

Investigating three patterns of new particles growing to cloud condensation nuclei size in Beijing's urban atmosphere

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List of Text:

Text S1 Model evaluation of organic matter and the inorganic species in PM_{2.5}.

List of Figures:

Fig. S1 Domains of the CMAQ simulation.

Fig. S2 Occurrence frequencies of difference growth patterns of NPF events in observation months.

Fig. S3 Contour plots of Class I (a), Scenario 1 (b), Scenario 2 (c), Scenario 3 (d) and Scenario 4 (e) of Class II NPF events.

Fig. S4 NPF events occurred on 12 and 13 July 2014 ((a, e) contour plots of the particle number concentration; (b, f) time series of the observed mixing ratios of SO₂ and NO₂+O₃; (c, g) time series of the modeled SOA, NO₃⁻ and NH₄⁺ in PM_{2.5}; (d, h) time series of ambient T and RH).

Fig. S5 NPF events occurred on 12 and 15 August 2014 ((a, e) contour plots of the particle number concentration; (b, f) time series of the observed mixing ratios of SO₂ and NO₂+O₃; (c, g) time series of the modeled SOA, NO₃⁻ and NH₄⁺ in PM_{2.5}; (d, h) time series of ambient T and RH).

Fig. S6 NPF events occurred on 25 July and 11 June 2014 ((a, e) contour plots of the particle number concentration; (b, f) time series of the observed mixing ratios of SO₂ and NO₂+O₃; (c) time series of the modeled SOA, semi-SOA, NO₃⁻ and NH₄⁺ in PM_{2.5}; (d, h) time series of ambient T and RH; (g) time

series of the observed OM, NO_3^- and NH_4^+ in $\text{PM}_{1.0}$.)

Fig. S7 Time series of daily mean concentrations of simulated and observed OM as well as inorganic species including NO_3^- , SO_4^{2-} and NH_4^+ .

List of Table:

Table S1 Model performance of organic matters as well as the inorganic species in $\text{PM}_{2.5}$ in Beijing

Text S1 Model evaluation of organic matter and the inorganic species in PM_{2.5}

The observed concentrations of organic matter (OM) as well as the inorganic species (including NO₃⁻, SO₄²⁻ and NH₄⁺) in PM_{1.0} measured by High-Resolution Time-of-Flight AMS (HR-ToF-AMS) in 10 minutes time-resolution from 3 June to 11 July 2014 (Xu et al., 2017) were used for model evaluation. The sampling site located at a Tower branch of the Institute of Atmospheric Physics in Beijing, China (39.98 N, 116.38 E). Three statistical parameters including Normalized Mean Bias (NMB), Normalized Mean Error (NME), and correlation coefficient (R) were used to evaluate the CMAQ model prediction, using the equations as following (US-EPA, 2007):

$$NMB = \frac{\sum_{i=1}^n (Sim_i - Obs_i)}{\sum_{i=1}^n Obs_i} \times 100\%$$
$$NME = \frac{\sum_{i=1}^n |Sim_i - Obs_i|}{\sum_{i=1}^n Obs_i} \times 100\%$$
$$R = \frac{\sum_{i=1}^n ((Sim_i - \overline{Sim}) \times (Obs_i - \overline{Obs}))}{\sqrt{\sum_{i=1}^n (Sim_i - \overline{Sim})^2 \times \sum_{i=1}^n (Obs_i - \overline{Obs})^2}}$$

in which, Sim_i represents the concentrations simulated by CMAQ, and Obs_i represents the observation concentrations.

The temporal variations of daily mean concentrations of simulated and observed OM, NO₃⁻, SO₄²⁻ and NH₄⁺ were shown in Fig. S7. The model simulation well replicated the temporal variations of OM, NO₃⁻, SO₄²⁻ and NH₄⁺ concentrations during the study period. The model results generally could meet the benchmark criteria of above four species (US-EPA, 2007), with correlations of higher than 0.51 (Table S1). The concentrations of SO₄²⁻ and NH₄⁺ had been slightly overestimated (with NMBs and 12%, 6%), while the concentrations of NO₃⁻ and OM were underestimated (with NMBs of -29% and -42%). HR-ToF-AMS detected only chemical species in particles less than 1.0 μm, while the accumulation mode of SO₄²⁻ and NH₄⁺ can extend to 1-2 μm. (Yao et al., 2003). The HR-ToF-AMS was set closer to an elevated highway as well as a moderate traffic road behind. The observational values may contain a large contribution from on-road vehicle emissions, and subsequently result in an under-prediction of NO₃⁻ and OM in modeling against them. NO₃⁻ concentrations in PM_{2.5} reportedly exhibited a larger spatial heterogeneity than that of SO₄²⁻ in Beijing (Yao et al., 2002). More under-prediction of OM can be also related to the underestimation of secondary organic aerosols (SOA). Underestimation of SOA is the common weakness of model simulation because a fraction of SOA

precursors were not involved such as aromatic volatile organic compounds, SOA yields was underestimated and some key formation pathways of SOA may still missed in current air quality models (Appel et al., 2008; Baek et al., 2011; Hallquist et al., 2009; Knote et al., 2014).

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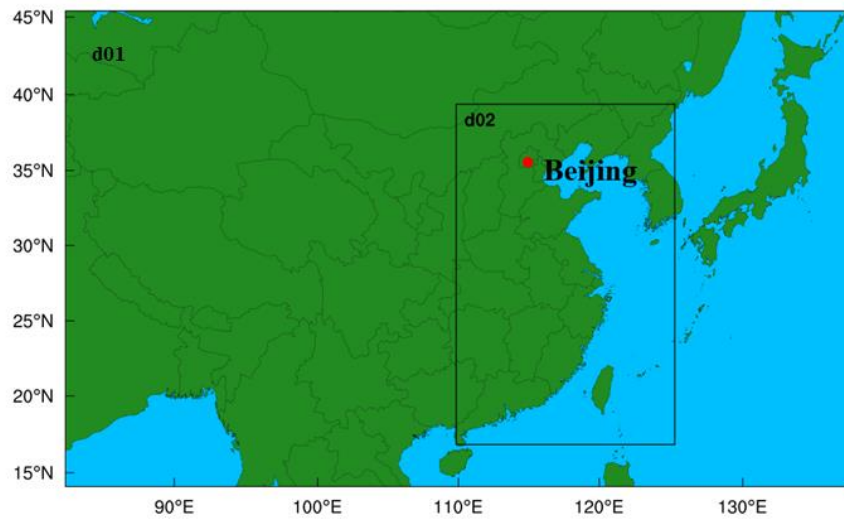


Fig. S1 Domains of the CMAQ simulation

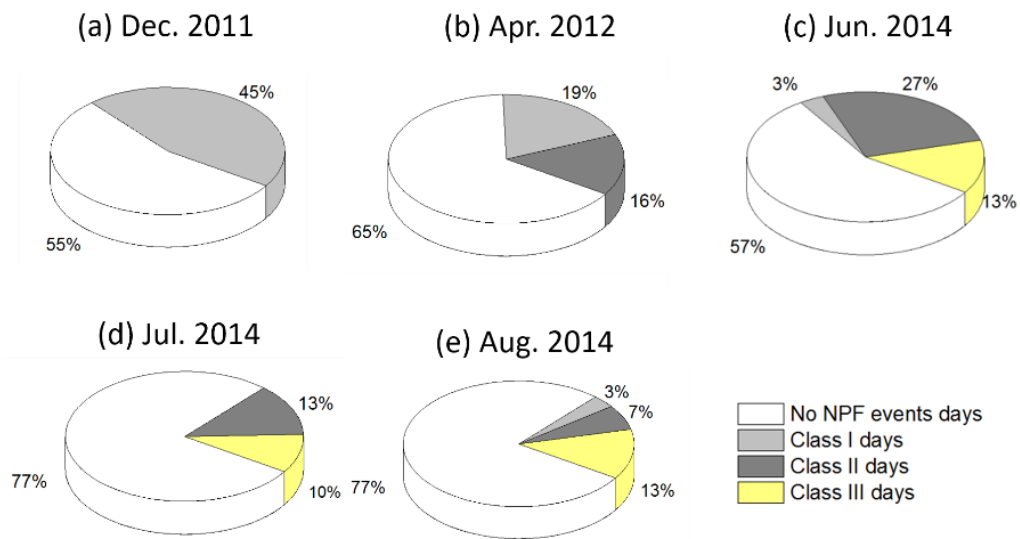


Fig. S2 Occurrence frequencies of difference growth patterns of NPF events in observation months.

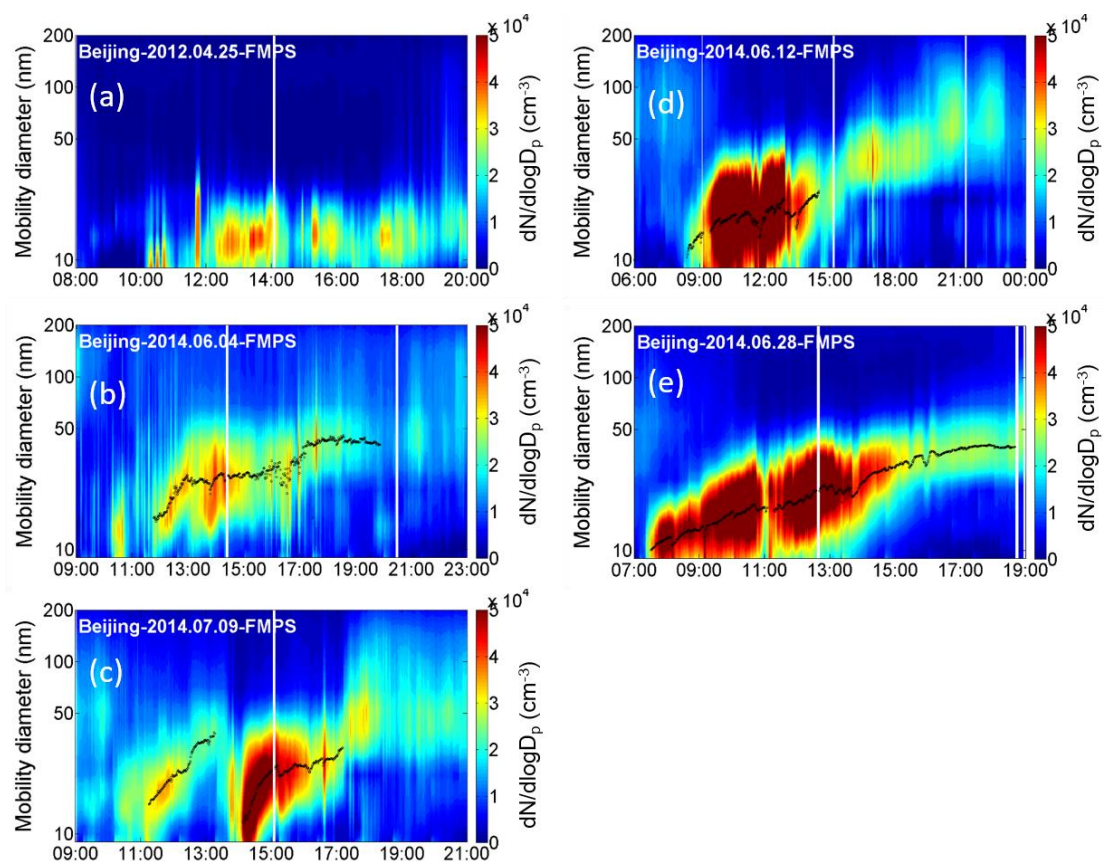


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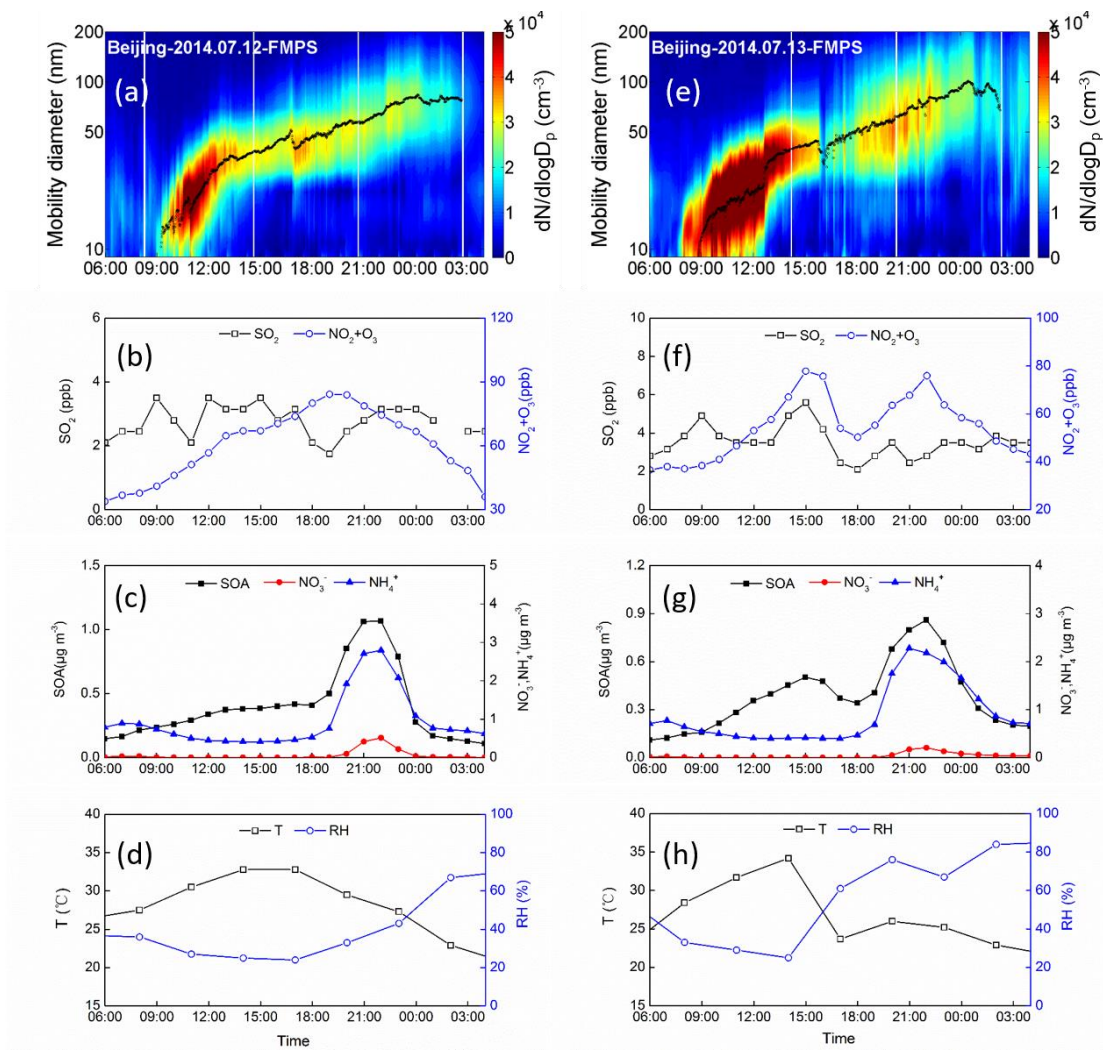


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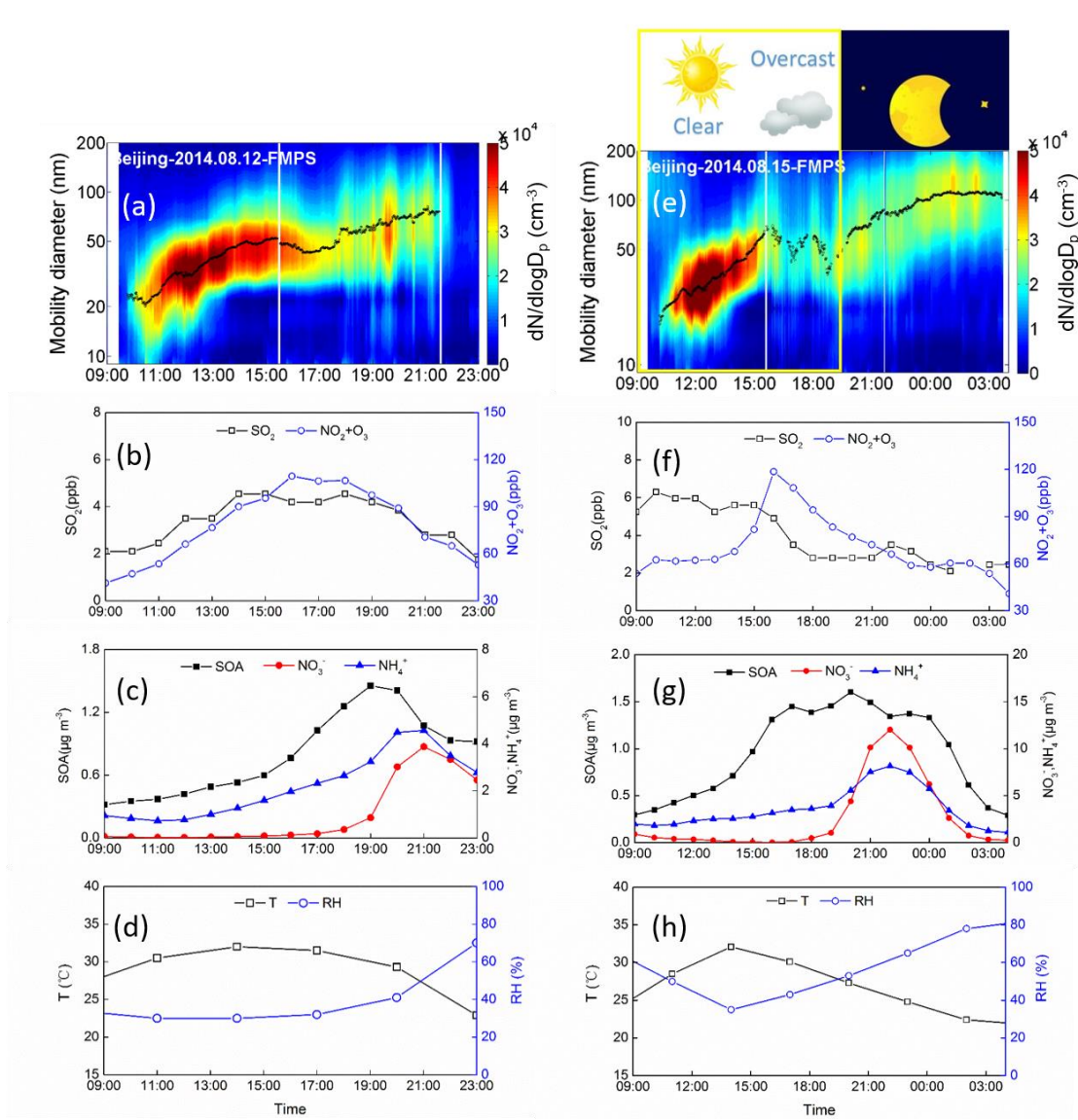


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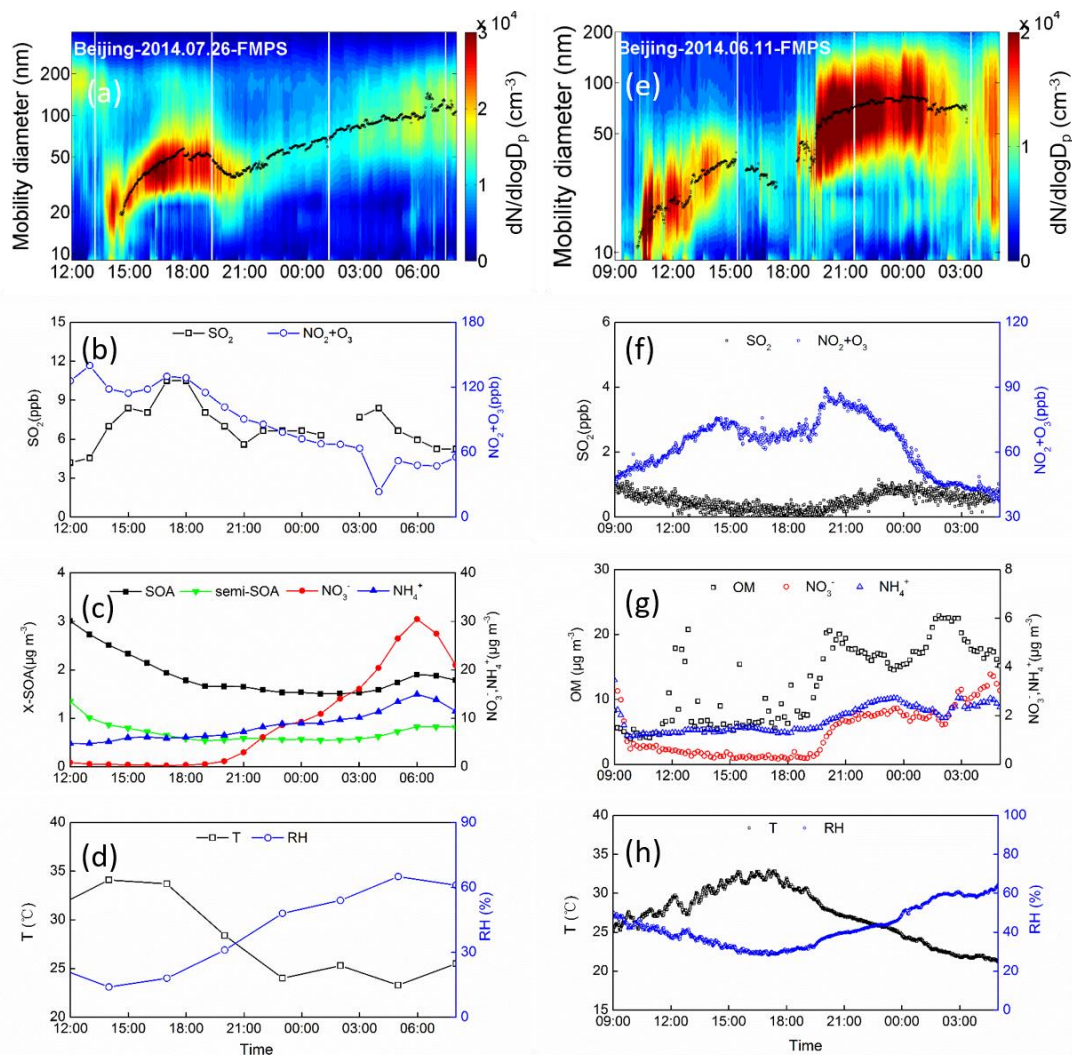


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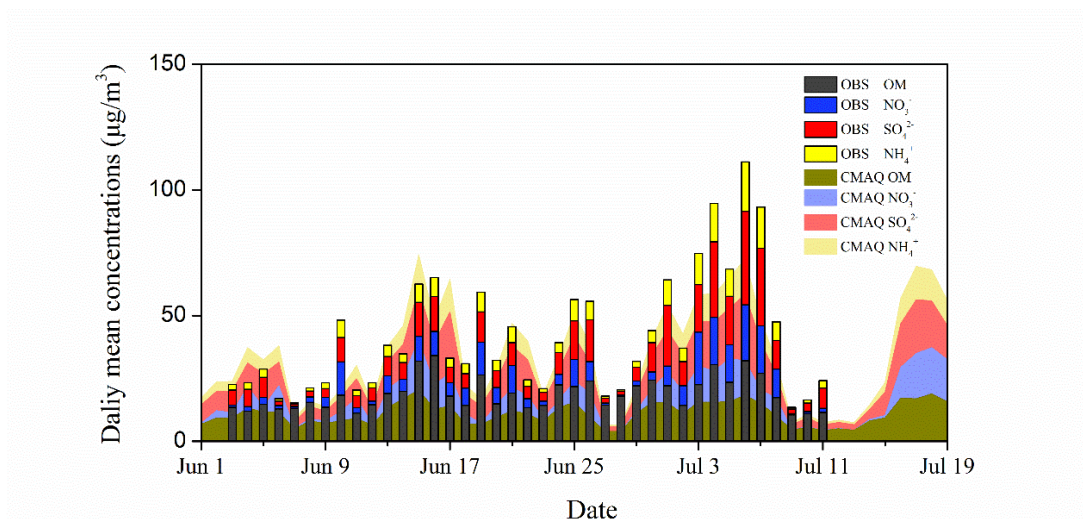


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	OM	NO ₃ ⁻	SO ₄ ²⁻	NH ₄ ⁺
NMB	-42%	-29%	12%	6%
NME	49%	72%	50%	53%
R	0.51	0.61	0.69	0.67