

Supplement of

Development of Four Dimensional Variational Assimilation System Based on GRAPES-CUACE Adjoint Model (GRAPES-CUACE-4D-Var V1.0) and Its Application in Emission Inversion

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3 Description of GRAPES-CUACE-4D-Var

3.2 Observations

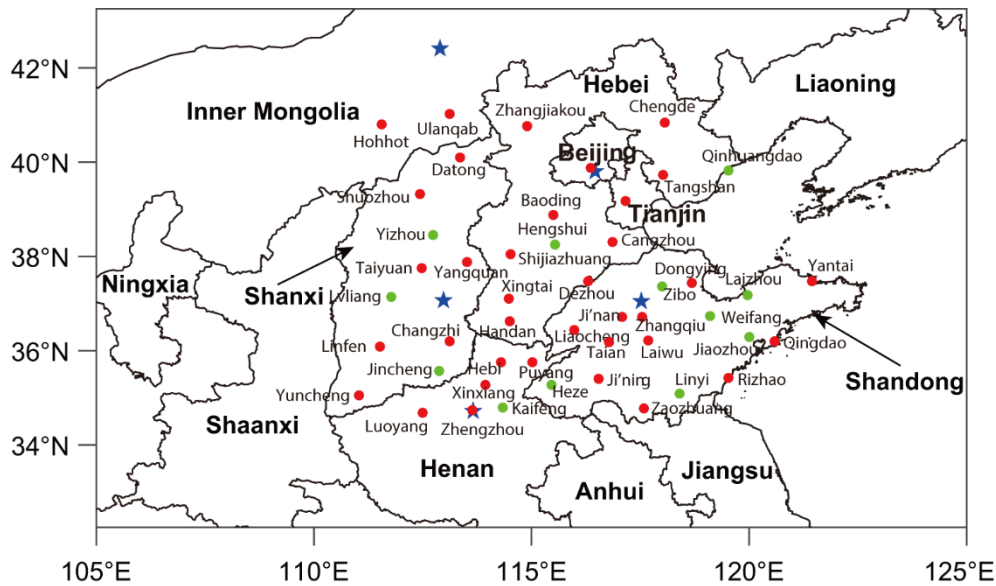


Figure S1. Simulation domain over North China, including Beijing City, Tianjin City, Hebei, Shanxi, Shandong, Shaanxi, Ningxia, Henan, and part of Inner Mongolia, Liaoning, Anhui and Jiangsu provinces. The blue stars denote locations of 5 BC surface monitoring sites from CAWNET. The details of the 5 sites in CAWNET are shown in Table S1. The dots denote locations of 48 PM_{2.5} surface monitoring sites from MEE with the city names labelled around. The red dots represent the 36 cities that are put into the assimilation system, and the green dots represent the 12 cities that are not put into the assimilation system and are used for validation of the effect of emission inversion.

Table S1. Information of the 5 sites in CAWNET.

Station	Longitude	Latitude
Beijing	116.47°E	39.8°N
Zhurihe	112.9	42.4
Yushe	112.98	37.07
Huimin	117.53	37.05
Zhengzhou	112.9	42.4

To improve the performance of emission inversion, adequate observations are needed for constraining the model. Due to the limited BC monitoring sites in North China, we used the surface $PM_{2.5}$ concentrations at 48 cities described above and the BC/ $PM_{2.5}$ ratio to obtain the hourly BC concentrations for July 1-31, 2016 at 48 cities in North China.

First of all, under the premise that the observations at the BC sites can represent a regional condition, we divided the region where the 5 BC sites are located into 5 areas (Beijing Area, Zhurihe Area, Yushe Area, Huimin Area, and Zhengzhou Area, Table S1), and considered each BC site to be the center of the area (Fig. S2). Then for 48 $PM_{2.5}$ sites, we calculated the distance between each $PM_{2.5}$ site and the 5 BC sites, and divided the $PM_{2.5}$ site into the area where the nearest BC site is located (Fig. S2). In each area, we used the observations at the BC site and its nearest $PM_{2.5}$ site to calculate the BC/ $PM_{2.5}$ ratio, and we assumed that all $PM_{2.5}$ sites in the same area share the same BC/ $PM_{2.5}$ ratio. Finally, we used the BC/ $PM_{2.5}$ ratios and $PM_{2.5}$ concentrations to calculate BC concentrations at the 48 sites where $PM_{2.5}$ sites are located.

The BC/ $PM_{2.5}$ ratio calculated in this study was compared with other documents. The BC/ $PM_{2.5}$ ratios in Zhurihe Area and Huimin Area are about 2%, which are consistent with Xu et al. (2020) and Yang (2008). The BC/ $PM_{2.5}$ ratios in Beijing Area, Yushe Area and Zhengzhou Area are relatively higher, with the values about 6-7%, which are consistent with He et al. (2001), Yang et al. (2011), Chen et al. (2016), Liu et al. (2018) and Xu et al. (2020).

In addition, we compared the monthly BC concentrations in July 2016 calculated in this study and from the MERRA-2 (Modern-era Retrospective Analysis for Research and Applications, Vision2) reanalysis data (Fig.S3). It can be seen that the values of BC concentration calculated in this study ($1-5 \mu g/m^3$) is a little lower than that of MERRA-2 data ($1-8 \mu g/m^3$), but the spatial distribution of BC concentration calculated in this study is highly consistent with the MERRA-2 data. The highest BC concentrations are mainly located in Beijing Area. The BC concentrations in Zhengzhou Area and Yushe Area are also relatively high. While the BC concentrations in Zhurihe Area and Huimin Area are much lower. Overall, the BC concentration calculated by the BC/ $PM_{2.5}$ ratio method in this study is reasonable.

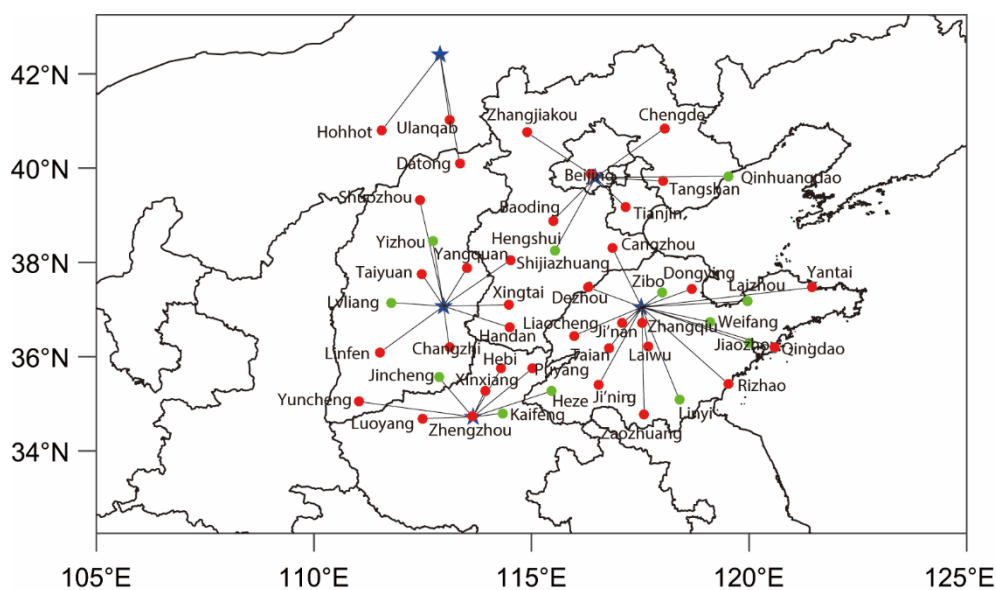


Figure S2. The distance between the BC sites and the neighbouring $PM_{2.5}$ sites.

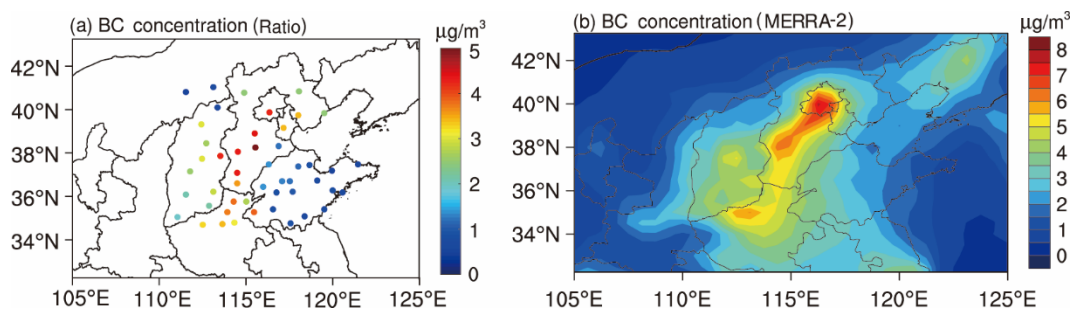


Figure S3. The comparison of monthly BC surface concentration in July 2016 (a) calculated in this study and (b) from the MERRA-2 (Modern-era Retrospective Analysis for Research and Applications, Vision2) reanalysis data. The monthly MERRA-2 products containing BC surface concentration, with the horizontal resolution of $0.5^{\circ} \times 0.625^{\circ}$, can be accessed through NASA website (<https://daac.gsfc.nasa.gov>).

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