Evaluating model simulated tropospheric ozone sources in the upper troposphere

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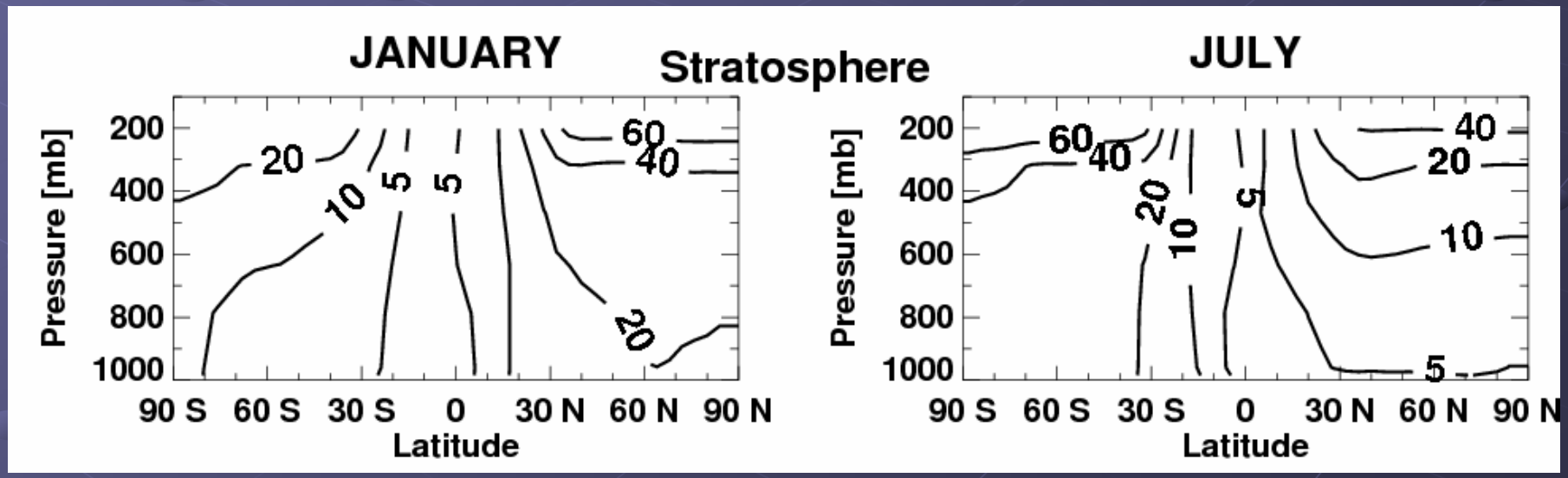
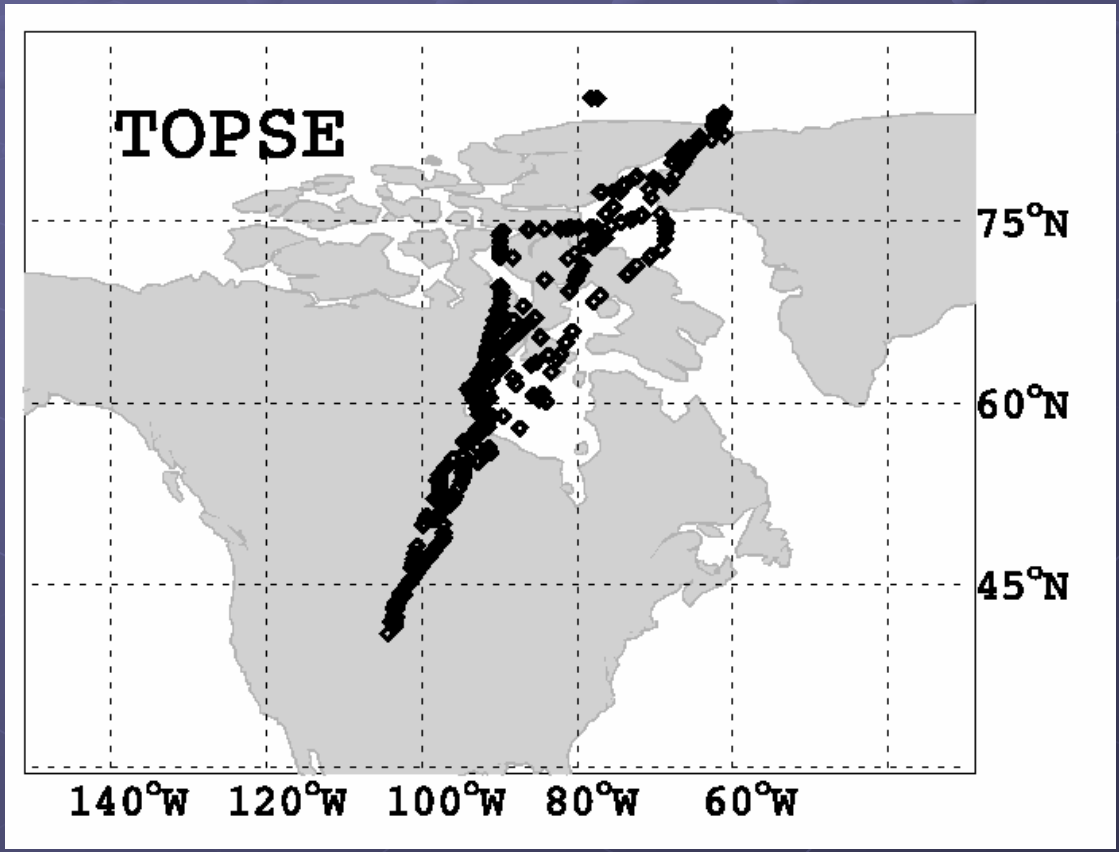
- Upper tropospheric O_3 mixing ratios are strongly affected by transport from the stratosphere
- 3-D models are often used in the assessments. However, direct evidence from the measurements remains elusive
- Interpretations of in situ measurement data tend to diverge



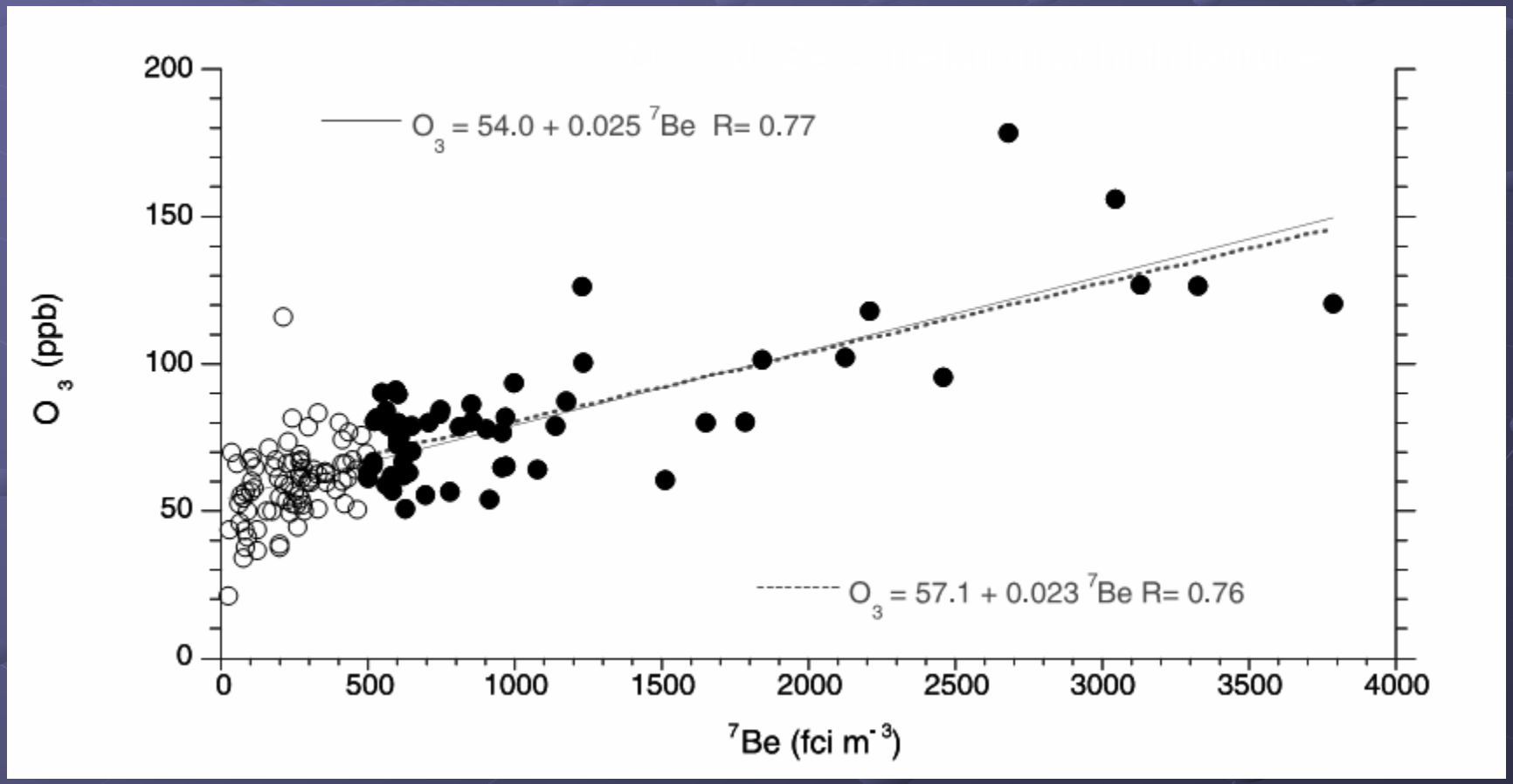
(Wang et al., 1998)

- TOPSE measurements from February to May, 2000
- Stratospheric ozone flux maximizes in spring at mid-high latitudes



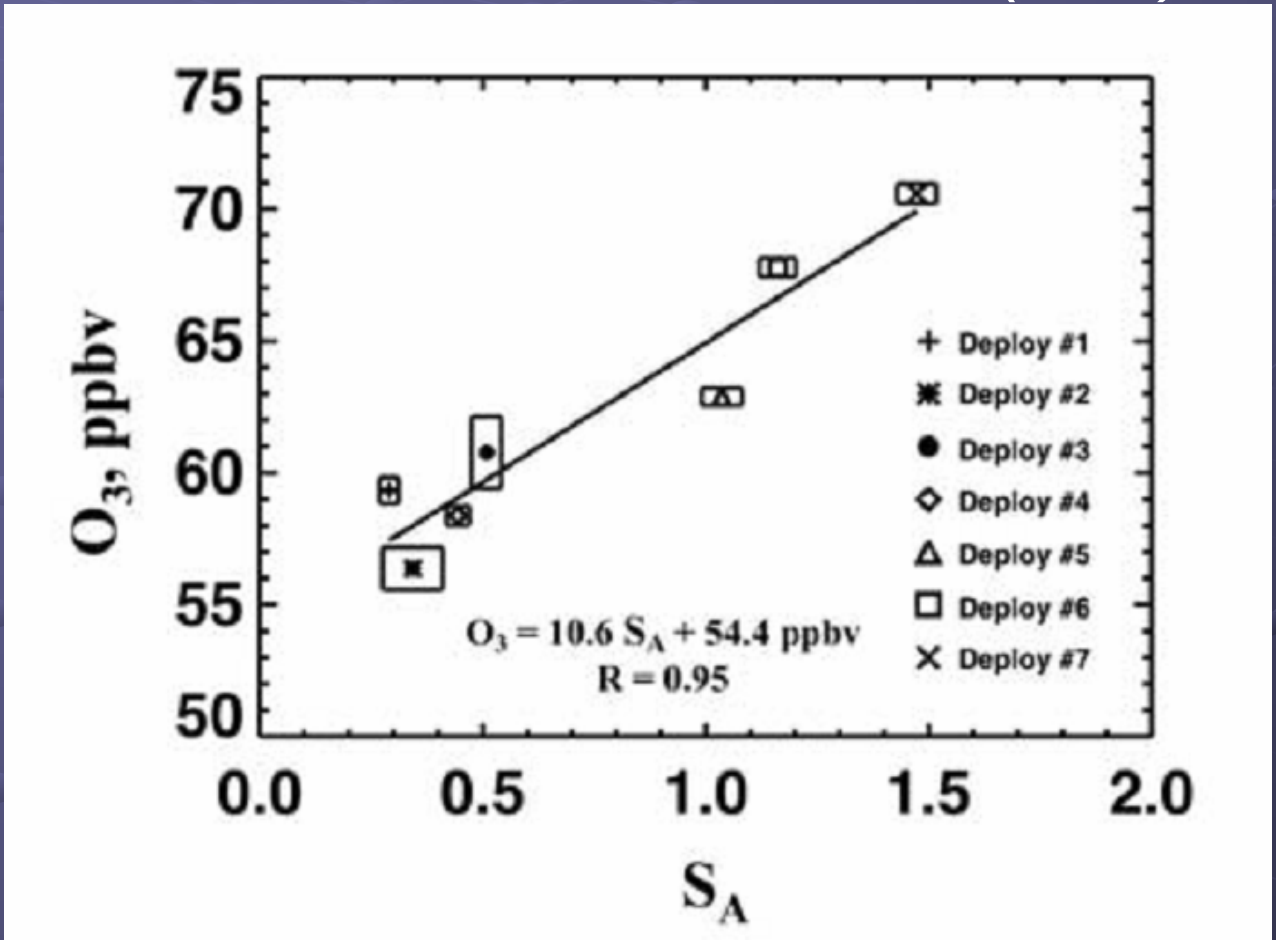
"…the stratospheric source can account for a dominant fraction (> 85%) of in situ O_3 throughout TOPSE…"

Dibb et al. (2003)



"The dominant source of the free tropospheric O_3 trend (>80%) was found to be photochemical O_3 production"

Browell et al. (2003)



Correlation between O_3 and IR aerosol scattering ratio at 60-85 N, 4-6 km,

Allen et al. (2003)

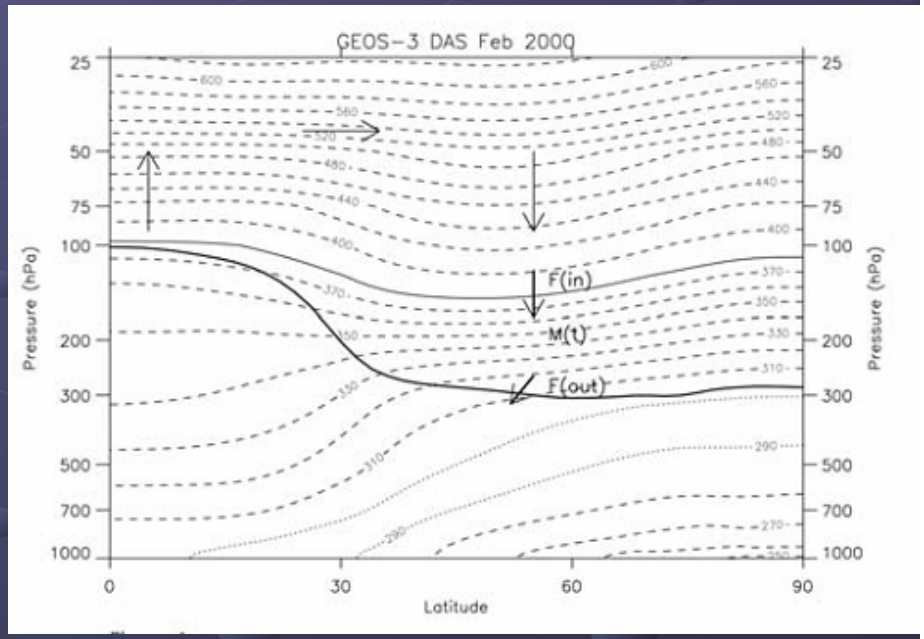
- Correlations of ^{7}Be and O_3 are used

$$dO_3/dt = d(\text{strat-}^{7}\text{Be})/dt * f_{strat}(O_3)$$

- Stratospheric contribution to O_3 trends is estimated at 20-60%

Emmons et al. (2003)

- Stratospheric flux is 16-33% of the total flux (including horizontal influx and production)
- Stratospheric O_3 fraction is 31-56%



Model evaluations

- Budget/fraction calculations in the model cannot be compared directly with available measurements
- However, tracer correlations can be directly evaluated
- Correlation of single-pair species can be biased

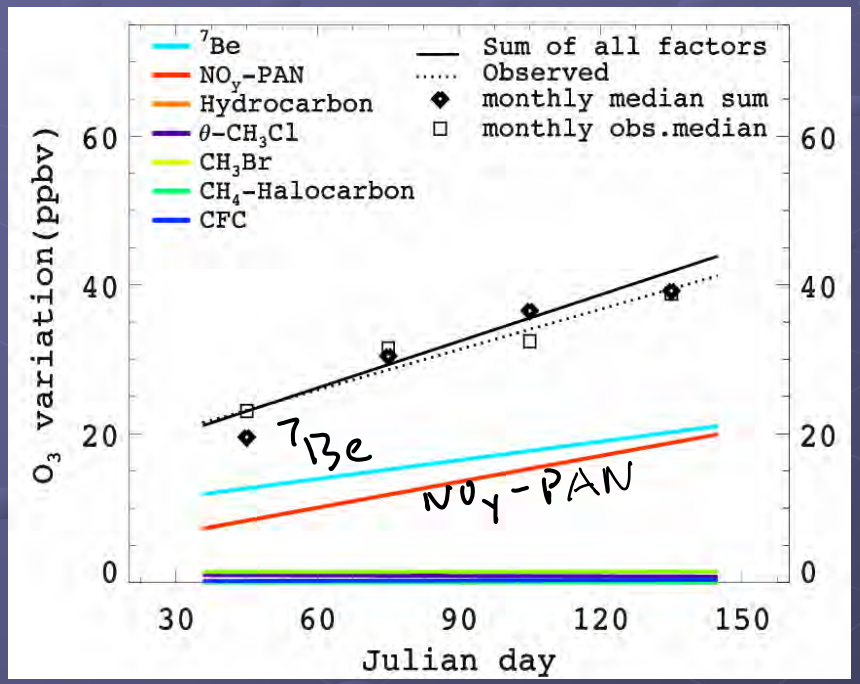
Positive matrix factorization

$$x_{ij} = \sum_{k=1}^{p} g_{ik} f_{kj} + e_{ij}$$

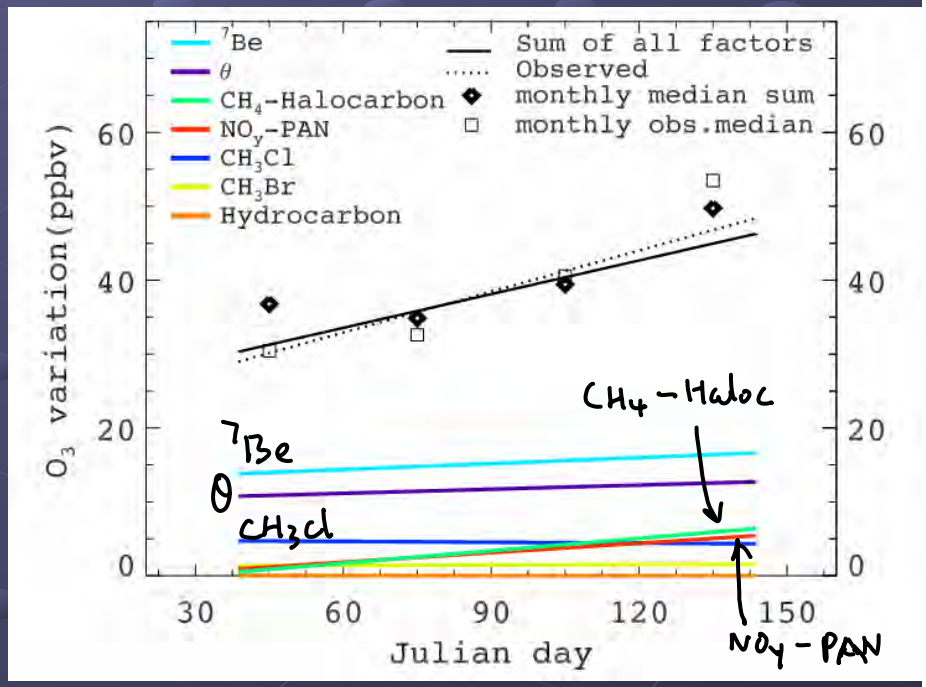
- "Objective" multivariate analysis
- O_3
- ^7Be
- Potential temperature
- NOy, PAN
- CO, C_2H_2, C_3H_8
- CH_4
- CH_3Cl, CH_3Br
- C_2Cl_4, CFC-11, HCFC-141B, Halon-1211

(*Wang et al., 2003*)

- Factors contributing to O_3 fractions may not contribute to its trend
- Long-range O_3 transport in nitrogen-poor air masses is very important for high latitudes
- The number of species needed to resolve the factors is not that large



Mid latitudes



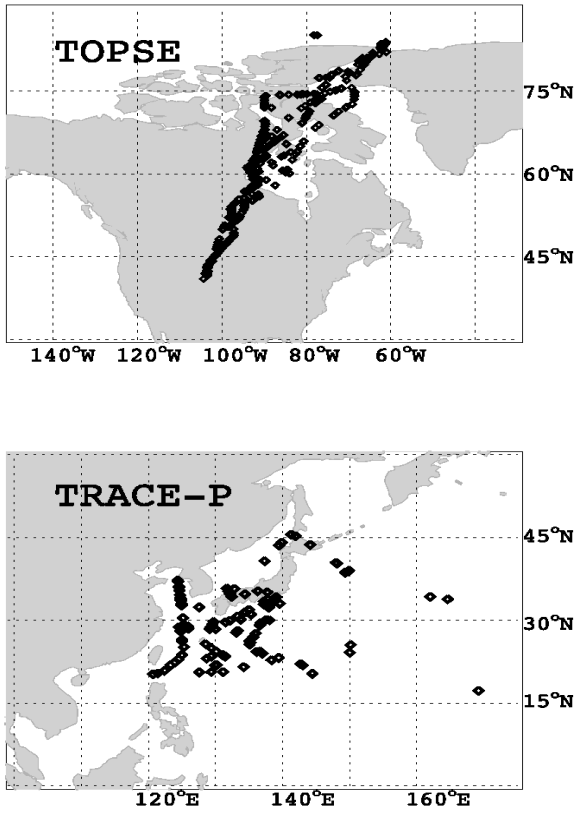
High latitudes

Model evaluation of O_3 contributions

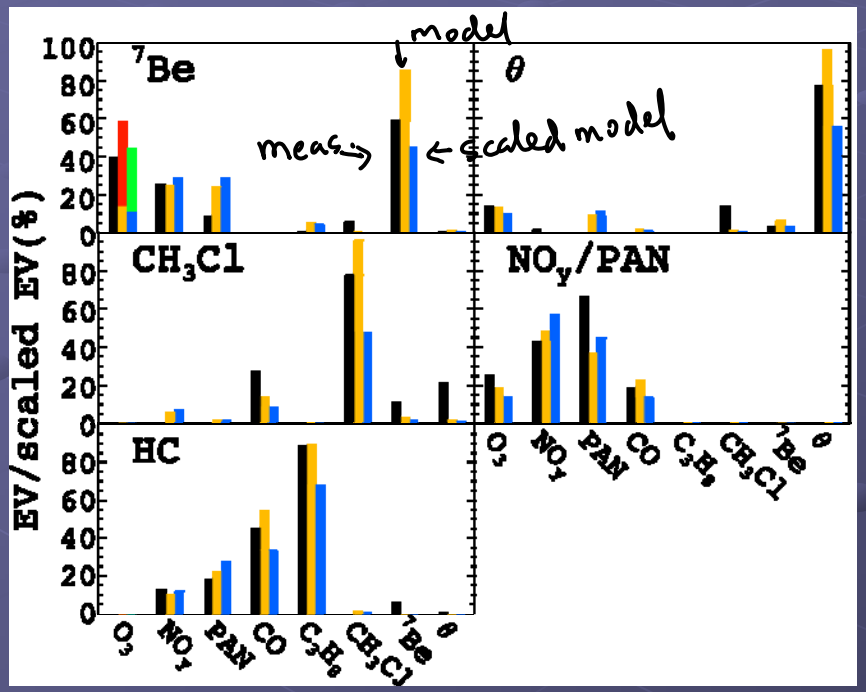
- Measurements from TOPSE and TRACE-P (GEOS-CHEM using GEOS-3 met data)
- O_3
- ^7Be (Liu et al., 2002)
- Potential temperature
- NOy, PAN
- CO, C_3H_8
- CH_3Cl (Yoshida et al., 2004,2006)

- Upper and middle troposphere (limited by ^7Be)

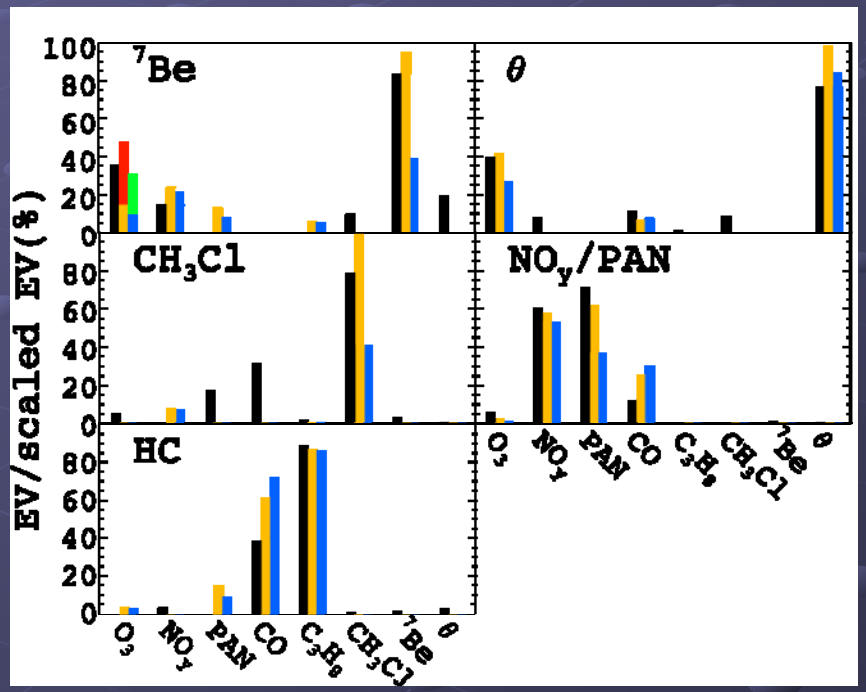
(*Shim et al, ACP, 2008*)



- Simulated factor profiles are in good agreement with the measurements
- 80% of O_3 in the ^7Be factor is stratospheric

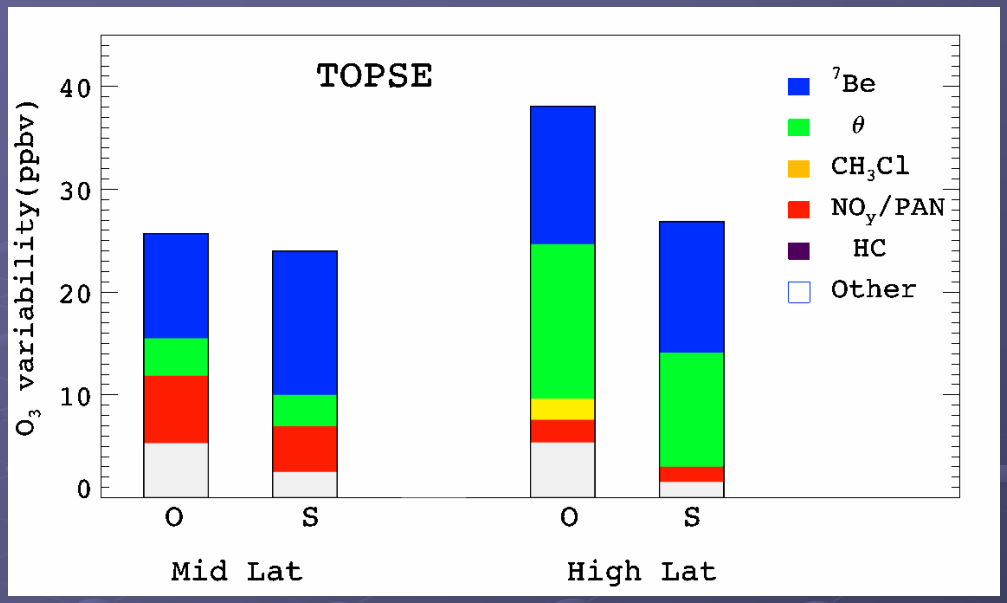


TOPSE mid latitudes



High latitudes

The factor contributions to O_3 are simulated.

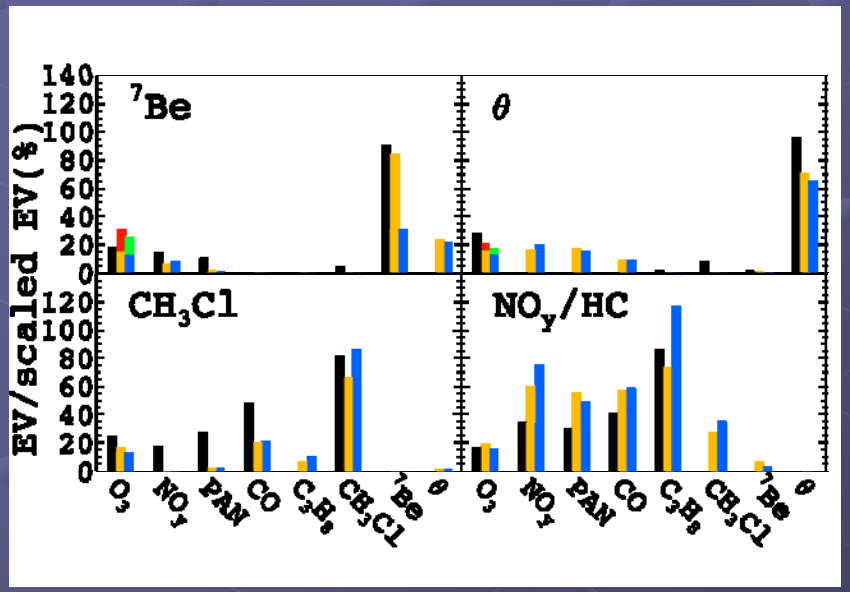


However, the O_3 trends are underestimated by a factor of 2-3.

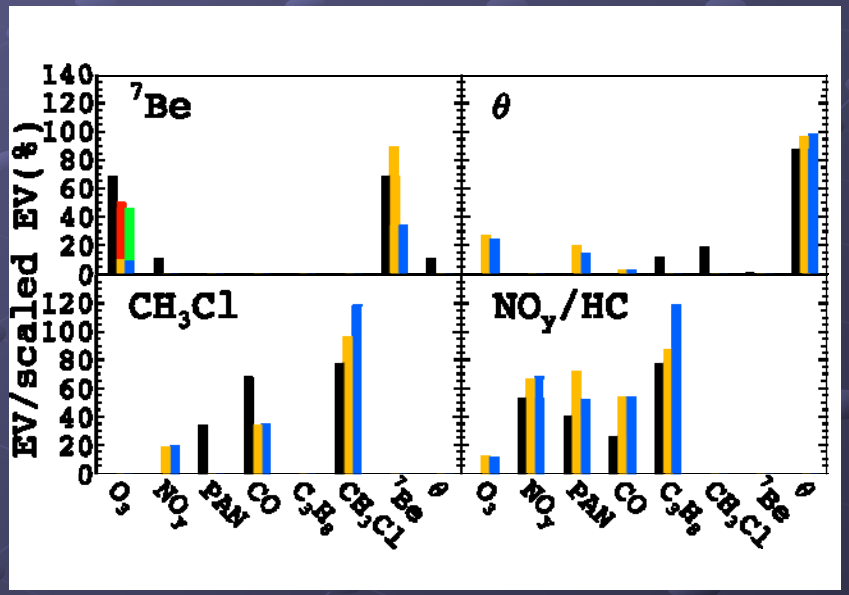
	Mid latitudes		High latitudes	
	Obs	Mod	Obs	Mod
^{7}Be	2.7	1.3	1.8	0.8
Θ	0.3	0.4	1.2	0.8
CH_3Cl	0	0	0.3	0
NO_y/PAN	3.5	1.3	1.1	0.1
HC	0	0	0	-0.4
Total	6.5	3.0	4.3	1.3

Factor contributions to O_3 seasonal increase (ppbv/month) for TOPSE.

- Factor profiles are reasonably simulated
- Contribution from the stratospheric (^{7}Be) factor is small at lower latitudes
- ^{7}Be source is too low

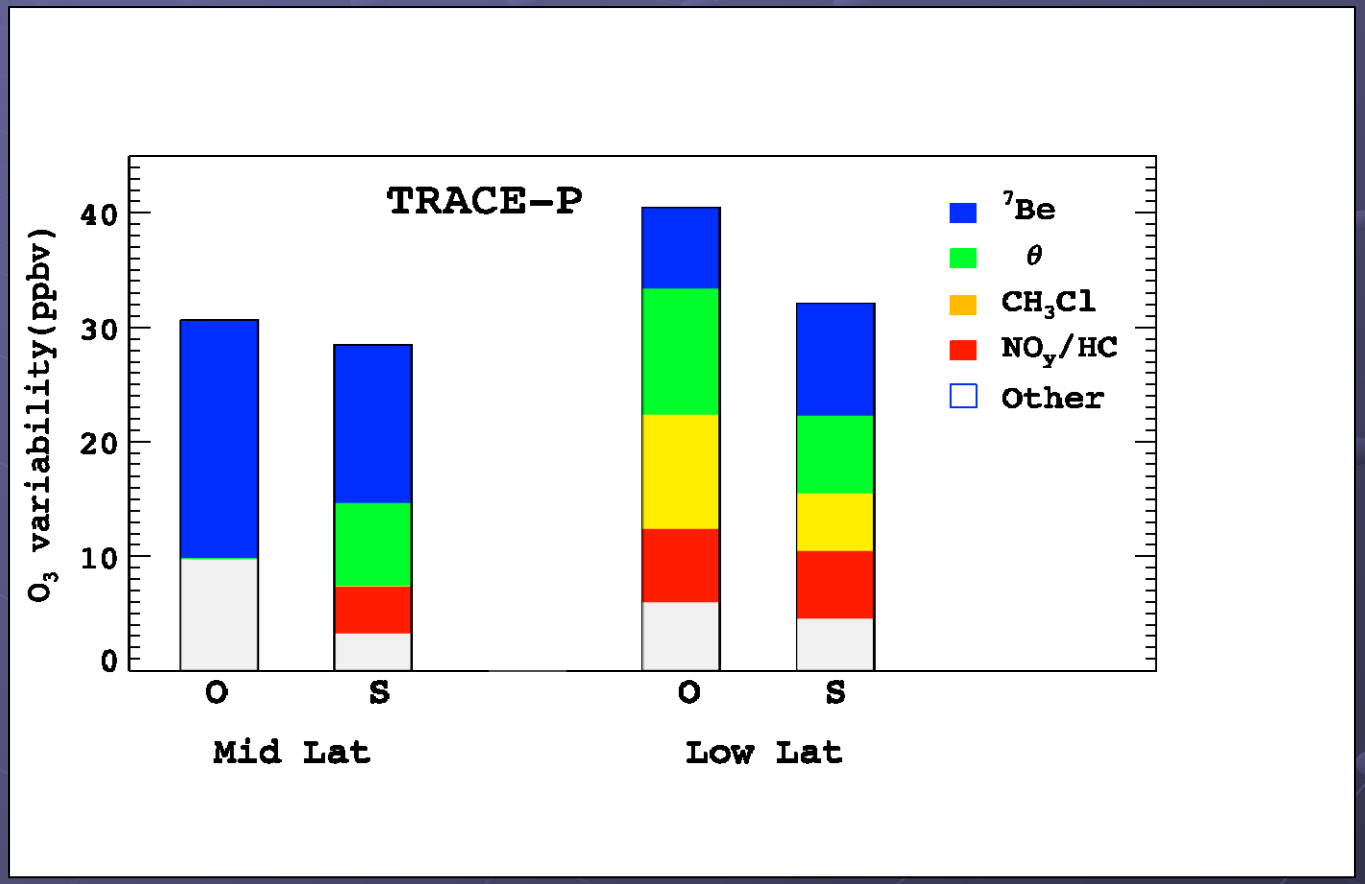


TRACE-P 15-30 N



30-45 N

Latitudinal difference in long-range transport factors (^7Be, θ, and CH_3Cl) is lower in the model. One possibility is that mixing between mid (30-45 N) and lower (15-30 N) latitudes appears to be too fast



Conclusions

- Simulated O_3 source contributions are only indirectly constrained by measurements
- Factor analysis is a promising method to quantify measurement-based constraints
- The average O_3 contributions are simulated much better than their temporal trends