atmosphere

Supplementary Materials:

Quantification of SO_2 Emission Variations and the Corresponding Prediction Improvements Made by Assimilating Ground-Based Observations

Jingyue Mo [1,2], Sunling Gong [2,*], Jianjun He [2], Lei Zhang [2,*], Huabing Ke [1,2] and Xingqin An [2]

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[1] Climate and Weather Disasters Collaborative Innovation Center, Nanjing University of Information Science &Technology, Nanjing 210044, China; mojingyue@nuist.edu.cn (J.M.); khb19940418@163.com (H.K.)
[2] State Key Laboratory of Severe Weather & Key Laboratory of Atmospheric Chemistry of CMA, Chinese Academy of Meteorological Sciences, Beijing 100081, China; hejianjun@cma.gov.cn (J.H.); anxq@cma.gov.cn (X.A.)
* Correspondence: gongsl@cma.gov.cn (S.G.); leiz09@cma.gov.cn (L.Z.)

The flowchart, code structure, and other details of the updated WRF-CUACE and its adjoint model were presented in this supplementary material.

Figure S1 shows the code structure of the updated WRF-CUACE and its adjoint model. The whole of WRF-CUACE-ADJ include WRF-CUACE and the backward adjoint and each part includes transport, gas and aerosol modules.

Figure S2 shows the flowchart of the WRF-CUACE-ADJ model. The relationship of each time step between forward simulation and backward simulation is shown directly. Adjoint forcing is the difference between observation and modeled concentration, and the adjoint operator is calculated by the adjoint code. Both of them drive the WRF-CUACE-ADJ to calculate the gradient of the cost function.

The simulation time of the WRF-CUACE-ADJ is about four times that of the normal WRF-CUACE. The storage of WRF-CUACE-ADJ at every time step is about 230 MB with 38 gas state variables, 73 aerosol state variables, and 25 transport-related variables as the model domain introduced in the main text. For example, a single adjoint simulation shown in Fig. S2 for one day with five minutes time step needs 66 GB storage. Accordingly, the corresponding optimization process needs 8 to 15 times computation resources.

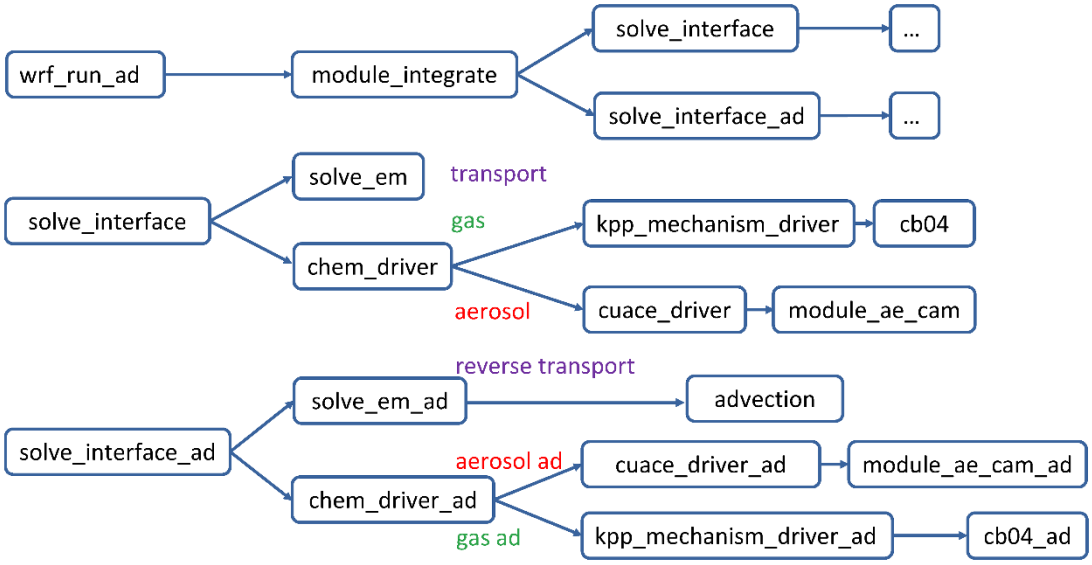


Figure S1. The code structure of the updated WRF-CUACE and its adjoint model.

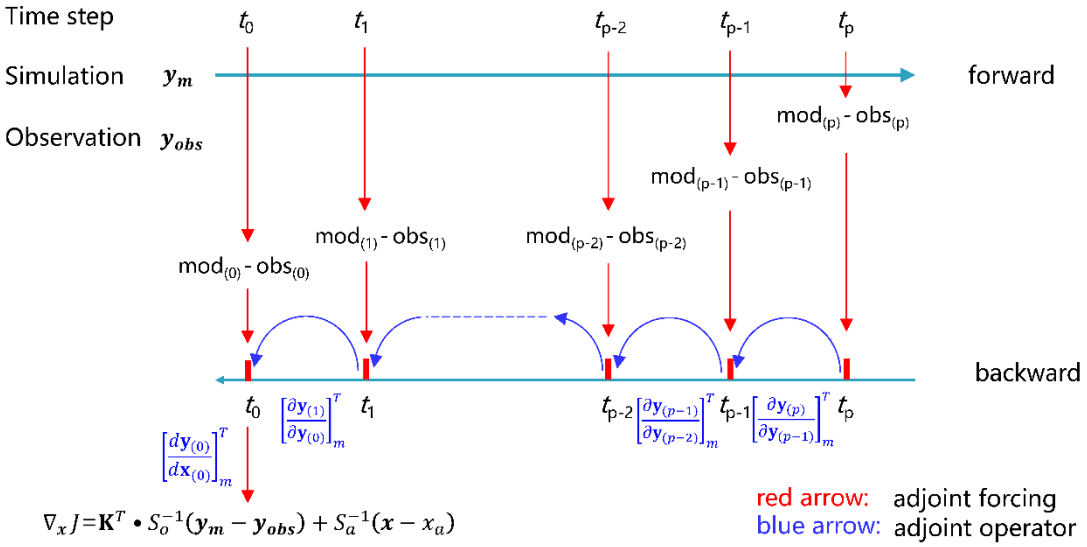


Figure S2. The flowchart of the WRF-CUACE-ADJ model.