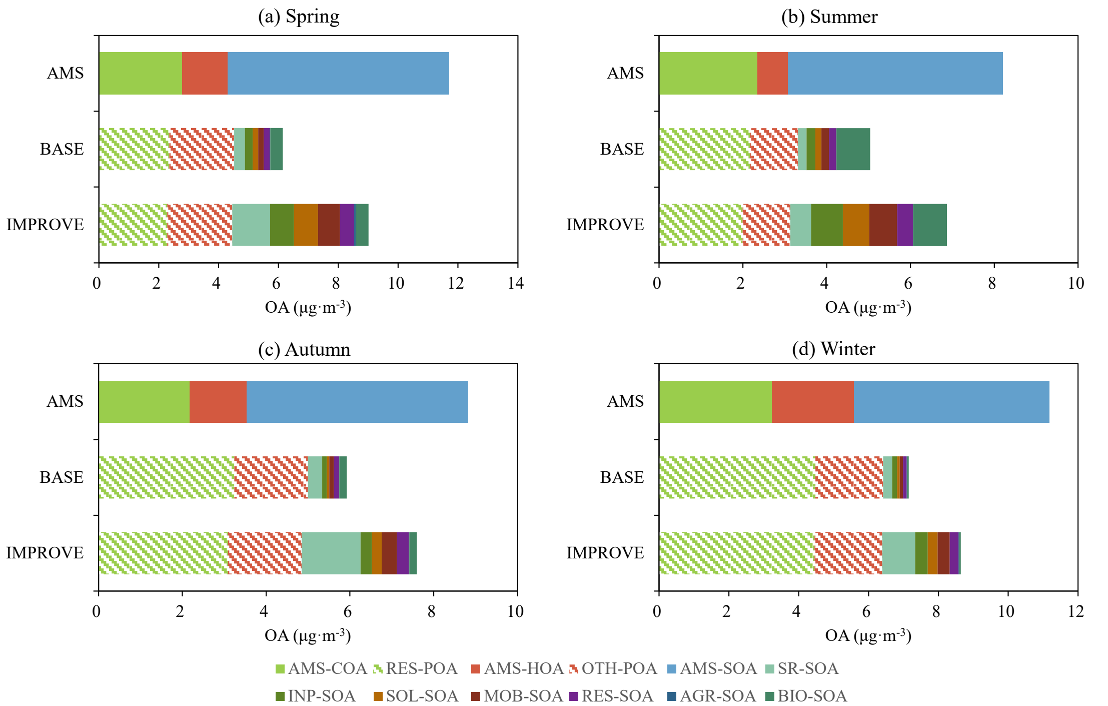


**Figure S5.** Comparisons of modeled POA and SOA source contributions with PMF results by AMS in different seasons in the BASE and IMPROVE simulations at the SAES supersite in Shanghai.