Evaluation of model simulated source contributions to tropospheric ozone with aircraft observations in the factor projected space

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Tropospheric O_3: Sources and seasonal trends

Major known sources

- **Stratospheric input**
- **Photochemical production**
- **Long-range/intercontinental transport**

- **Previously, using receptor modeling (positive matrix factorization (PMF)), we estimated the source contributions to TOPSE O_3 and found that the observed increase during springtime is mainly due to the intercontinental transport of O_3 and its precursors [Wang et al., 2003].**

- **This approach is useful because multiple observed tracers can be analysed in a consistent manner and the resulting attributions do not carry explicit a priori assumptions.**

! However, direct comparison of simulated attributions with the observation is lacking.

Objectives

Evaluation of 3-D global chemical transport model (GEOS-Chem) simulated tracers with TOPSE and TRACE-P measurements in the projected factor space. Specifically, the contributions from tropospheric photochemical production, tropospheric long-range transport, and transport from the stratosphere are investigated.

PMF analysis

PMF results represent the source characteristics and their variability of the captured samples based on covariance between them.

It is an advanced factor analysis method.

Measurements & Simulations

Measurements

Select relatively long-lived chemical tracers including O_3, NOy, PAN, CO, C_3H_8, CH_3Cl, and Beryllium-7,and one dynamic tracer (potential temperature).

I. TOPSE

Mid latitudes (40˚N – 60˚N, 87˚W – 104˚W), High latitudes (60˚N – 85˚N, 61˚W – 94˚W).The selected data has a bias towards high altitudes of 5 – 8 km (~70% of the data) due to the availability of 7Be measurements (150 – 200 points).

II. TRACE-P

Low latitudes (< 30˚N, 115˚E – 160˚W), Mid latitudes (30˚N – 45˚N, 115˚E – 160˚W). The selected data has a bias towards high altitudes of 7 – 12 km (~50% of the data) due to the availability of 7Be measurements (70 – 90 points).

Measurements & Simulations

Global chemical transport model (GEOS-Chem)

- **Using assimilated meteorological data from GMAO with horizontal resolution of 2˚x2.5˚ and 30 vertical layers (GEOS-3)**
- **Including comprehensive chemical mechanisms of tropospheric O_3-NOx-VOCs (version 7.01)**
- **Separate ^{7}Be and CH_3Cl simulations are conducted.**
- **Tagged O_3 simulation results are used in order to estimate stratospheric O_3 contributions in the model.**

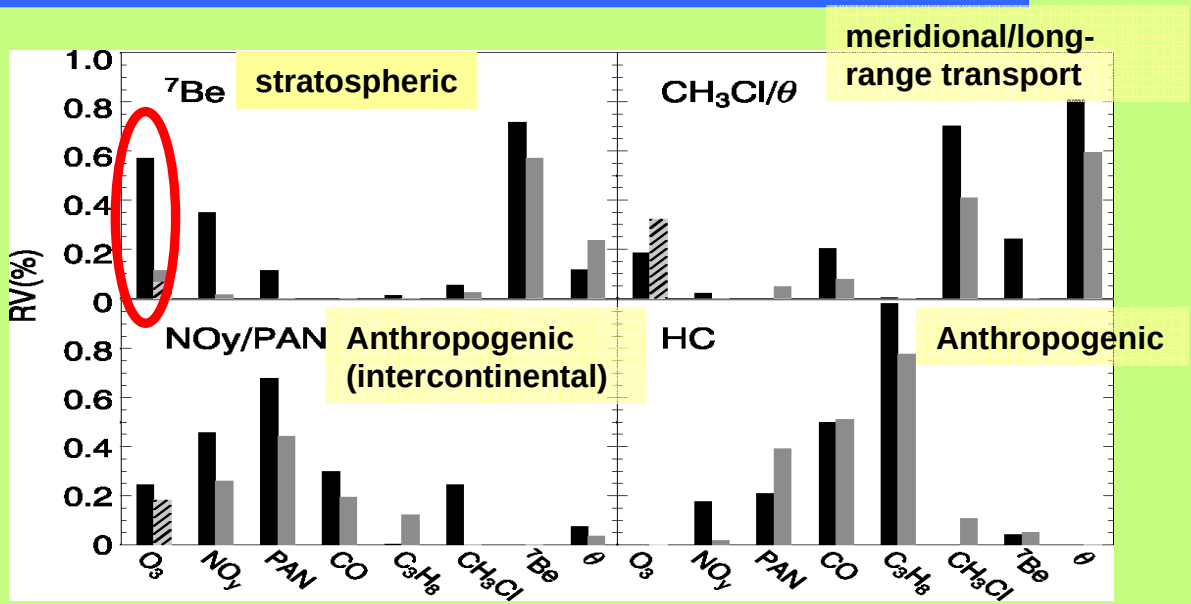
Back trajectory analysis

- **The back trajectories of high factor score-points in each factor are useful in some cases to identify its characteristic.**

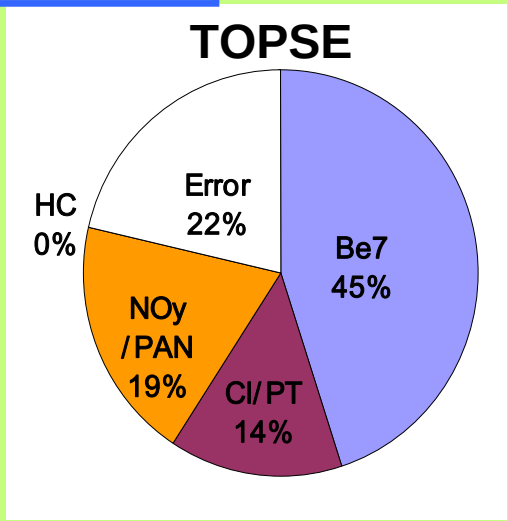
Result: TOPSE Middle latitudes

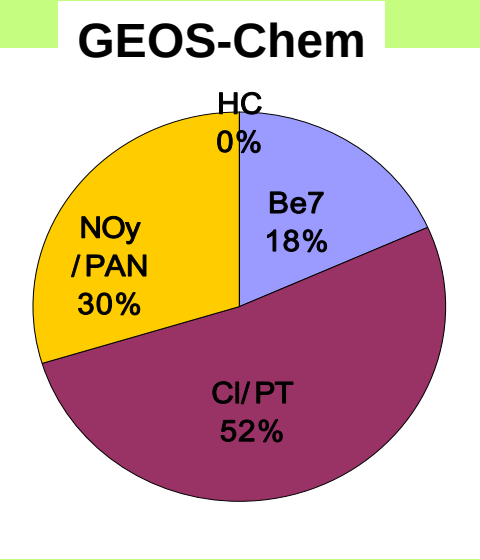
Relative factor loadings (scaled by measurement absolute variability) for 4 identified factors

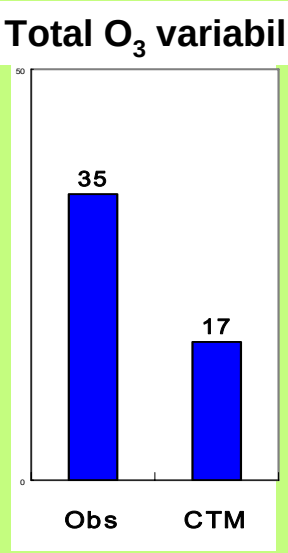
***Black*: Obs.**
***Gray*: GEOS-Chem**
***Strips on O_3*: tropospheric fraction**



Fractions of O_3 variability





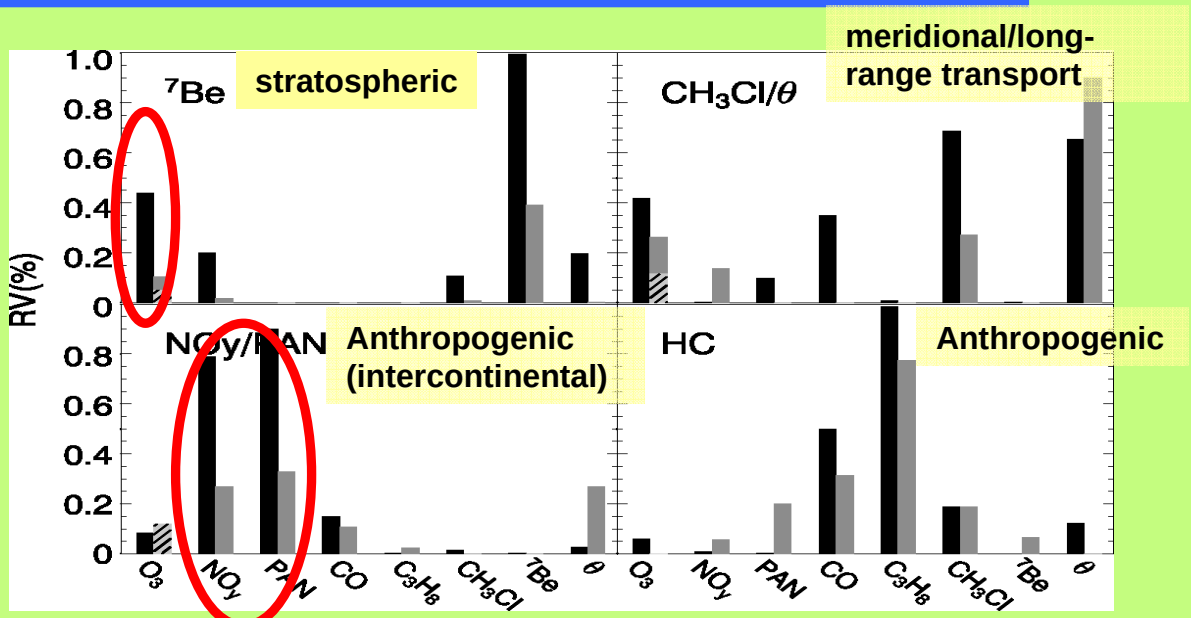


* HC: Hydrocarbon, Cl: CH_3Cl, PT: potential temperature

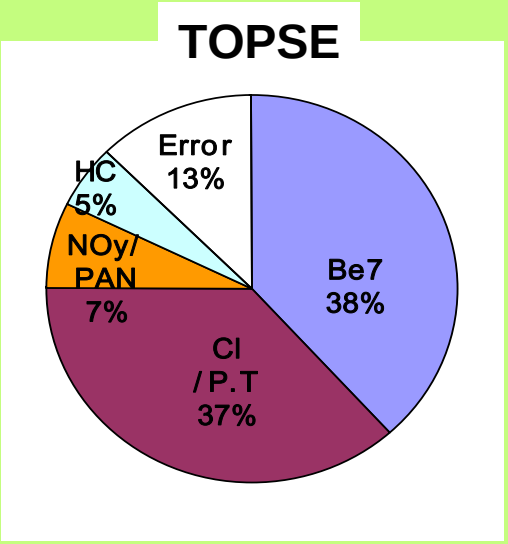
Result: TOPSE High latitudes

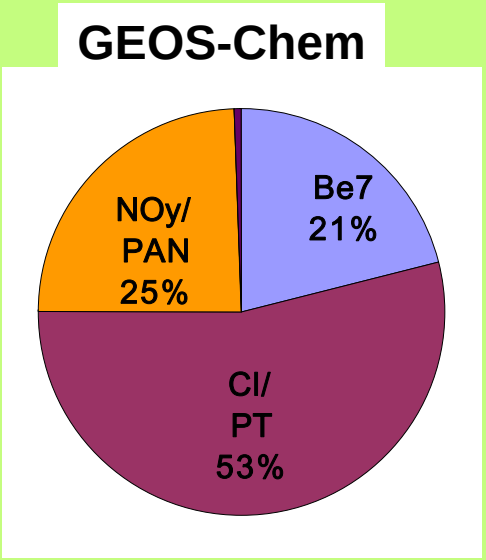
Relative factor loadings for 4 identified factors

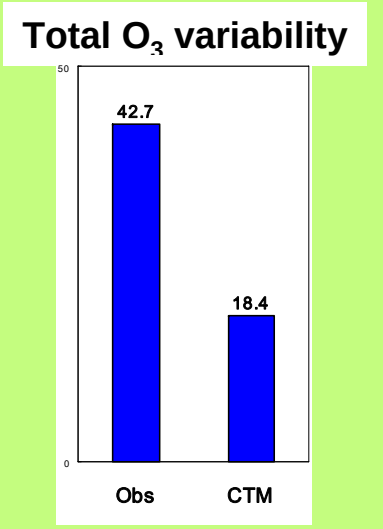
***Black*: Obs.**
***Gray*: GEOS-Chem**
***Strips on O_3*: tropospheric fraction**



Fractions of O_3 variability





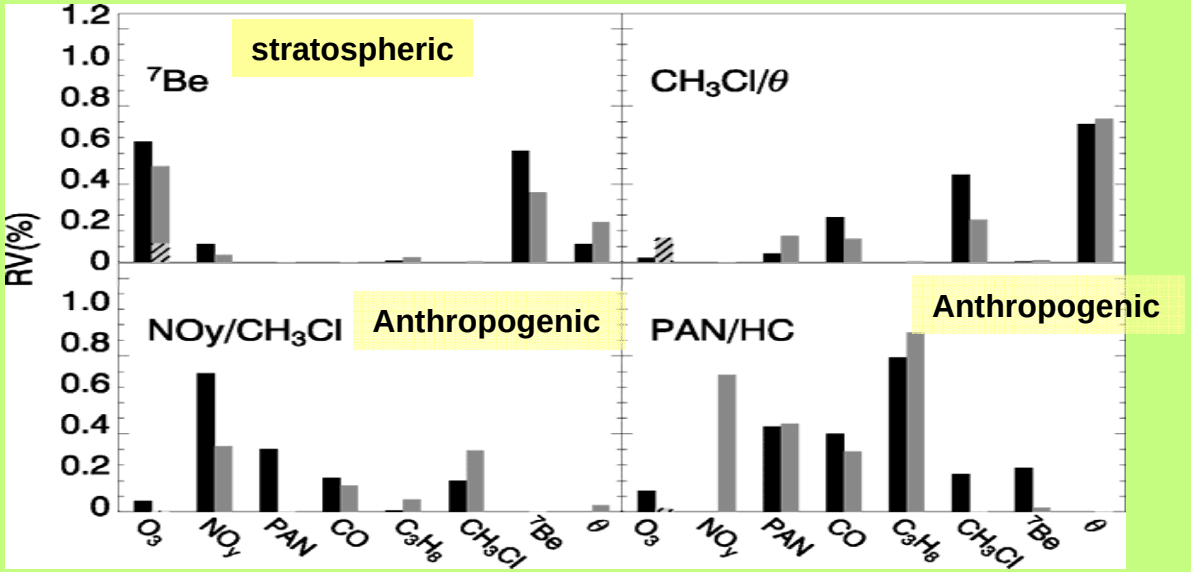


* HC: Hydrocarbon, Cl: CH_3Cl, PT: potential temperature

Result: TRACE-P Middle latitudes

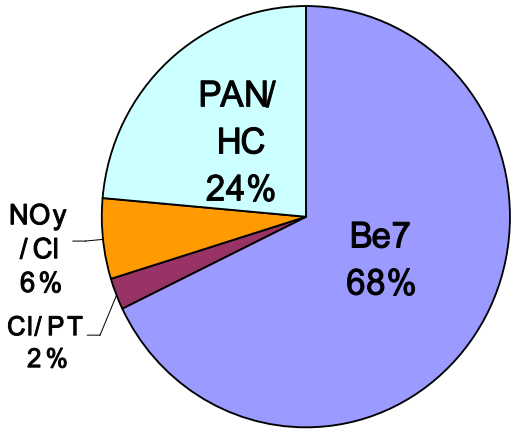
Relative factor loadings for 4 identified factors

***Black*: Obs.**
***Gray*: GEOS-Chem**
***Strips on O_3*: tropospheric fraction**

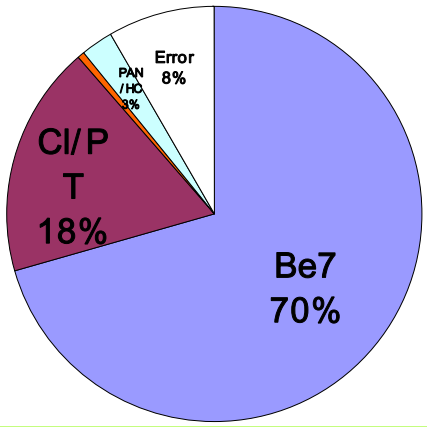


Fractions of O_3 variability

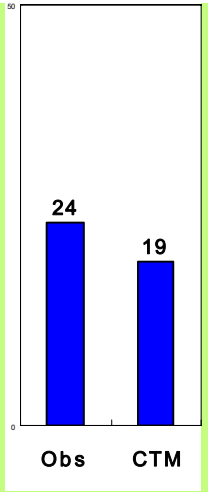
TRACE-P



GEOS-Chem



Total O_3 variability

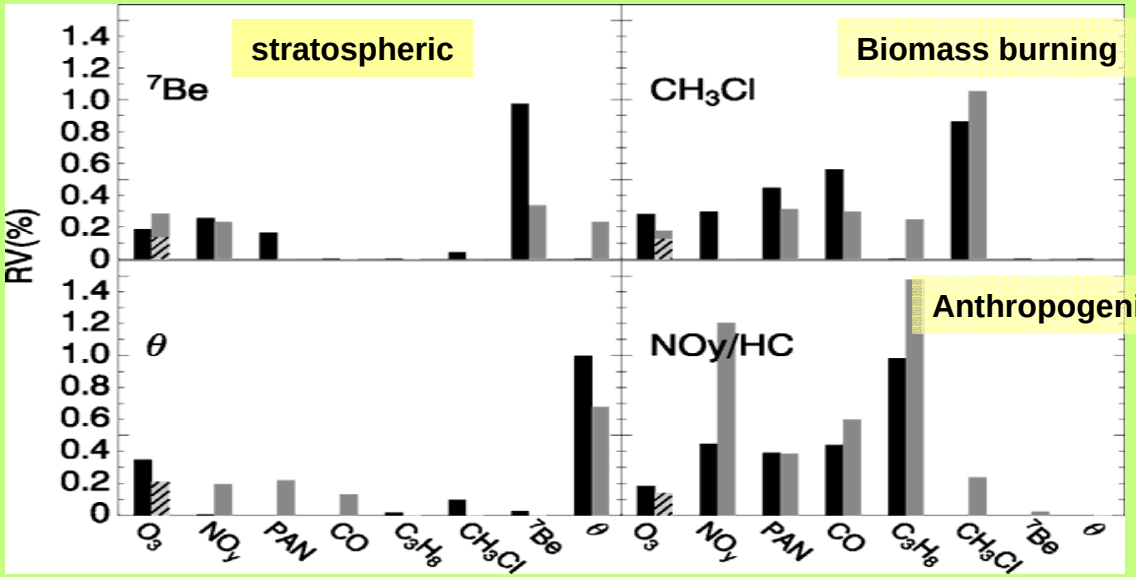


* HC: Hydrocarbon, Cl: CH_3Cl, PT: potential temperature

Result: TRACE-P Low latitudes

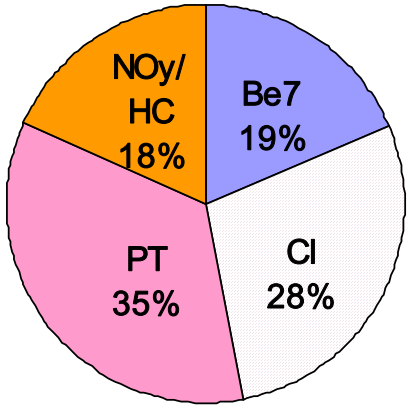
Relative factor loadings for 4 identified factors

***Black*: Obs.**
***Gray*: GEOS-Chem**
***Strips on O_3*: tropospheric fraction**

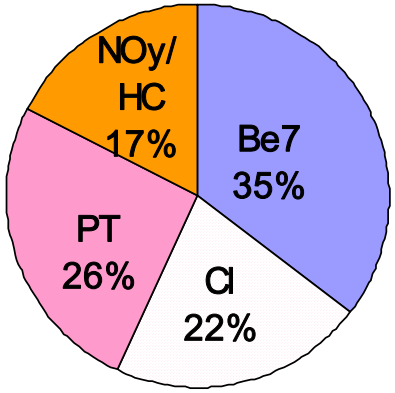


Fractions of O_3 variability

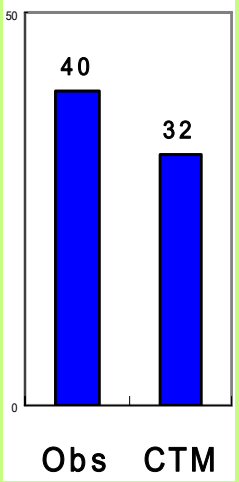
TRACE-P



GEOS-Chem



Total O_3 variability



* HC: Hydrocarbon, Cl: CH_3Cl, PT: potential temperature

Results: O_3 fractions (ppbv)

TOPSE O_3 Mid (ppbv)		
Factors	**Obs**	**CTM**
^{7}Be	**15.7**	3.1
Cl/θ	5.0	8.8
NOy/PAN	6.7	5.0
HC	0.0	0.0

TOPSE O_3 High (ppbv)		
Factors	**Obs**	**CTM**
^{7}Be	**16.4**	3.9
Cl/θ	15.6	9.9
NOy/PAN	3.1	4.5
HC	2.2	0.0

TRACE-P O_3 Mid (ppbv)		
Factors	**Obs**	**CTM**
^{7}Be	17.3	13.7
Cl/θ	0.6	3.5
NOy/Cl	1.6	0.1
PAN/HC	**6.0**	0.5

TRACE-P O_3 Low (ppbv)		
Factors	**Obs**	**CTM**
^{7}Be	7.6	11.7
Cl	11.6	7.3
θ	14.2	8.5
NOy/HC	7.5	5.8

Conclusions

- During TOPSE, the stratospheric contribution of ~ 16 ppbv to tropospheric O_3 variability from the measurements is much higher than that of the model (only 3 – 4 ppbv), indicating a large model underestimation.

- In contrast, the stratospheric contribution for TRACE-P is comparable between the measurements and model (8 – 17 ppbv and 12 – 14 ppbv, respectively).

- At mid latitude during TRACE-P, the model result indicates that most of ozone in the ^{7}Be factor originates from the stratospehere.

- Measurements and model simulation for TRACE-P at low latitudes suggest substantial contributions to O_3 from photochemical production in biomass burning and convective (with lightning) air masses.