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Global Simulation of Tropospheric Ozone and Related Tracers: Description and Evaluation of MOZART, Version 2

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Abstract

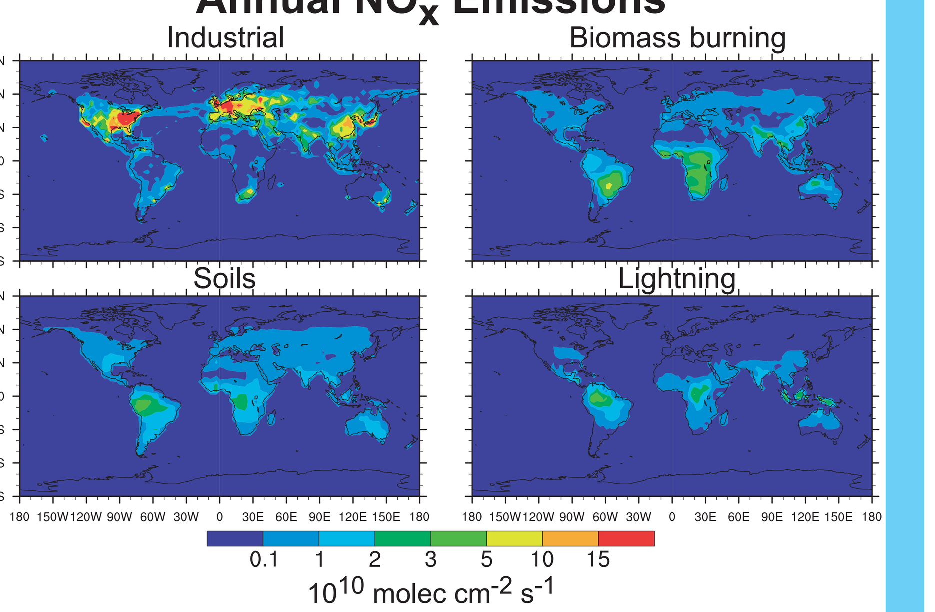
We have developed a global three-dimensional chemical transport model to simulate tropospheric ozone and its precursors. The model, called MOZART-2 (Model for OZone and Related chemical Tracers, version 2), includes a detailed representation of ozone-NO_x-NMHC chemistry. The model is built on the framework of the NCAR MATCH transport model, and can be run using a variety meteorological input datasets. Surface emissions are based on recent emission inventories. We have extensively evaluated the results of MOZART-2 by comparison with observations. MOZART-2 successfully simulates most features of the observed distributions of ozone, carbon monoxide, nitrogen oxides, and other related species. We present an analysis of the global budget of tropospheric ozone in MOZART-2, including estimates of the in situ chemistry, transport from the stratosphere, and surface deposition.

Model Description

Resolution: 2.8° lat x 2.8° long; 34 hybrid vertical levels (surface-5 mb)
Timestep: 20 minutes for all processes
Meteorology: From MACCM3, every 6 hours
Photochemistry: 58 chemical species, 132 kinetic + 31 photolysis rxns
Surface emissions: Anthropogenic emissions, EDGAR [*Olivier et al.*, 1996]
Biomass burning [*Hao and Liu*, 1994; *Müller*, 1992; *Granier et al.*, 1999]
Biogenic emissions GEIA [*Guenther et al.*, 1995]
Soil emissions [*Yienger and Levy*, 1995]
Oceanic emissions [*Brasseur et al.*, 1998]
Lightning: NO_x source in convective clouds (4 TgN/y) [*Price et al.*, 1997; *Pickering et al.*, 1998]
Advection: Flux-form semi-Lagrangian scheme [*Lin and Rood*, 1996]
Convection: Rediagnosed using *Zhang & MacFarlane* [1995] and *Hack* [1994]
Dry deposition: Velocities calculated using *Gao and Wesely* [1995], based on 10 years of 6-hourly NCEP meteorological data
Wet deposition: Based on *Giorgi and Chameides* [1985]
Boundary layer diffusion: Based on *Holtslag and Boville* [1993]

Emissions

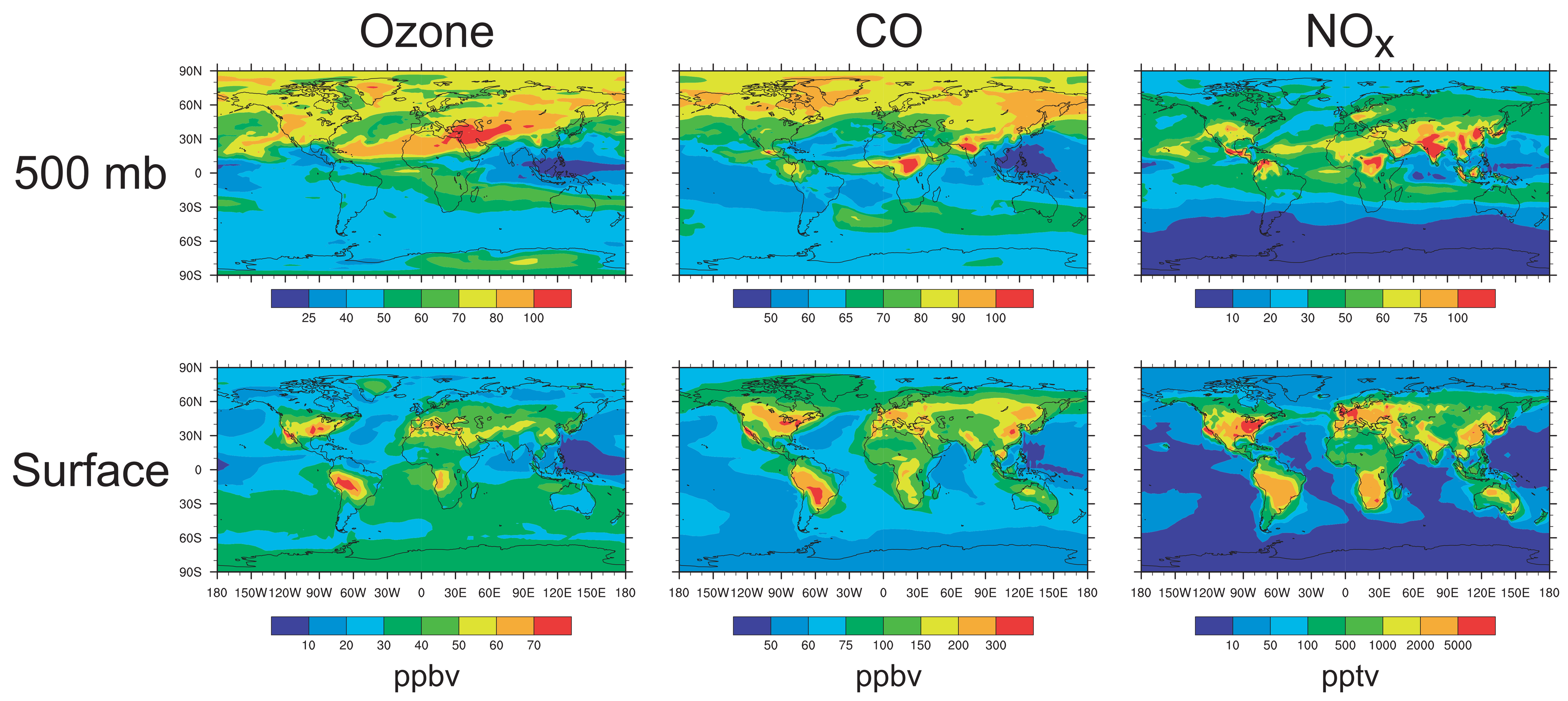
Annual NO_x Emissions



Annual mean NO_x source from fossil fuel combustion and industrial activities, biomass burning, soil emissions, and lightning (above). Summary of surface emission sources in MOZART-2 (below).

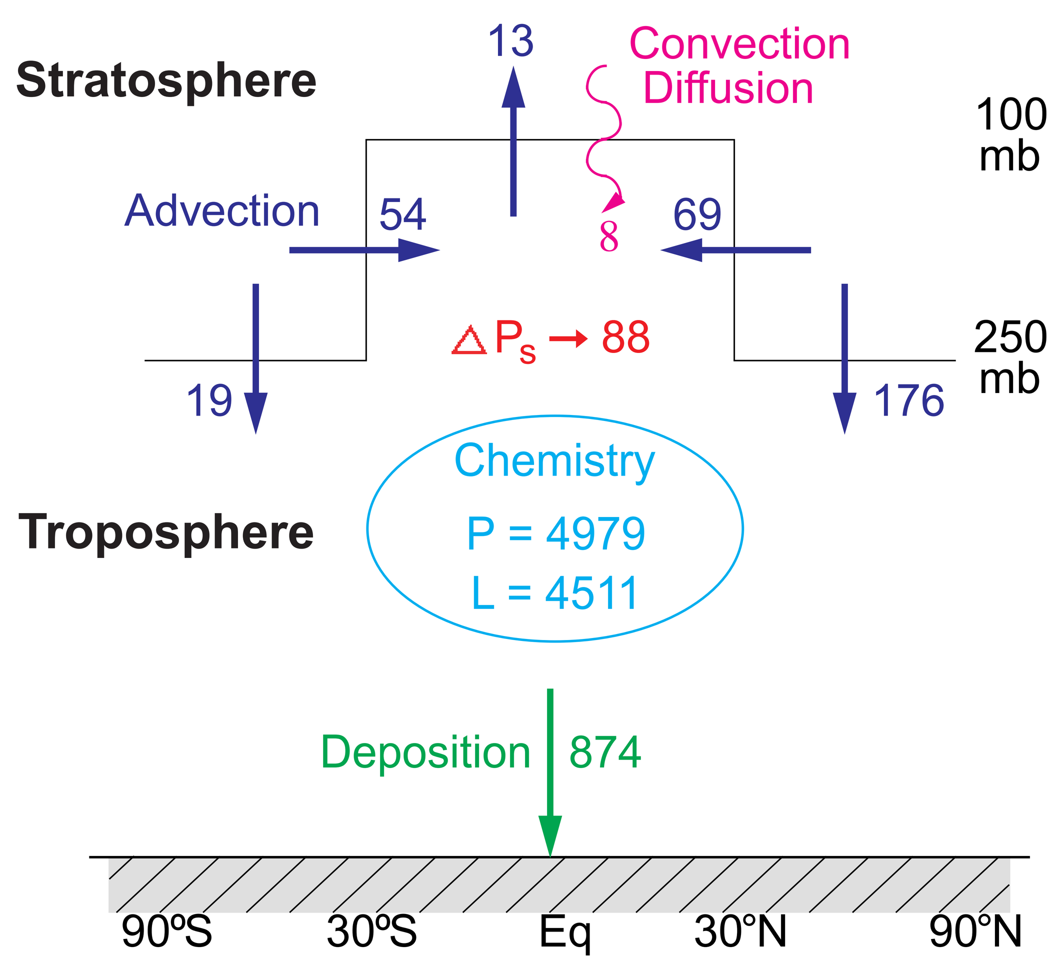
Species	Fossil fuel / Industrial	Biomass burning	Biogenic / Soil	Oceans	Total
NO (TgN/y)	23.1	8.7	6.6	0	38.4
CO (Tg/y)	306.9	711.2	181.0	10.0	1209.1
C_2H_6 (TgC/y)	6.4	4.5	0.8	0.1	11.7
C_3H_8 (TgC/y)	10.0	2.2	1.6	0.1	14.00
C_2H_4 (TgC/y)	2.0	12.3	4.3	2.1	20.7
C_3H_6 (TgC/y)	0.9	5.6	0.9	2.5	9.8
C_4H_{10} (TgC/y)	22.2	23.0	21.4	6.3	72.9
CH_3COCH_3 (Tg/y)	1.0	10.0	20.0	19.8	50.8
Isoprene (TgC/y)	0	0	411.6	0	411.6
$C_{10}H_{16}$ (TgC/y)	0	0	129.1	0	129.1

Simulated Concentrations (July)



Mixing ratios of ozone (ppbv), CO (ppbv), and NO_x (pptv) at approximately 500 mb and the surface.

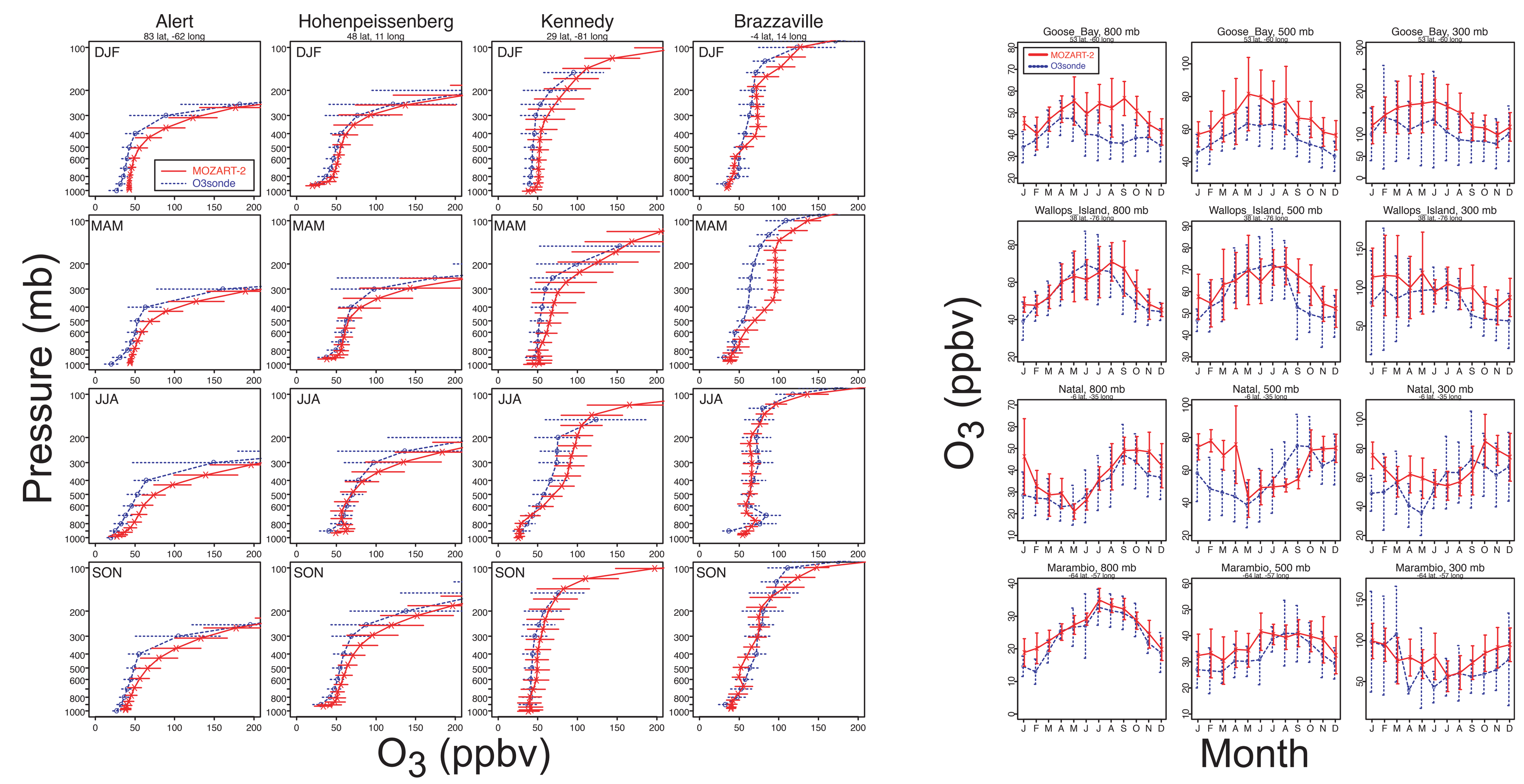
Tropospheric ozone budget



Budget of ozone in the troposphere calculated by MOZART-2, in units of Tg O_3/y. Terms included are: advective fluxes, chemical production and loss, dry deposition to surface, convection and vertical diffusion, and mass consistency correction in the advection scheme. The "net" source from transport is 401 Tg O_3/y. Net chemical production in the troposphere is 468 Tg/y. For this budget, the troposphere was defined as extending up to 100 mb in the tropics (30°S-30°N) and 250 mb in the extratropics.

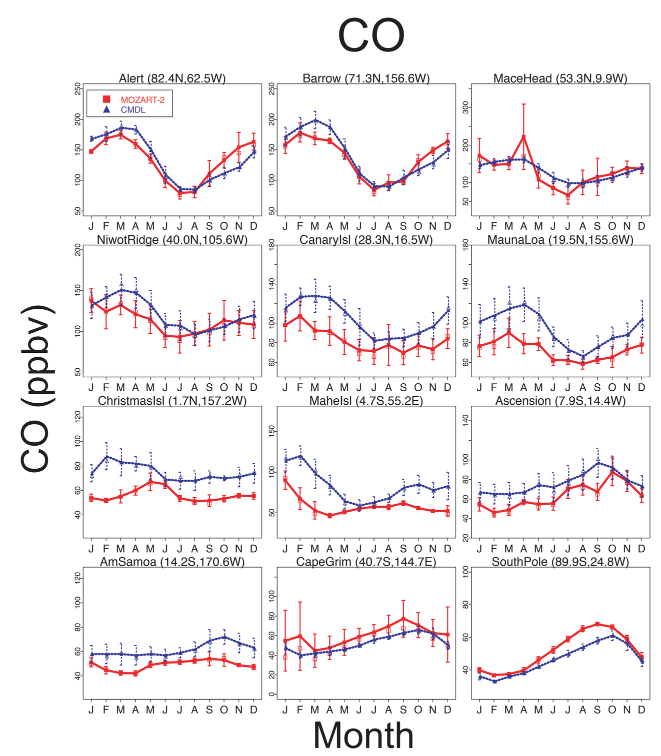
Model Evaluation

Ozonesondes



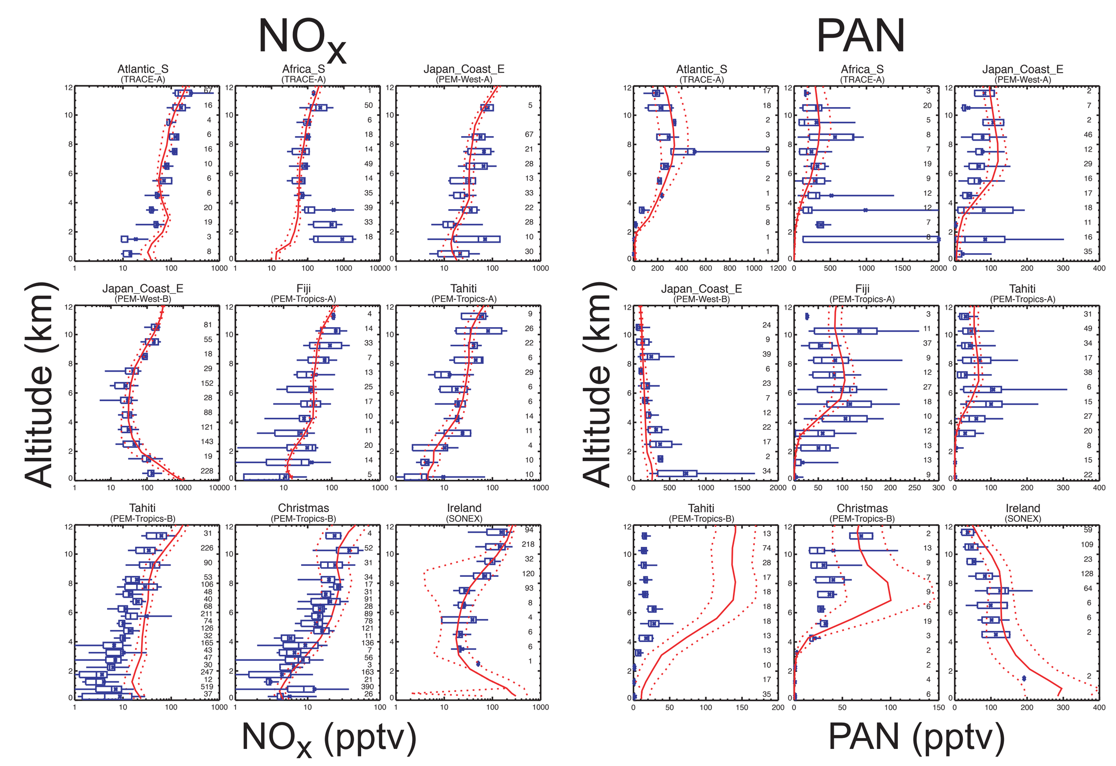
Comparison of simulated ozone (in ppbv) from MOZART-2 (solid red) with ozonesonde observations (dotted blue) [*Logan*, 1999]. Plots show vertical profiles of seasonal means (left) and monthly means at three pressure levels (right).

CO



Comparison of simulated monthly mean CO (ppbv) from MOZART-2 (solid red) with observations from CMDL (dotted blue) [*Novelli et al.*, 1998].

NO_x / PAN



Mean observed (blue bars) and simulated (red lines) regional vertical profiles of NO_x (left) and PAN (right) (pptv). Observations are from NASA aircraft campaigns.

Conclusions

- MOZART-2 successfully simulates the major features of the observed distributions of ozone, CO, NO_x, PAN, and related species (including peroxides and carbonyls, not shown). Horizontal and vertical gradients and seasonality generally agree well with observations.
- Discrepancies with observations include an underestimate of CO at tropical surface sites, and an overestimate of PAN in the upper troposphere at some sites. In addition, nitric acid (not shown) is overestimated by the model at many locations.
- The calculated budget of tropospheric ozone is within the range found in previous global chemical transport model studies. The photochemical production and loss rates of ozone in the troposphere are higher than found in many earlier modelling studies.
- The net influx of ozone from the stratosphere is at the low end of the range found in recent chemical transport modelling studies. This influx shows significant hemispheric asymmetry, especially in the extratropics.
- The large source of ozone due to the mass consistency correction in the advection scheme (88 Tg/y in the troposphere) indicates a significant problem for offline chemical transport models.

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