

Supplement

5 **Development of the global chemistry-climate coupled model BCC-GEOS-Chem v2.0: improved atmospheric chemistry performance and new capability of chemistry-climate interactions**

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20 **Table S1.** Comparison of global annual emissions in BCC-GEOS-Chem v2.0

| Main species | BCC-GEOS-Chem v2.0 | BCC-GEOS-Chem v1.0 | BCC-AGCM-Chem | Classic GEOS-Chem ^a |
|-----------------|--------------------|--------------------|---------------|--------------------------------|
| NO ^b | 118.1 | 111.1 | 110.3 | 113.6 |
| CO | 926.2 | 925.5 | 1140.6 | 925.9 |
| ISOP | 389.4 | 410.0 | 410.8 | 367.2 |
| Other species | BCC-GEOS-Chem v2.0 | BCC-GEOS-Chem v1.0 | BCC-AGCM-Chem | Classic GEOS-Chem |
| ALK4 | 54.7 | 44.0 | \ | 52.9 |
| BC | 8.0 | 9.2 | 9.2 | 8.0 |
| BENZ | 7.8 | 6.7 | \ | 7.8 |
| C2H6 | 13.2 | 9.3 | \ | 14.4 |
| C3H8 | 14.5 | 7.2 | \ | 14.4 |
| CH2O | 6.5 | 5.7 | 5.7 | 6.5 |
| OC | 29.5 | 31.0 | 31.0 | 29.5 |
| PRPE | 28.0 | 16.8 | \ | 30.6 |
| SO2 | 128.2 | 123.7 | 123.7 | 130.0 |
| TOLU | 8.5 | 7.8 | \ | 8.5 |
| XYLE | 7.8 | 7.5 | \ | 7.8 |

^a Results from the standard version of GEOS-Chem v13.3.1 with aircraft emissions excluded (Wang et al., 2022). ^b Total NO emissions including lightning NO. All values are averaged over 2012-2014 in Tg yr⁻¹.

Table S2. Meteorological variables needed for GEOS-Chem v14.0.1.

| NO. | Variables | Description | Usage | Unit |
|---------------|-----------|--|----------------------------|--------------------------------|
| 2-D variables | | | | |
| 1 | ALBD | Surface albedo | Dry deposition | 1 |
| 2 | CLDFRC | Cloud fraction | Photolysis | 1 |
| 3 | EFLUX | Latent heat flux | Diagnostics | W m ⁻² |
| 4 | FRSEAICE | Fraction of sea ice | Hg simulation | 1 |
| 5 | GWETROOT | Root soil wetness | Diagnostics | 1 |
| 6 | GWETTOP | Top soil moisture | CH ₄ simulation | 1 |
| 7 | HFLUX | Sensible heat from turbulence | Dry deposition | W m ⁻² |
| 8 | FRLAND | Fraction of land/ocean/surface/snow/lake/land ice type in grid box | Chemistry | 1 |
| | FROCEAN | | | |
| | FRLAKE | | | |
| | FRLANDIC | | | |
| | FRSNO | | | |
| 9 | LAI | Leaf area index | Diagnostics | m ² m ⁻² |

| | | | | |
|----|---------------------|---|--------------------------|--------------------------------|
| 10 | PBLH | Planetary boundary layer height | PBL mixing | m |
| 11 | PRECCON | Convective precipitation | Wet deposition | mm day ⁻¹ |
| 12 | PRECTOT | Total precipitation | Wet deposition | mm day ⁻¹ |
| 13 | PARDR | Direct photosynthetically active radiation | Biogenic emissions | W m ⁻² |
| 14 | PARDF | Diffuse photosynthetically active radiation | Biogenic emissions | W m ⁻² |
| 15 | PHIS | Surface geopotential height | Diagnostics | m ² s ⁻² |
| 16 | TROPP | temperature based tropopause pressure | Grid setting | hPa |
| 17 | TS | Surface temperature | Chemistry, deposition | K |
| | TSKIN | Surface skin temperature | Sea salt emissions | K |
| 18 | TAUCLI | Optical depth of ice clouds | Diagnostics | 1 |
| 19 | TAUCLW | Optical depth of water clouds | Diagnostics | 1 |
| 20 | SUNCOS | Zenith angle | Chemistry | 1 |
| 21 | SNODP | Snow deposition | Diagnostics | m |
| 22 | SNOMAS | Snow mass | Dry deposition | kg m ⁻² |
| 23 | SWGDN | Surface incident radiation | Soil NOx; dry deposition | W m ⁻² |
| 24 | U10M | 10m east-west wind speed | Dry deposition | m s ⁻¹ |
| 25 | USTAR | Friction velocity | Dry deposition | m s ⁻¹ |
| 26 | UVALBEDO | UV albedo | photochemistry | 1 |
| 27 | TO3 | Total overhead O ₃ column | Photolysis | DU |
| 28 | V10M | 10m south-north wind speed | Dry deposition | m s ⁻¹ |
| 29 | Z0 | Roughness length | Dry deposition | m |
| 30 | AREA_m ² | Grid box surface area | Many locations | m ² |
| 31 | XLAII | Leaf Area Index | Dry deposition | 1 |
| 32 | LANDTYPEFRAC | Olson fraction per land type | Dry deposition | 1 |

3-D variables on level edge

| | | | | |
|----|---------|---|------------------|------------------------------------|
| 33 | PFILSAN | 3-D flux of ice non-convective precipitation | Wet deposition | kg m ⁻² s ⁻¹ |
| 34 | PFICU | 3d flux of ice convective precipitation | Wet deposition | kg m ⁻² s ⁻¹ |
| 35 | PFLLSAN | 3-D flux of liquid non-convective precipitation | Wet deposition | kg m ⁻² s ⁻¹ |
| 36 | PFLCU | 3d flux of liquid convective precipitation | Wet deposition | kg m ⁻² s ⁻¹ |
| 37 | CMFMC | Upward moist convective mass flux | Cloud convection | kg m ⁻² s ⁻¹ |
| 38 | PEDGE | Pressure edge for each grid | Grid setting | hPa |

3-D variables on level center

| | | | | |
|----|---------|------------------------------|------------------|-------------------------------------|
| 39 | CLDF | 3-D cloud fraction | Chemistry | 1 |
| 40 | DTRAIN | Detrainment cloud mass flux | Cloud convection | kg m ⁻² s ⁻¹ |
| 41 | DQRLSAN | Large-scale rainwater source | Wet deposition | kg kg ⁻¹ s ⁻¹ |
| 42 | DQRCU | Convective rainwater source | Cloud convection | kg kg ⁻¹ s ⁻¹ |
| 43 | QI | Cloud ice water mixing ratio | Chemistry | kg kg ⁻¹ |

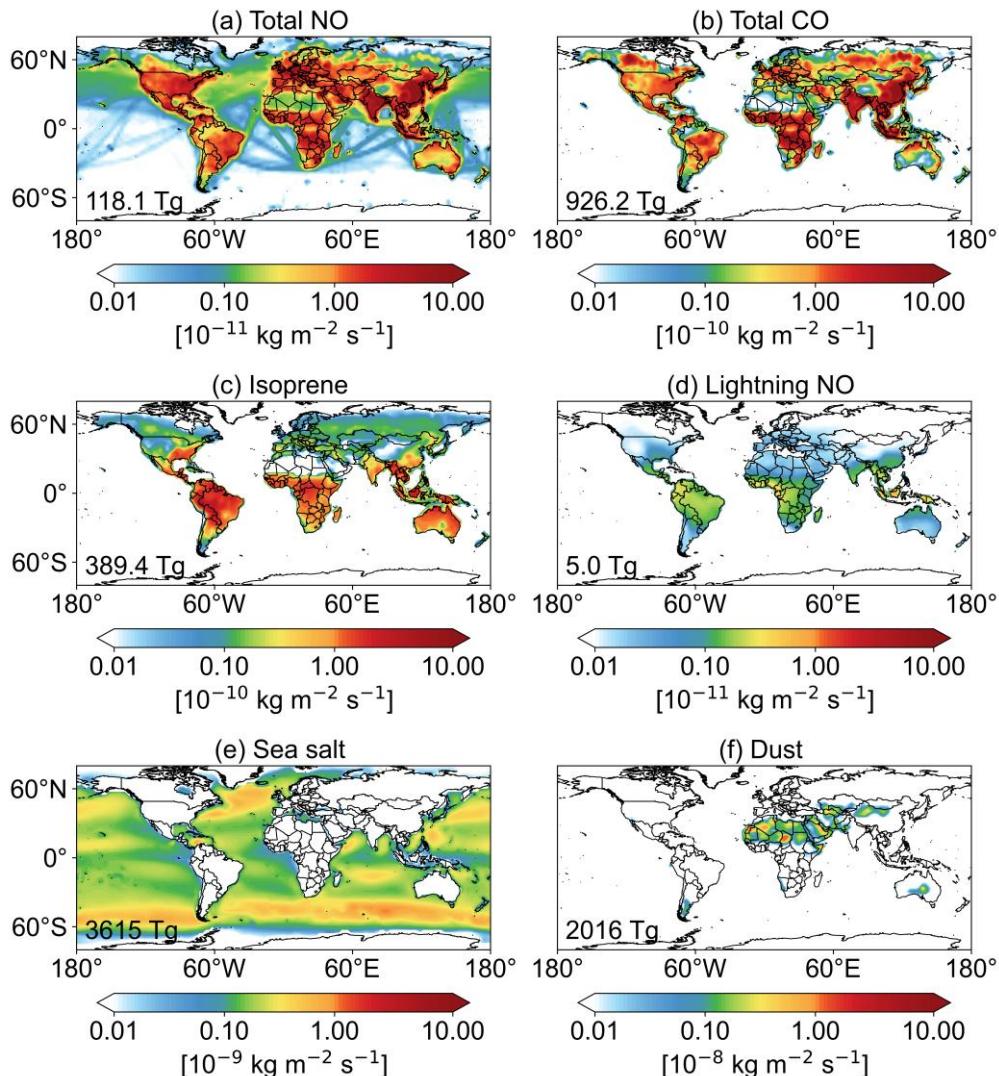
| | | | | |
|----|----------|--|-------------------------|-----------------------------------|
| 44 | QL | Cloud liquid water mixing ratio - anvils | Aerosol microphysics | kg kg^{-1} |
| 45 | RH | Relative humidity | Many locations | 1 |
| 46 | SPHU | Specific chemistry | Chemistry | kg kg^{-1} |
| 47 | T | Temperature | Chemistry | K |
| 48 | U | East-west component of wind | Advection | m s^{-1} |
| 49 | V | North-south component of wind | Advection | m s^{-1} |
| 50 | OMEGA | Updraft velocity | Diagnostics | Pa s^{-1} |
| 51 | REEVAPLS | Evaporation of precipitating LS & anvil condensate | Wet deposition | $\text{kg kg}^{-1} \text{s}^{-1}$ |
| 52 | REEVAPN | Evaporation of precipitating convection condensate | Wet deposition | $\text{kg kg}^{-1} \text{s}^{-1}$ |
| 53 | OPTD | Cloud optical depth | Photolysis | 1 |

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Table S3. Observations and reanalysis data used for model evaluation

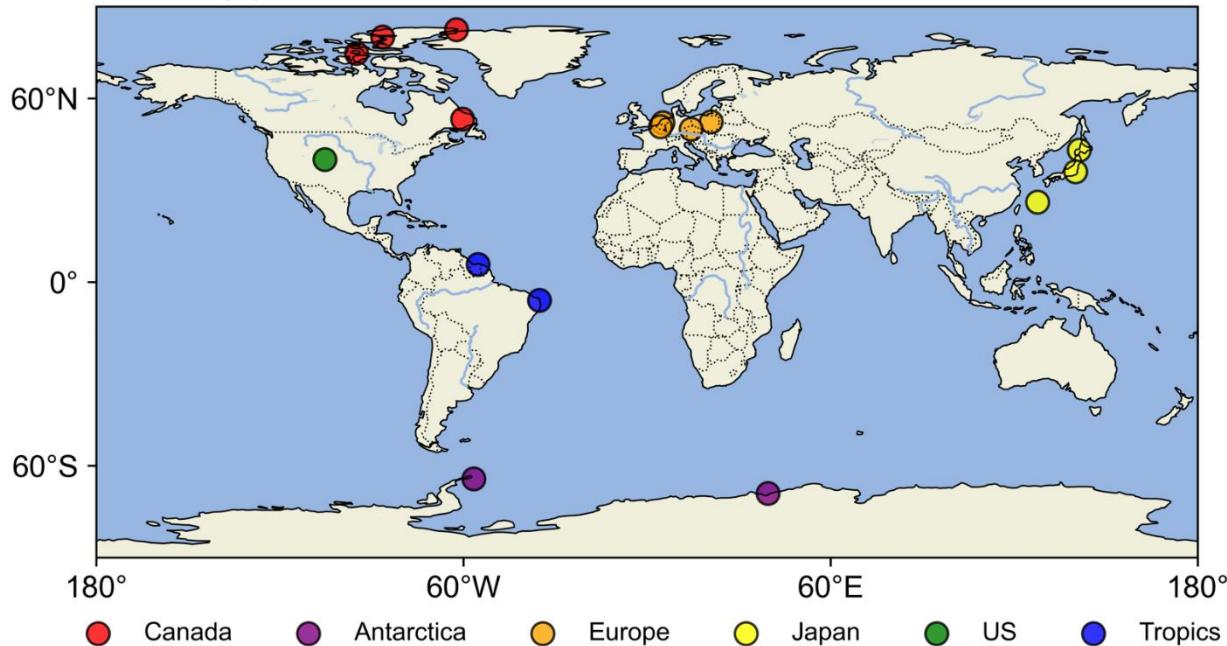
| Variables | Data sources or reference | |
|---------------------|-------------------------------------|---|
| Ozone | WOUDC network | http://woudc.org/data.php (last access: 1 Apr 2025) |
| | National monitoring networks | Wang et al. (2024) |
| | OMI satellite (Level 2) | Liu et al. (2010) |
| | OMI gridded total column ozone | https://disc.gsfc.nasa.gov/datasets/OMTO3d_003/summary (last access: 1 Apr 2025); Ziemke et al. (2017) |
| NO ₂ | OMI satellite (Level 3) | https://disc.gsfc.nasa.gov/datasets/OMNO2d_003/summary (last access: 1 Apr 2025); Lamsal et al. (2021) |
| CH ₂ O | OMI satellite (Level 3) | https://h2co.aeronomie.be/ (last access: 1 Apr 2025); De Smedt et al. (2015) |
| CO | MOPITT satellite (Level 3) | https://terra.nasa.gov/data/mopitt-data (last access: 1 Apr 2025); Deeter et al. (2021) |
| PM _{2.5} | Satellite-derived PM _{2.5} | https://sites.wustl.edu/acag/datasets/surface-pm2-5/#TOOLS (last access: 1 Apr 2025); Shen et al. (2024) |
| SWDOWN | CERES | https://ceres.larc.nasa.gov/data/ (last access: 1 Apr 2025); Kato et al. (2018) |
| OLR | | |
| SWCRF | | |
| LWCRF | | |
| Total precipitation | GPCP | https://psl.noaa.gov/data/gridded/data.gpcp.html (last access: 1 Apr 2025); |

| | | |
|--------------------|---------|---|
| TS | MERRA-2 | https://disc.gsfc.nasa.gov/datasets?keywords=MERRA-2&page=1 (last access: 1 Apr 2025) |
| Cloud fraction | | |
| Cloud liquid water | | |

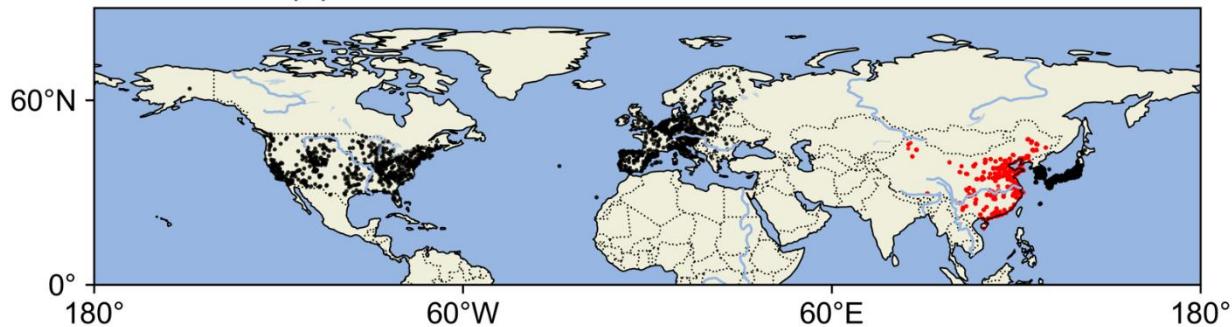


30 **Figure S1. Spatial distributions of annual total emissions used in the study compared to Figure 2 in Lu et al. (2020):** (a) total NO emissions, (b) total CO emissions, (c) biogenic isoprene emissions, (d) lightning NO emissions, (e) sea salt emissions, and (f) mineral dust emissions. Values are averaged over 2012–2014.

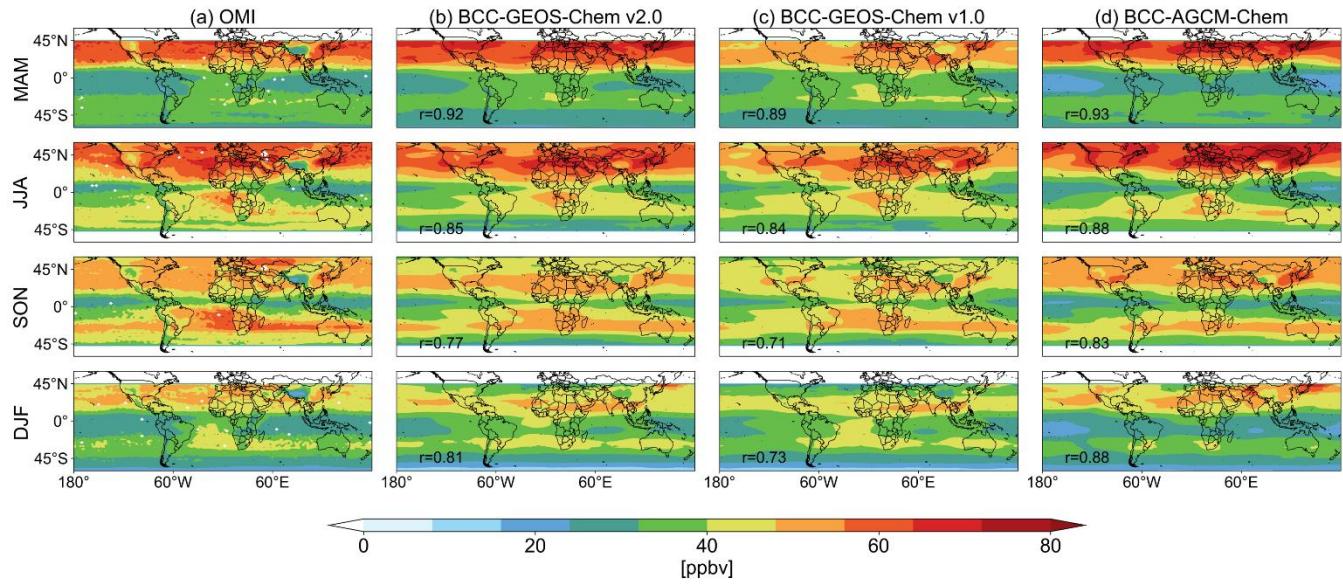
(a) Locations of selected ozonesonde observations



(b) Locations of surface ozone observations

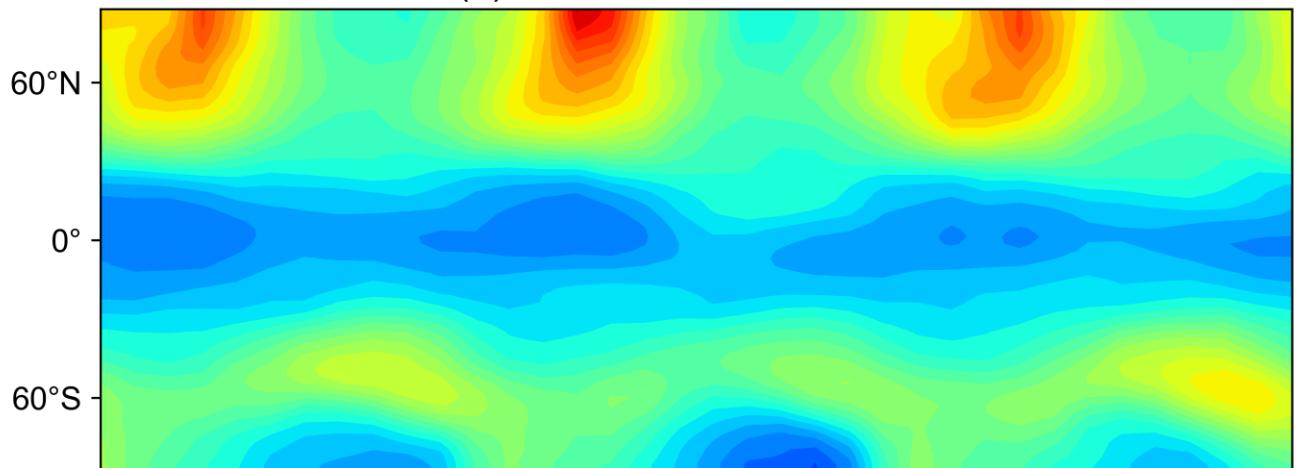


35 Figure S2. Locations of (a) selected ozonesonde observations, and (b) surface ozone observations used in this study. The black dots in panel b represent rural sites, which are used to evaluate surface ozone at T42L26 simulation, as we do not expect a coarse resolution simulation can resolve urban air pollution. The red dots represent observation sites in China used in Figure 10f. These sites are mostly located at urban or suburban regions.

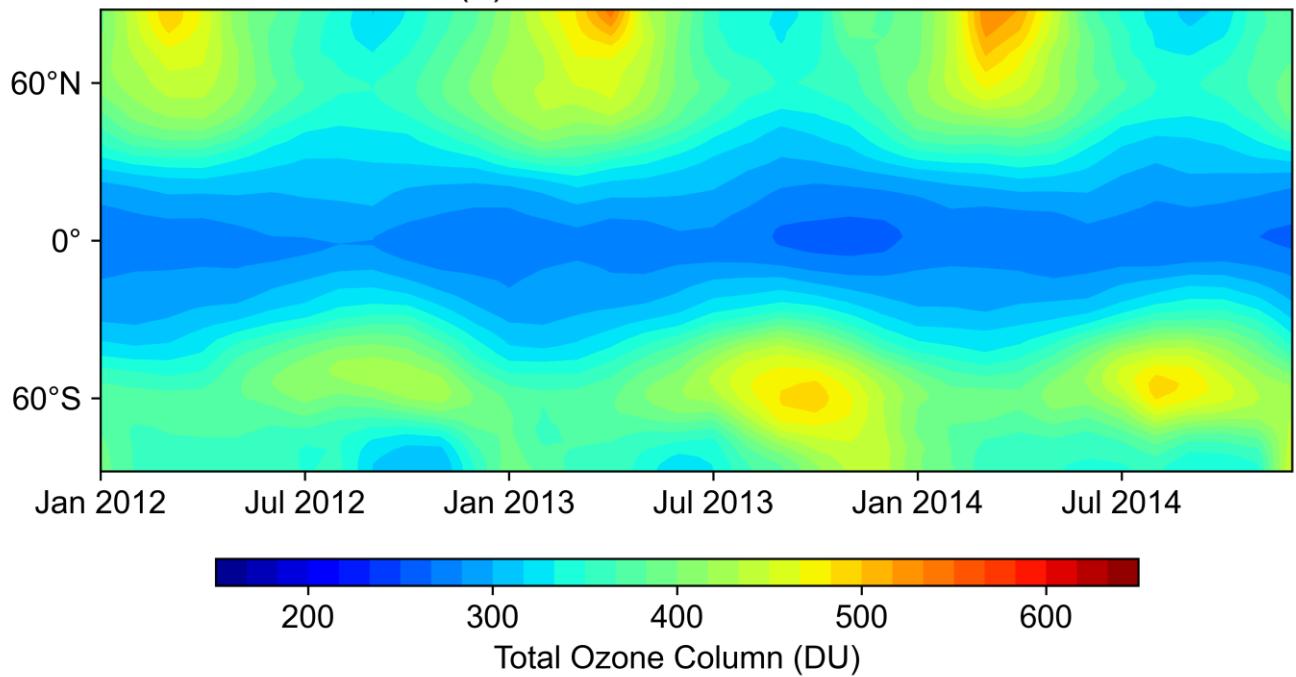


40 **Figure S3. Spatial and seasonal distributions of global mid-tropospheric ozone averaged for 700–400hPa over 2012–2014 from (a) OMI satellite observation, (b) BCC-GEOS-Chem v2.0, (c) BCC-GEOS-Chem v1.0, and (d) BCC-AGCM-Chem. All model outputs are applied with OMI averaging kernels for a proper comparison with the observations.**

(a) BCC-GEOS-Chem v2.0



(b) BCC-GEOS-Chem v1.0



45 Figure S4. Zonal-mean column ozone over 2012-2014 from (a) BCC-GEOS-Chem v2.0, and (b) BCC-GEOS-Chem v1.0.