

Improving Ozone Simulations in Asia via Multisource Data Assimilation: Results from an Observing System Simulation Experiment with GEMS Geostationary Satellite Observations

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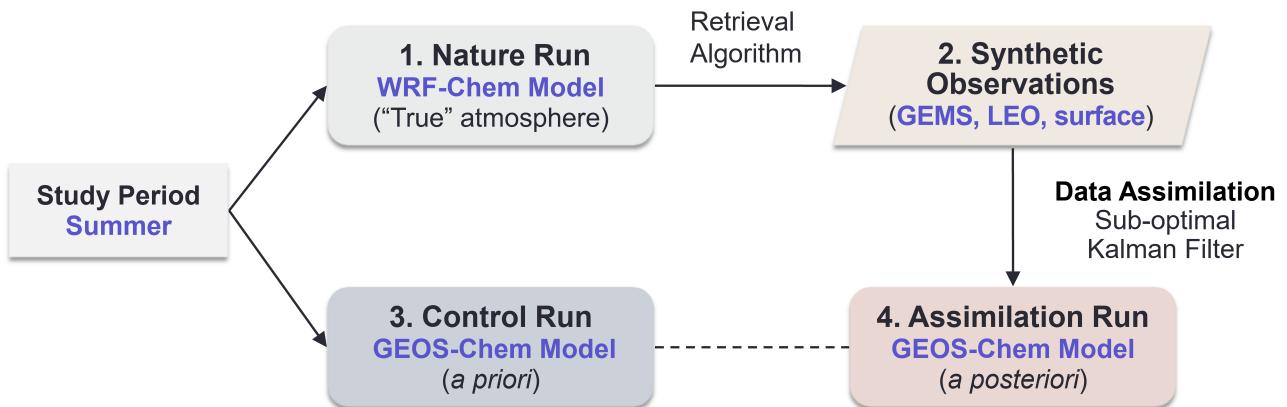
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Table S1

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Table S1. WRF-Chem and GEOS-Chem model configurations.

Configurations	(1) WRF-Chem v4.1	(2) GEOS-Chem v12.9.3
Global simulation	—	$2^\circ \times 2.5^\circ$ with 72 vertical layers up to 0.1 hPa, spin-up time of 1 year
Asian simulation	50 km \times 50 km (centered at 35°N, 103°E) with 34 vertical layers up to 50 hPa, spin-up time of 72 h	$0.5^\circ \times 0.625^\circ$ (11°S–55°N, 60°–150°E) with 47 vertical layers up to 0.1 hPa, boundary conditions updated every 3 h from the global simulation, spin-up time of 6 months
Meteorological conditions	National Centers for Environmental Prediction (NCEP) Final (FNL) operational global analysis (https://rda.ucar.edu/datasets/ds083.3 , last access: 28 October 2022), $0.25^\circ \times 0.25^\circ$	Modern-Era Retrospective Analysis for Research and Applications, Version 2 (MERRA-2) meteorological fields (Gelaro <i>et al.</i> , 2017)
Chemical initial and boundary conditions	Whole Atmosphere Community Climate Model (WACCM) 6 h outputs (Gettelman <i>et al.</i> , 2019)	—
Anthropogenic emission	Multi-resolution Emissions Inventory for China (MEIC) (Zheng <i>et al.</i> , 2018), $0.25^\circ \times 0.25^\circ$; Emissions Database for Global Atmospheric Research-Hemispheric Transport of Air Pollution (EDGAR-HTAP) (Janssens-Maenhout <i>et al.</i> , 2015) outside China, $1^\circ \times 1^\circ$	Community Emissions Data System (CEDS) (Hoesly <i>et al.</i> , 2018), substituted by MIX inventory (Li <i>et al.</i> , 2017) over Asia
Biogenic emission	Model of Emissions of Gases and Aerosols from Nature (MEGAN) (Guenther <i>et al.</i> , 2012)	MEGAN
Fire emission	Fire INventory from NCAR (FINN) version 1.5 (Wiedinmyer <i>et al.</i> , 2011)	the fourth-generation Global Fire Emissions Database (GFED4) (Giglio <i>et al.</i> , 2013)
Chemical mechanism	CBMZ chemical mechanism (Zaveri and Peters, 1999) for gas-phase chemistry and MOSAIC aerosol scheme configured with 4 sectional aerosol bins (Zaveri <i>et al.</i> , 2008)	HO _x -NO _x -VOC-ozone-aerosol-halogen tropospheric chemistry mechanism (Bey <i>et al.</i> , 2001; Park <i>et al.</i> , 2004; Mao <i>et al.</i> , 2013)



25 **Figure S1. The framework of the Observing System Simulation Experiment (OSSE). Modified from Shu *et al.* (2022).**

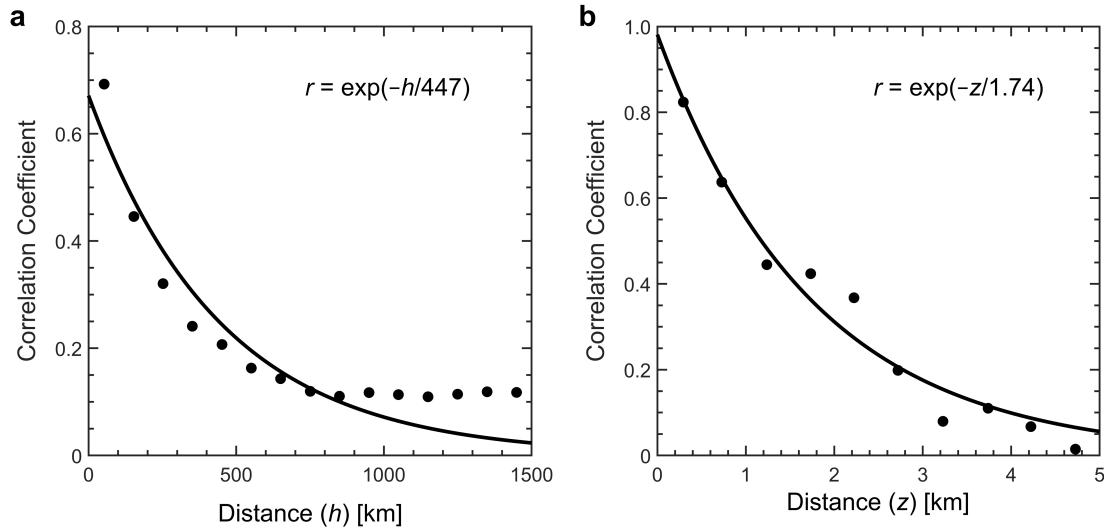


Figure S2. Horizontal and vertical error correlation length for the GEOS-Chem simulation of tropospheric ozone in Asia. The panel (a) shows the correlation coefficients (r) of the model errors between pairs of surface monitoring sites relative to surface ozone observations from the China National Environmental Monitoring Center (CNEMC; <http://www.cnemc.cn/>, last access: 28 October 2022) and plotted against the horizontal distance h (in km, binned every 100 km). The panel (b) shows the correlation coefficients of the model errors between pairs of vertical levels (from surface to 8 km altitude) relative to ozonesonde measurements (Shu *et al.*, 2022) and plotted against the vertical distance z (in km, binned every 500 m). Exponential fits based on the least-squares method to the data are shown inset.

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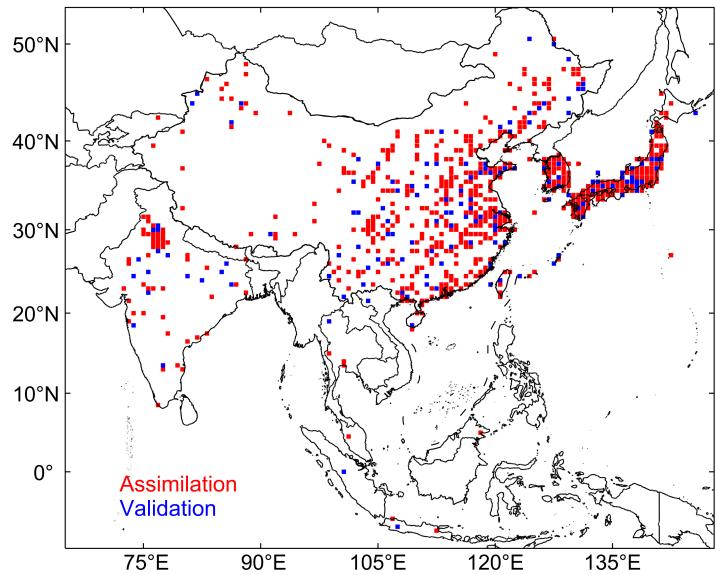
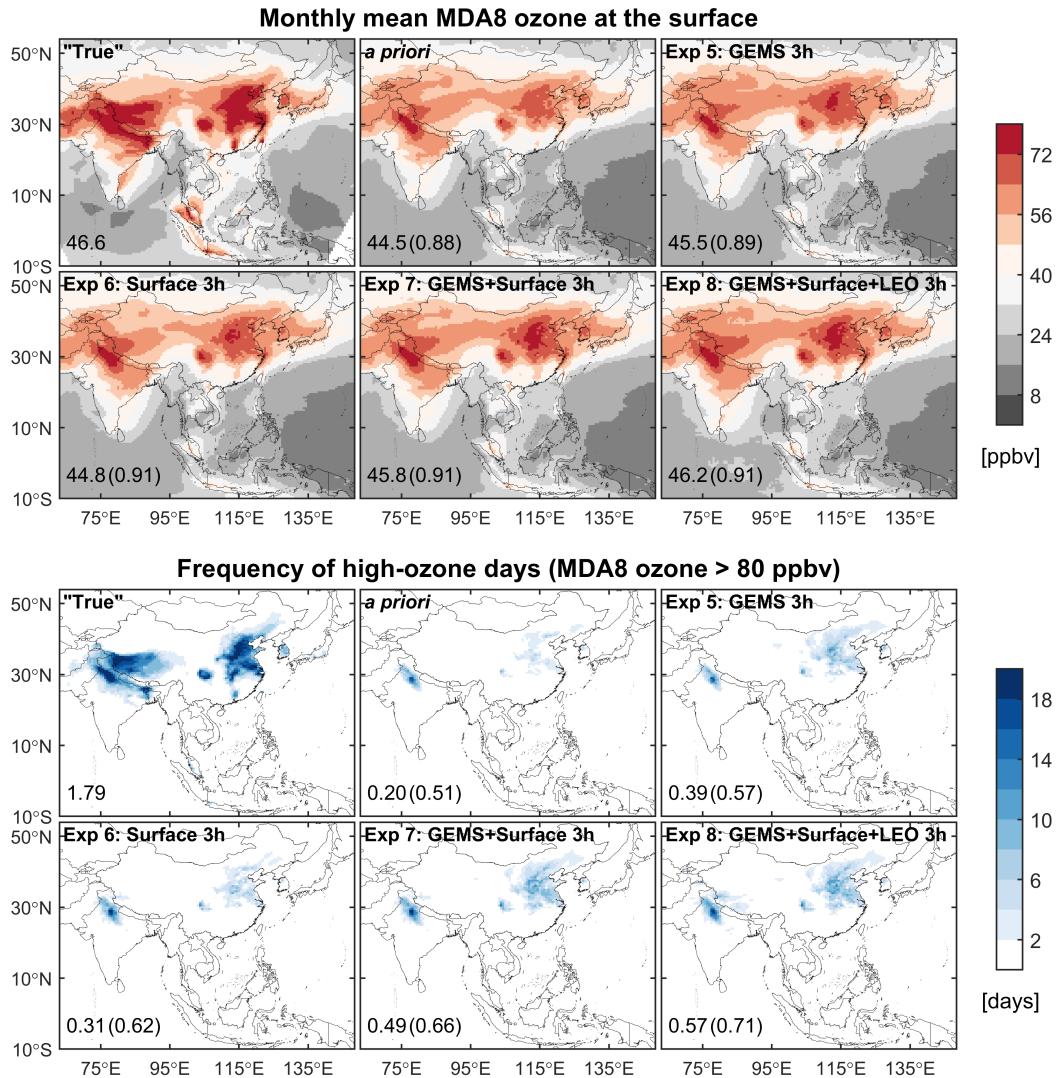


Figure S3. Distribution of super-observation grids for assimilation (red) and validation (blue) over the Asian domain.



40 **Figure S4.** Same as Fig. 4 but for assimilation runs with the assimilation time step of 3 h (Exp 5–8 in Table 1).

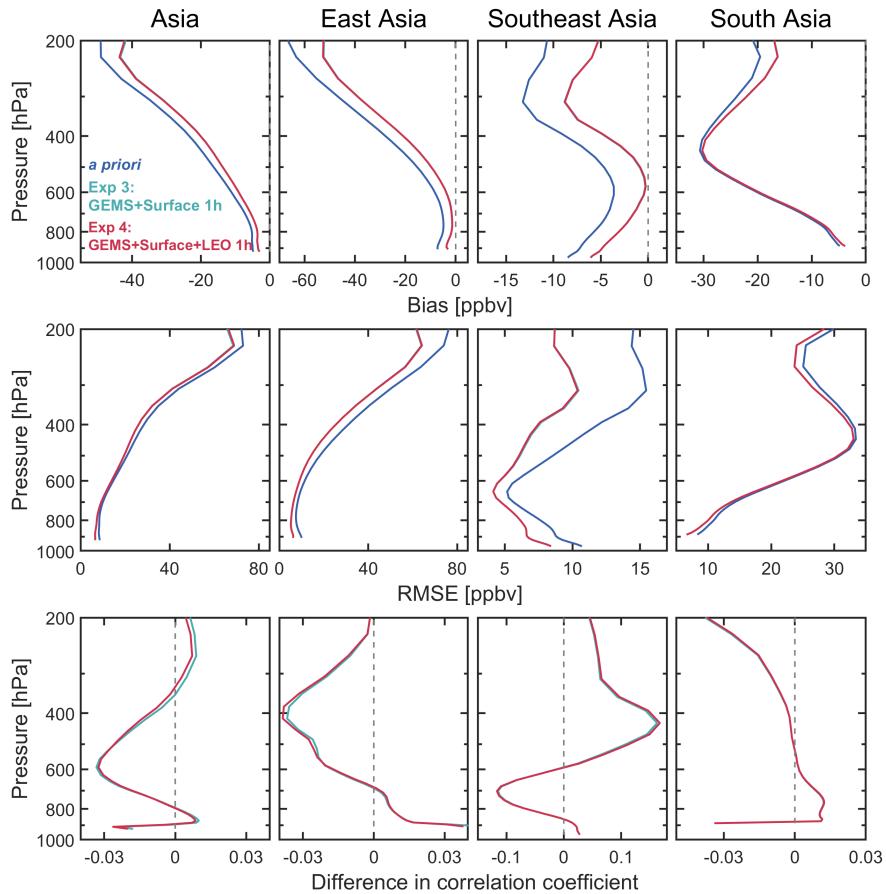
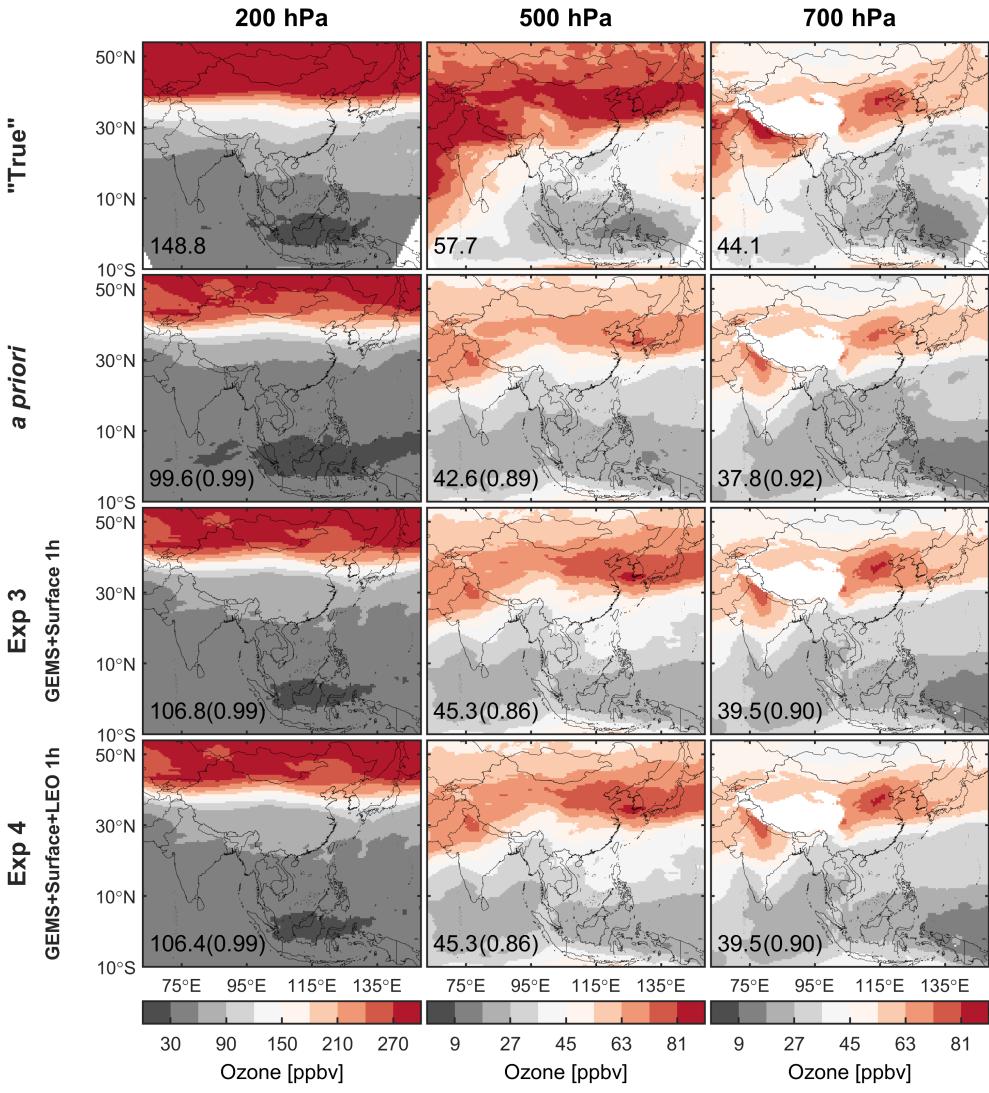


Figure S5. Same as Fig.7 but for *assimilation runs* with the assimilation time step of 1 h (Exp 3 and 4 in Table 1).



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Figure S6. Same as Fig. 8 but for assimilation runs with the assimilation time step of 1 h (Exp 3 and 4 in Table 1).

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