Using Meteorological Analyses for Off-Line Chemical Transport Modelling

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- Description of Off-Line Models
- Example CTM results
- Formulation of a TOMCAT/SLIMCAT models
    - Mass conservation
    - Vertical motion
    - Chemical data assimilation
- Summary

Off-Line Chemical Transport Modelling

Off-line CTM:

• Meteorology (winds, temperature, humidity?) specified from analyses.

• Model integrates chemical species.

• Model constrained to 'real' meteorology - good for comparison with observations.

• Computationally simpler (no internal variability) and cheaper than a coupled chemistry-GCM.

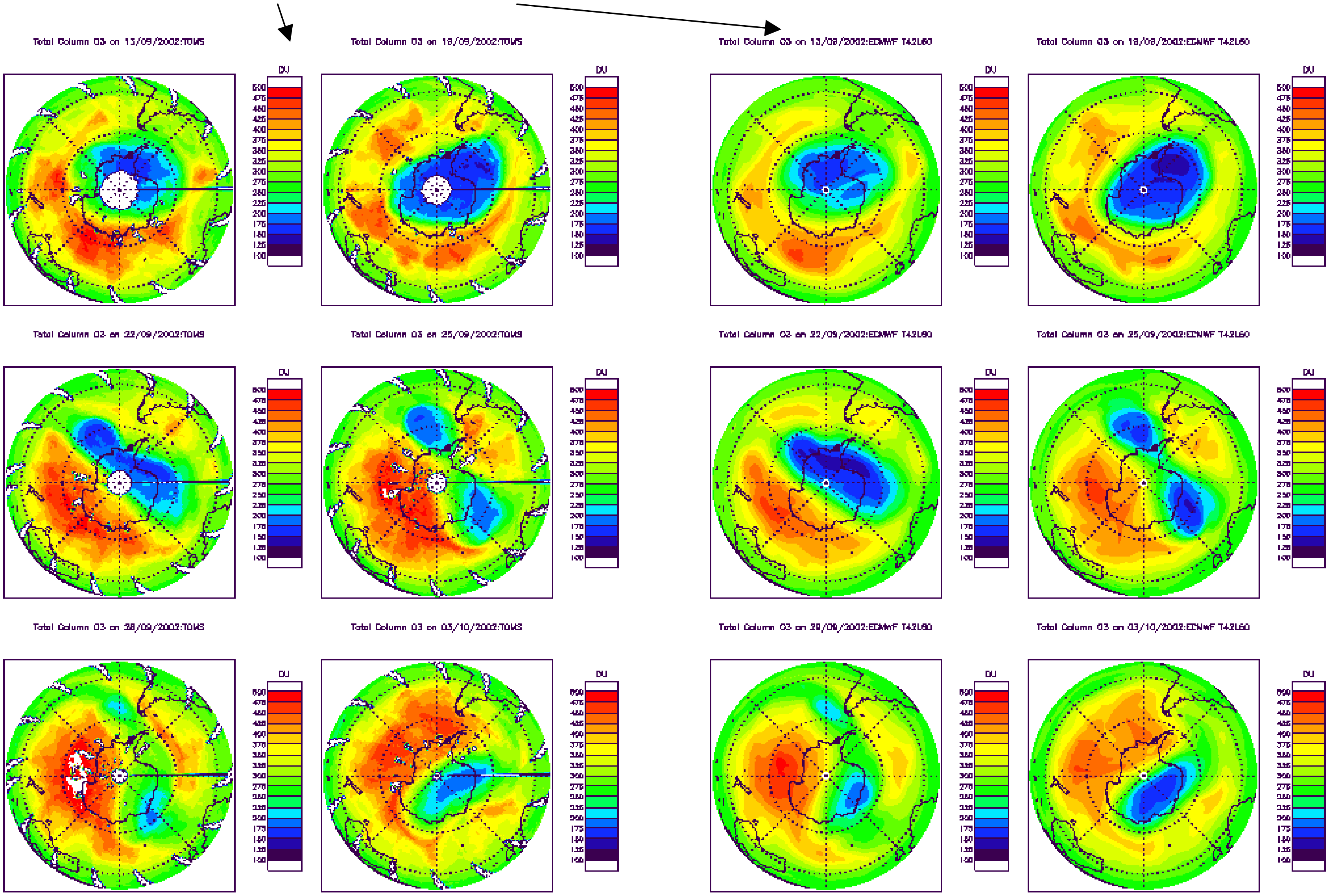
Principle of how a CTM works is simple - but in practice exactly how analyses are used is critical.

Off-line Chemical Modellers (+ trajectory modellers) are a large user group for meteorological analyses.

Experiences of CTM modellers provide useful information on quality of analyses.

Example CTM results 1: 2002 Antarctic O_3 Hole

TOMS v 3D CTM (SLIMCAT, ECMWF analyses)



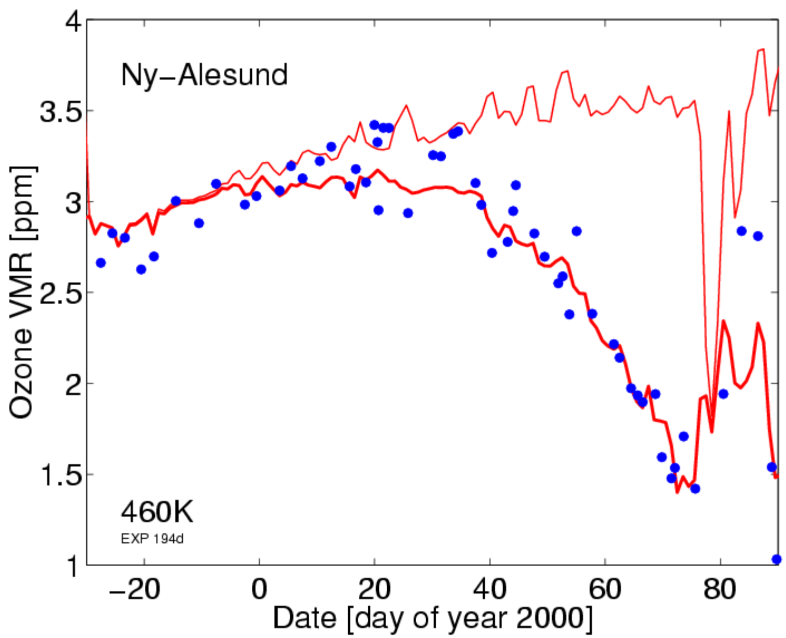
Analyses appear to capture unusual 2002 Antarctic dynamics well

Example CTM Results 2: Arctic O_3 Loss

SLIMCAT CTM. 5º x 5º.
UKMO winds.

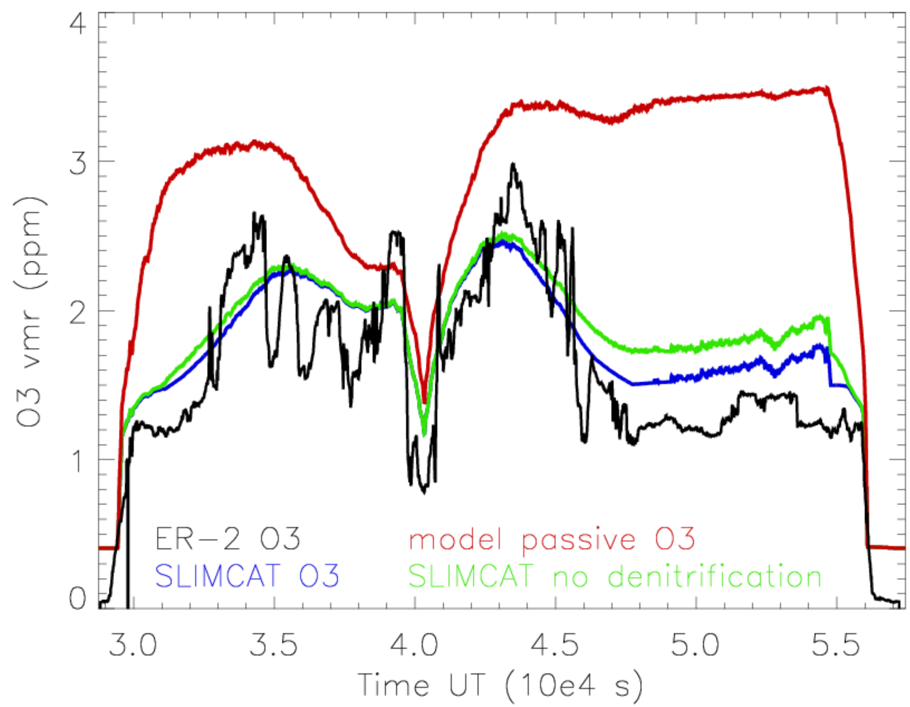
Arctic O_3 loss 1999/2000

3D CTM v O_3 sonde at Ny Alesund



3D CTM v ER-2 in-situ observations

(Arctic vortex flight March 2000 ~18 km)



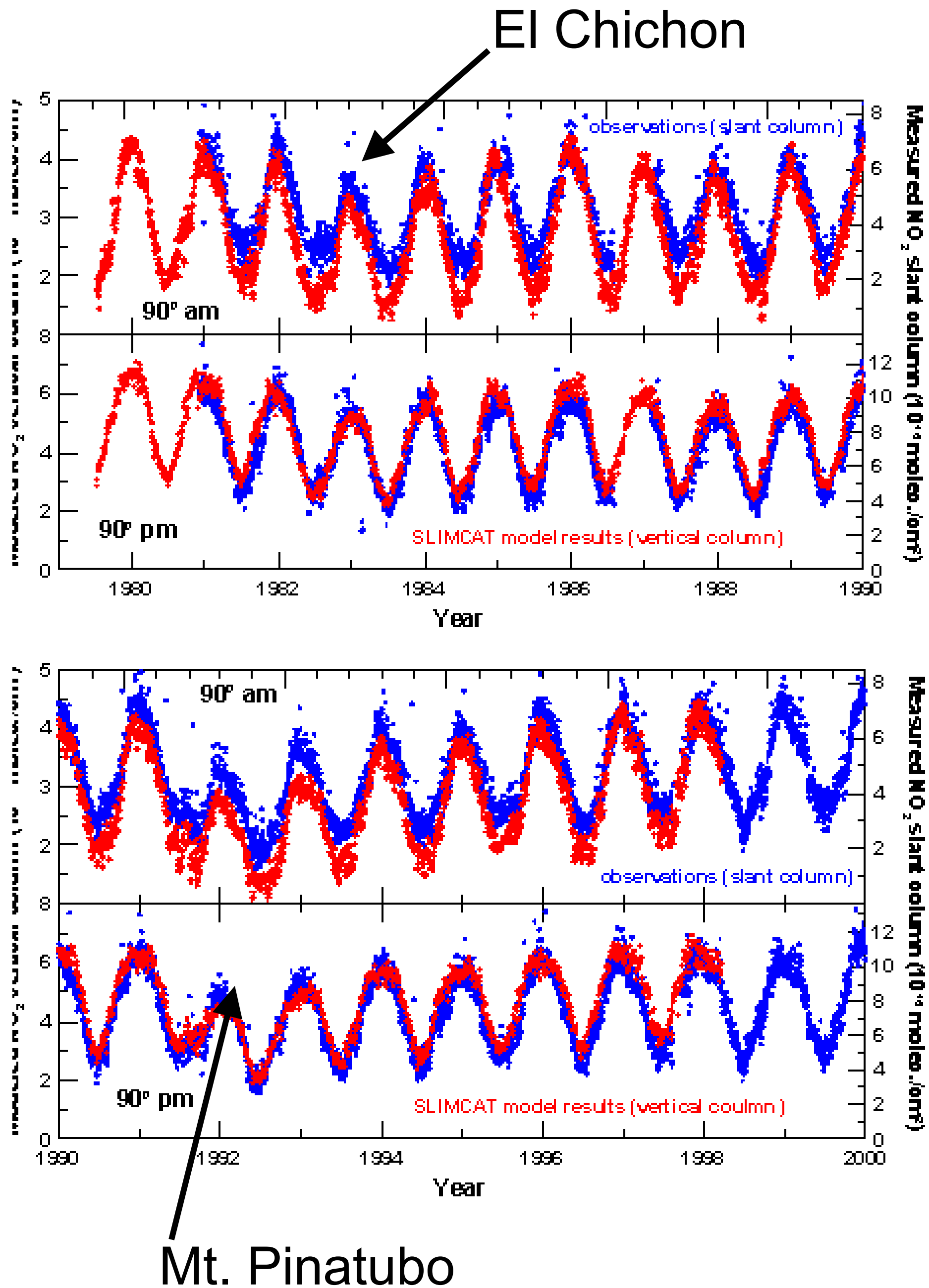
CTM 3: Long-Term NO_2 variations

Groundbased column NO_2 at Lauder (45°S)
(P. Johnston + K. Kreher)

v SLIMCAT 3D CTM (ECMWF ERA15 run to exploit long Lauder time series) (*assuming AMF=17*)

3D model captures: (i) seasonal cycle and (ii) aerosol-induced variability.

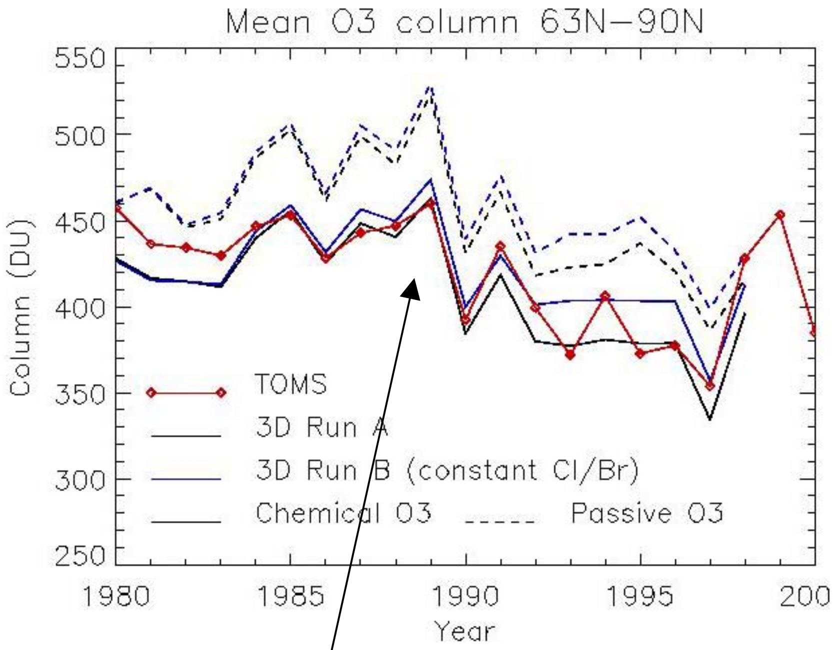
Also seems to capture a lot +6%/year trend (study on-going - see Kreher et al. AGU 2002).

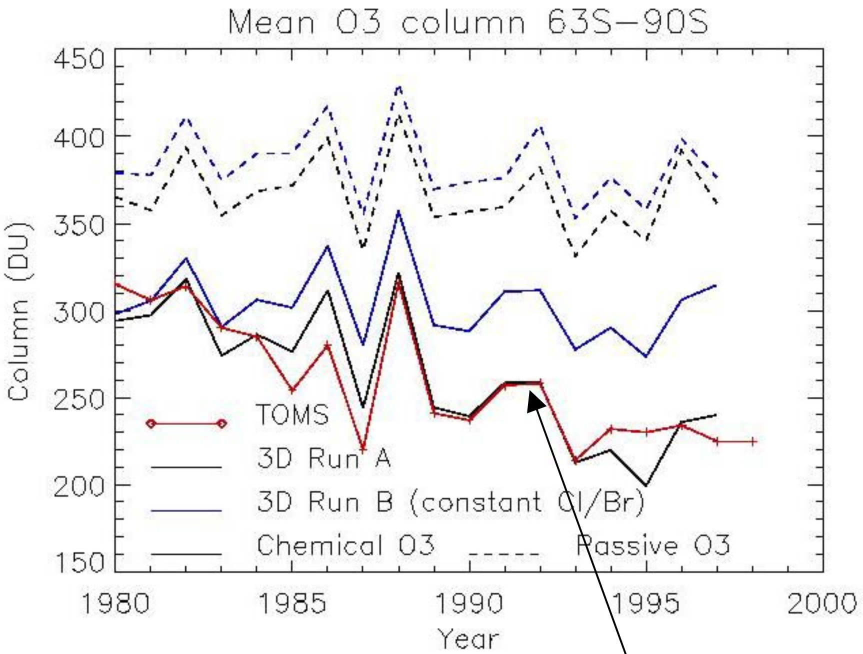


CTM Example 4: Polar O_3 Variability and Trend

Mean NH March/ SH October Column O_3 63°-90° v TOMS data (P. Newman)

SLIMCAT CTM forced by ERA15 (+ operational) winds.





Model captures interannual variability (esp. pre-1994 ERA period).

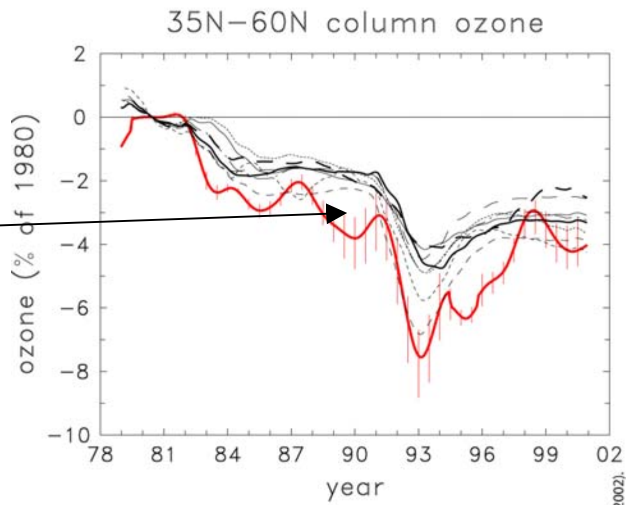
Chemical loss (trend) in SH ok. Models known to underestimate Arctic (polar) loss (see posters/Wednesday)

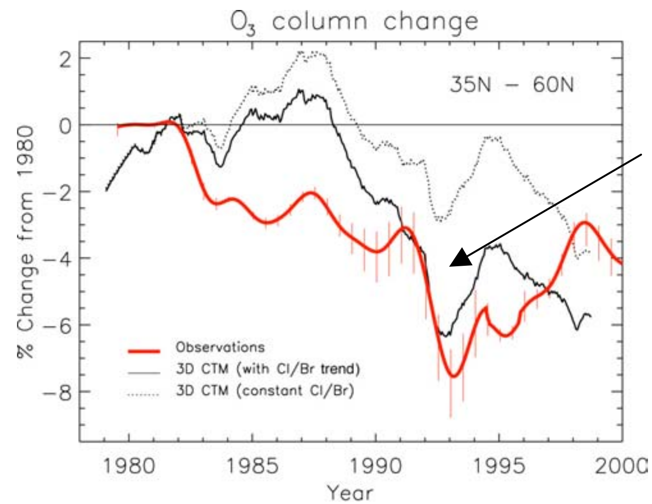
CTM Examples 5: Mid-Latitude O_3 Trends

2D Models - Cly/Bry trends; climatological winds; poor polar treatment.

SLIMCAT 3D CTM - analysed winds, better polar treatment. (ERA15 + op winds)

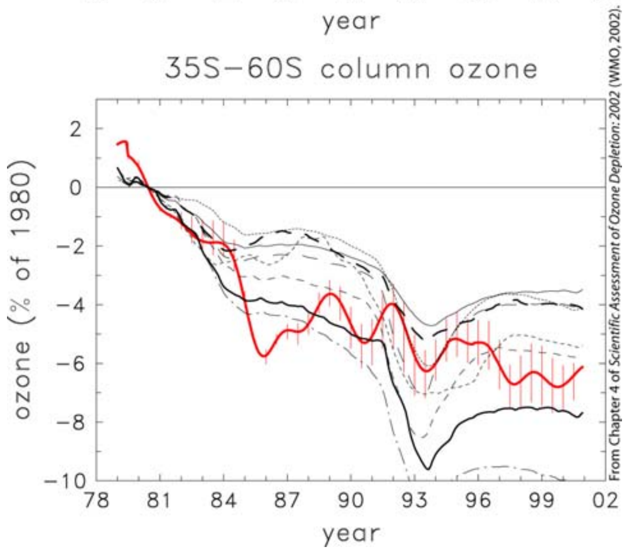
Aerosol chemistry

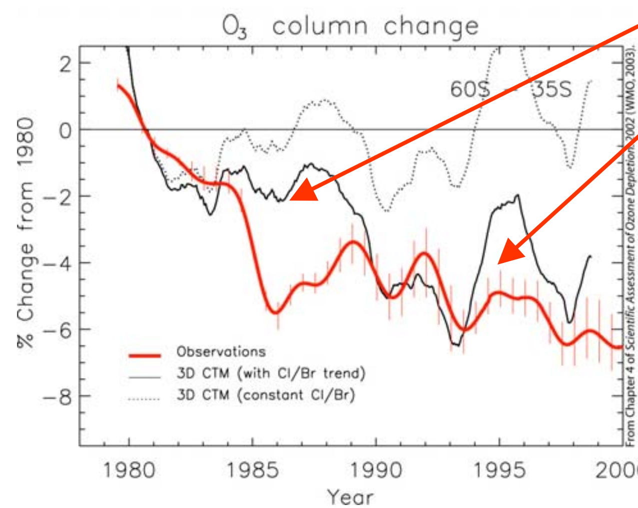




Chemistry/ dynamics

SH - 2D poor





Solar cycle??

TOMCAT/SLIMCAT 3D CTMs

Chipperfield and Simon, CNRM Toulouse, 1991/92.

Two related off-line CTMs (in fact same library):

- Horizontal/vertical resolution variable.
- Horizontal winds/temperatures from analyses (ECMWF, UKMO).
- Vertical coordinate: σ-p (TOMCAT), σ-θ (SLIMCAT).
- Vertical motion from either:

    Divergence (of mass flux).

    Diagnosed heating rates (SLIMCAT in θ coordinates).
- Default advection scheme: Prather [1986] - finite volume.
- Convection: Tiedtke [1989] - (only requires T, u, v, q).
- 'Full' chemistry schemes stratosphere/troposphere (TOMCAT Cambridge).
- Chemical data assimilation scheme: sub-optimal Kalman filter [Khattatov]

Why SLIMCAT?
- θ coordinates better in stratosphere (correct separation of horizontal/vertical motion; reduces numerical diffusion).
- Analysed vertical winds can be 'noisy'.

SLIMCAT/TOMCAT Stratospheric Chemical Scheme

Integrated shorter lived species	O_x (O_3 + $O(^3P)$ + $O(^1D)$) NO_x (N + NO + NO_2), NO_3, N_2O_5, HNO_3,HO_2NO_2 ClO_x (Cl + ClO + Cl_2O_2), OClO, HCl, $ClONO_2$, HOCl BrO_x (Br + BrO), HBr, $BrONO_2$, HOBr, BrCl CH_3OOH, CH_2O
Steady-state	H, OH, HO_2 CH_3O, CHO, CH3O_2
Long-lived species	CH_4, N_2O, H_2O, CO $CFCl_3$, CF_2Cl_2, CH_3Br

100 gas-phase reactions

20 photolysis reactions

~9 heterogeneous reactions on liquid sulphate aerosols and solid polar stratospheric clouds (PSCs).

CTM Vertical Coordinate

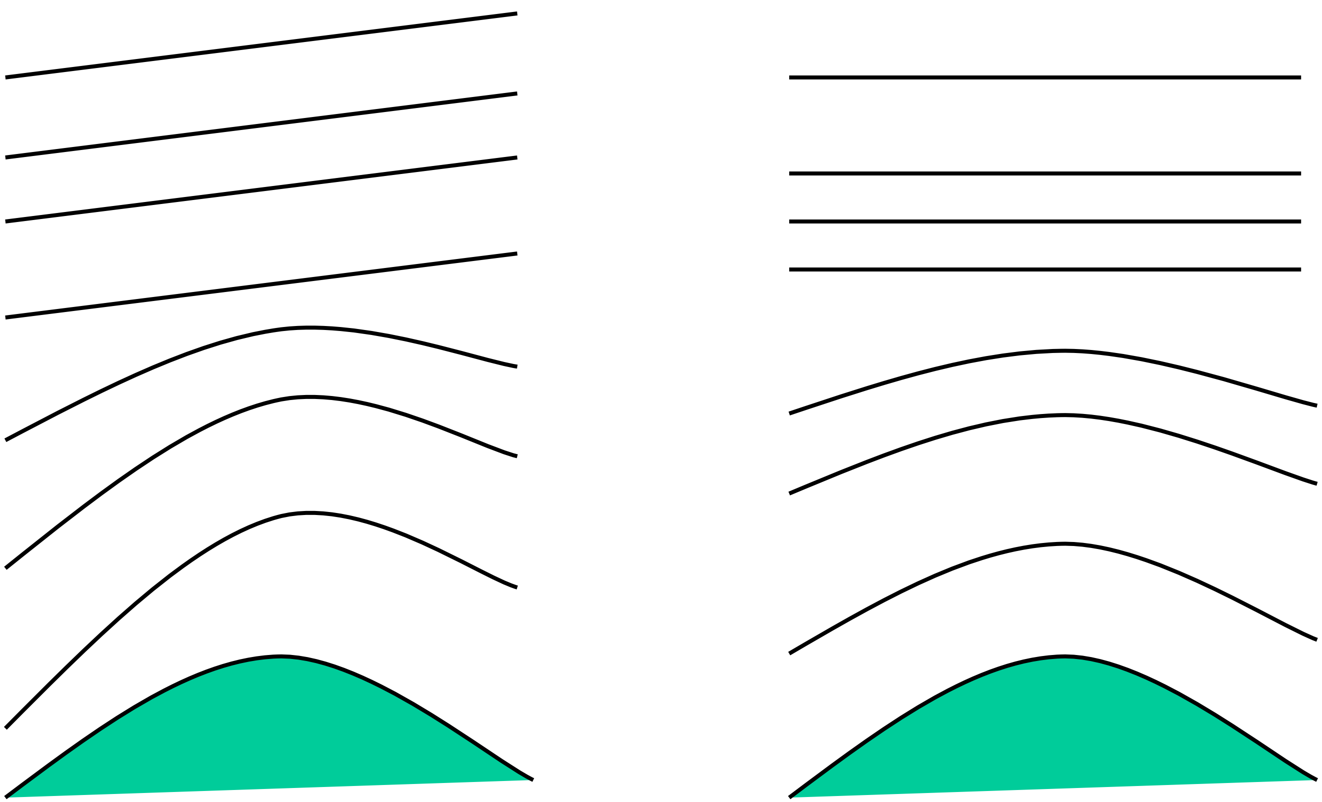
‘SLIMCAT’ mode

hybrid σ-θ

‘TOMCAT’ mode

hybrid σ-p

Lowest pure θ level = 350 K typically



Surface

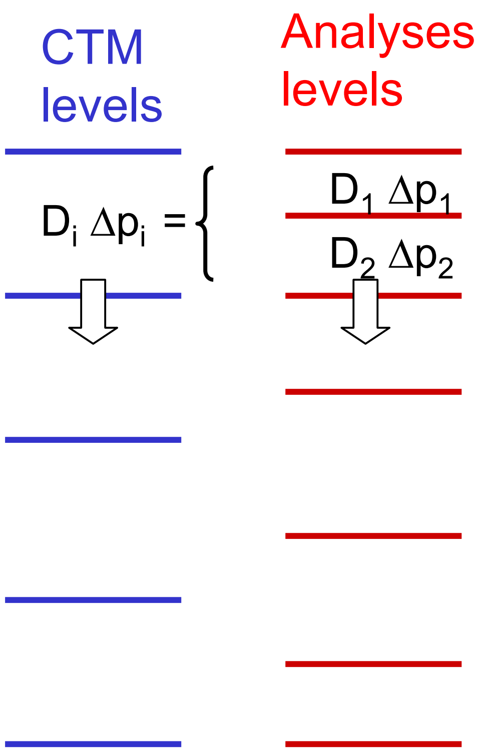
'Philosophy' of Off-Line Approach

Off-line model should replicate meteorological model (advection, convection)

Minimise manipulations (interpolation etc) of analyses, but CTM will likely want different grid (θ levels, irregular latitudes etc).

In SLIMCAT/TOMCAT when forced by ECMWF analyses:

- Model reads spectral coefficients of V, D, T, q, p_s (at any resolution - ideally on original analysis levels).
- V and D of winds converted to V and D of mass fluxes.
- Horizontally: Spectral transform of mass fluxes averaged over model grid cell edges.
- Vertically: Horizontal mass fluxes distributed over CTM model levels. (∫ D dp preserved).



Mass Conservation

A problem for off-line models. A few different aspects to this problem:

Necessary pre-requisites:

- Mass-conserving advection scheme.
- Conserving chemistry scheme.

Then, in addition, need good formulation of model:

- Transport defined in terms of mass fluxes.
- Vertical mass fluxes from divergence of horizontal mass fluxes.
- Conversion of analyses from analysis grid to model grid done in conserving way.

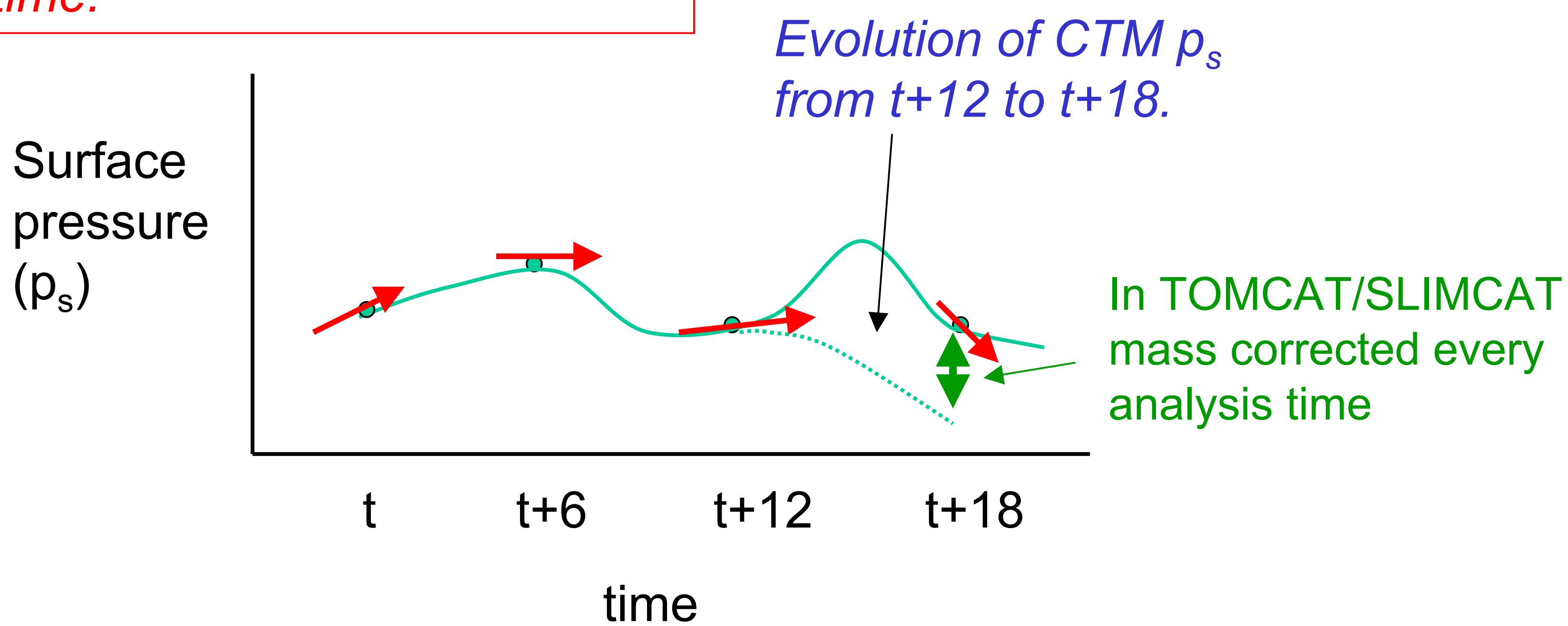
Mass Conservation (cont)

Even though mass fluxes may balance instantaneously, time discretisation will prevent complete mass conservation:

CTM only has 6-hourly fields (ps, dp_s/dt from divergence).

CTM interpolates fields linearly in time.

This local mass correction possible so long as analyses conserve mass (which they don't !)



Three Laws of Off-Line Modelling

1. All good CTMs should conserve mass exactly.

2. A CTM can only conserve mass properly if the analysis (meteorological) model conserves mass.

3. Analysis (meteorological) models don't conserve mass.

SLIMCAT/TOMCAT 3D CTM forced by ERA40 Analyses

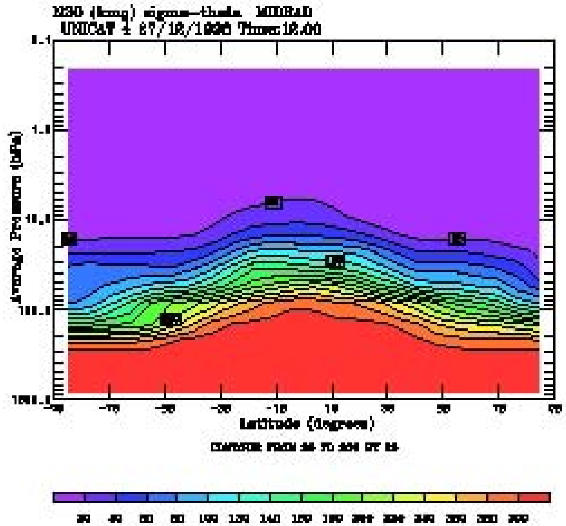
Different vertical coordinates and vertical motion

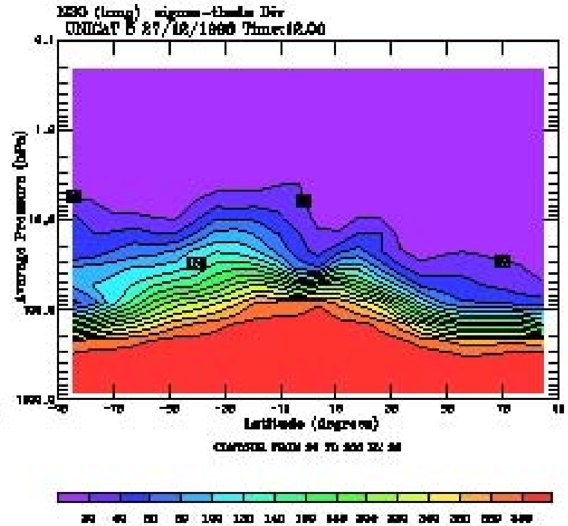
N_2O-like tracer.

27/12/1998.

Sigma-theta (σ-θ)

Heating rates (MIDRAD)



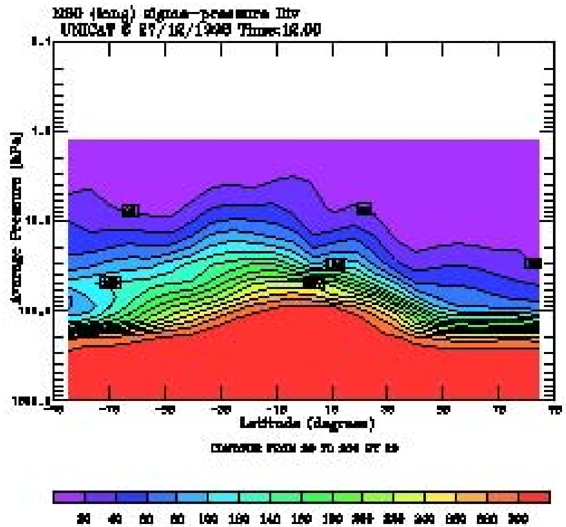


Sigma-theta (σ-θ)

Divergence

Sigma-pressure (σ-p)

Divergence

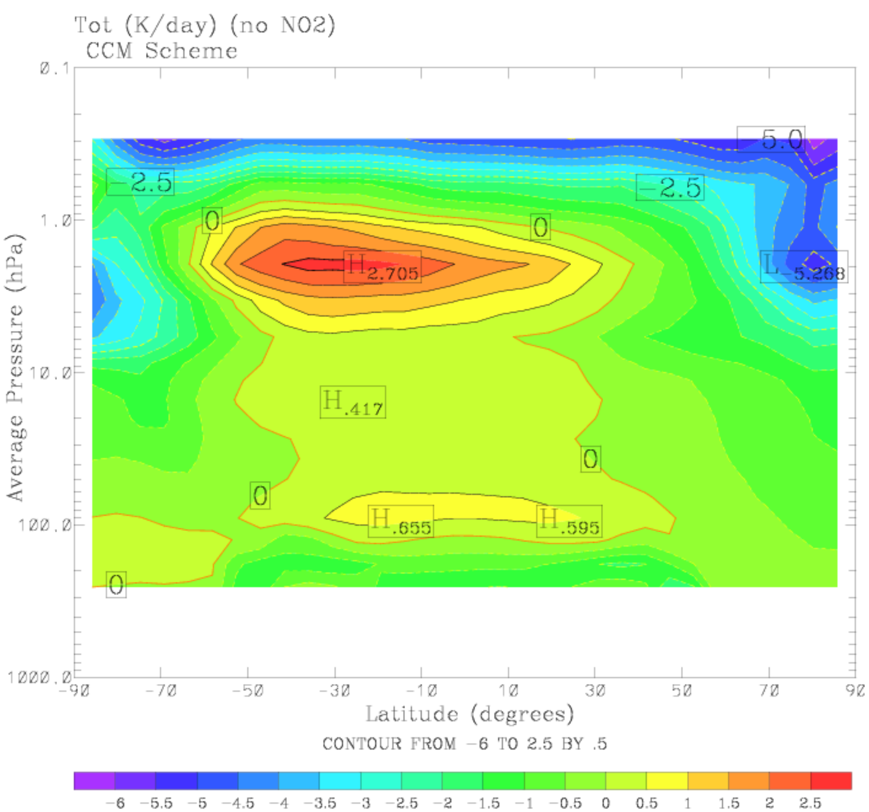


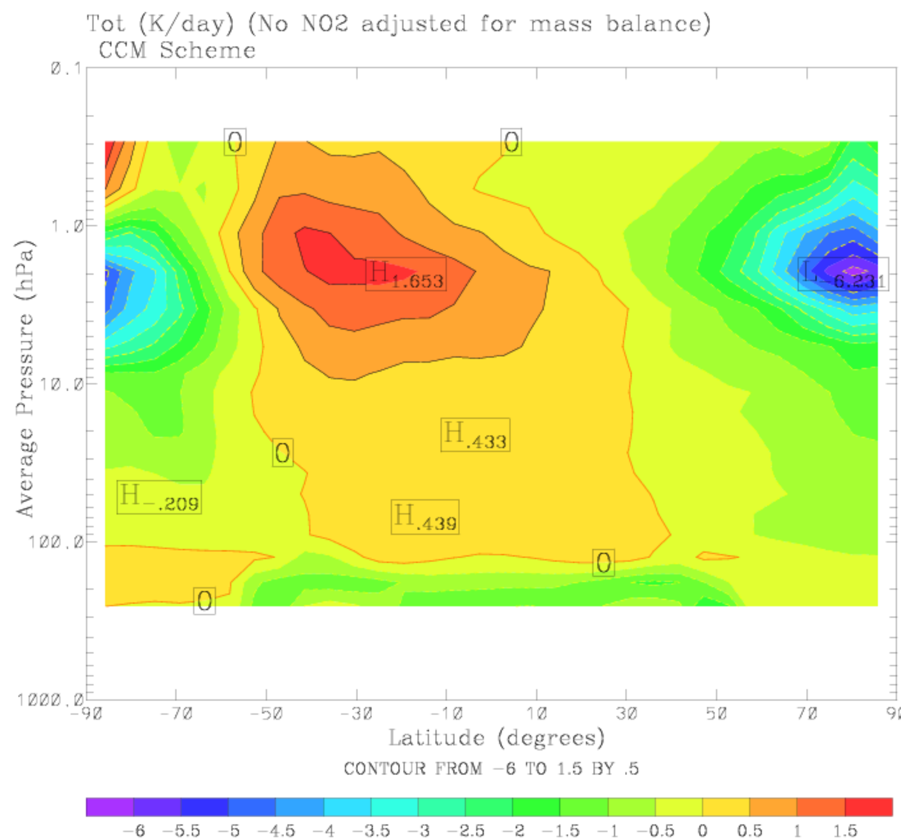
Diagnosing Vertical (Diabatic) Transport (Heating Rates)

SLIMCAT CTM.
CCM radiation scheme.
ERA-40 temperatures.

Net heating rate - with imposed mass balance

Net heating rate





Sequential Chemical Data Assimilation in a 3D CTM

Included sub-optimal Kalman filter chemical assimilation scheme (Khattatov, NCAR) into a full chemistry 3D atmospheric model (SLIMCAT).

A unique improvement of our scheme over previous uses of this scheme is the preservation of compact correlations during assimilation process.

Scheme is useful for assimilation long-lived tracers (not short-lived species)

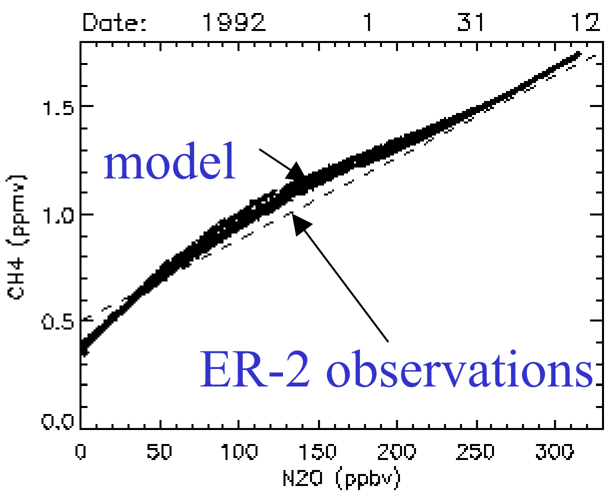
See Chipperfield et al., JGR, [2003].

Tracer-tracer correlations: CH_4 v N_2O from SLIMCAT 3D CTM

⇒ Long-lived tracers display compact correlations (e.g. Plumb + Ko, 1992)

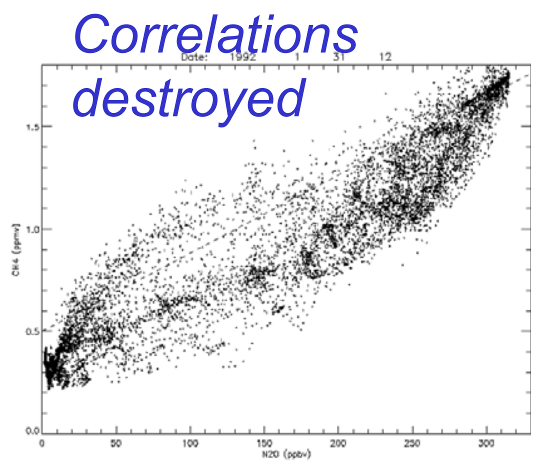
⇒ Total abundance of chemical species limited (e.g. ΣCl)

⇒ Chemical assimilation should make use of these constraints!



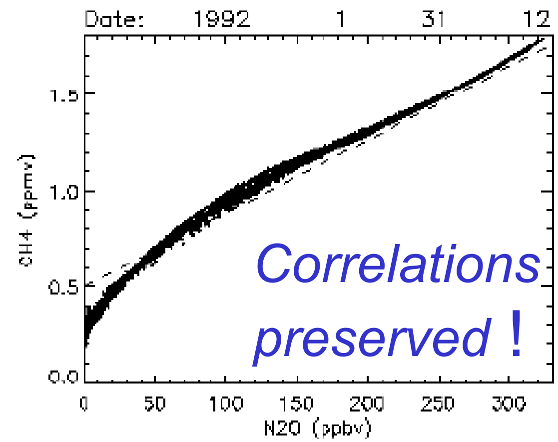
Basic (non - assimilation model)

CH_4



N_2O

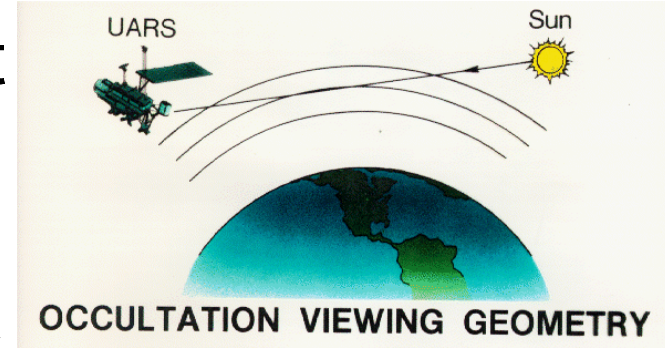
Naïve assimilation of HALOE CH_4 only.



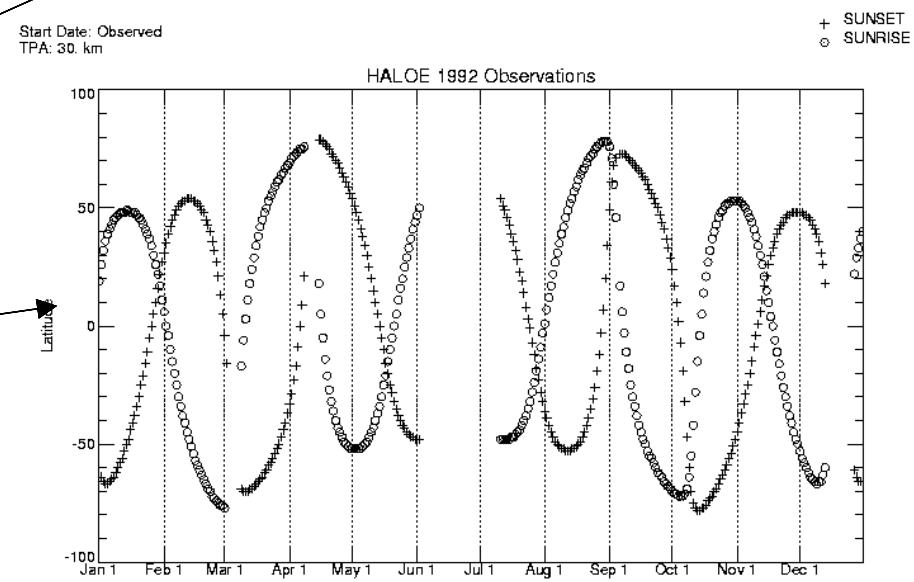
Assimilation of HALOE CH_4, and adjustment of N_2O to preserve correlation.

HALogen Occultation Experiment

(Russell et al.)



- Launched on Upper Atmosphere Research Satellite (UARS) - Sept 1991
- Solar occultation observations
- Latitude coverage over ~1 month
- Here we use profiles of O_3, CH_4, H_2O, and HCl



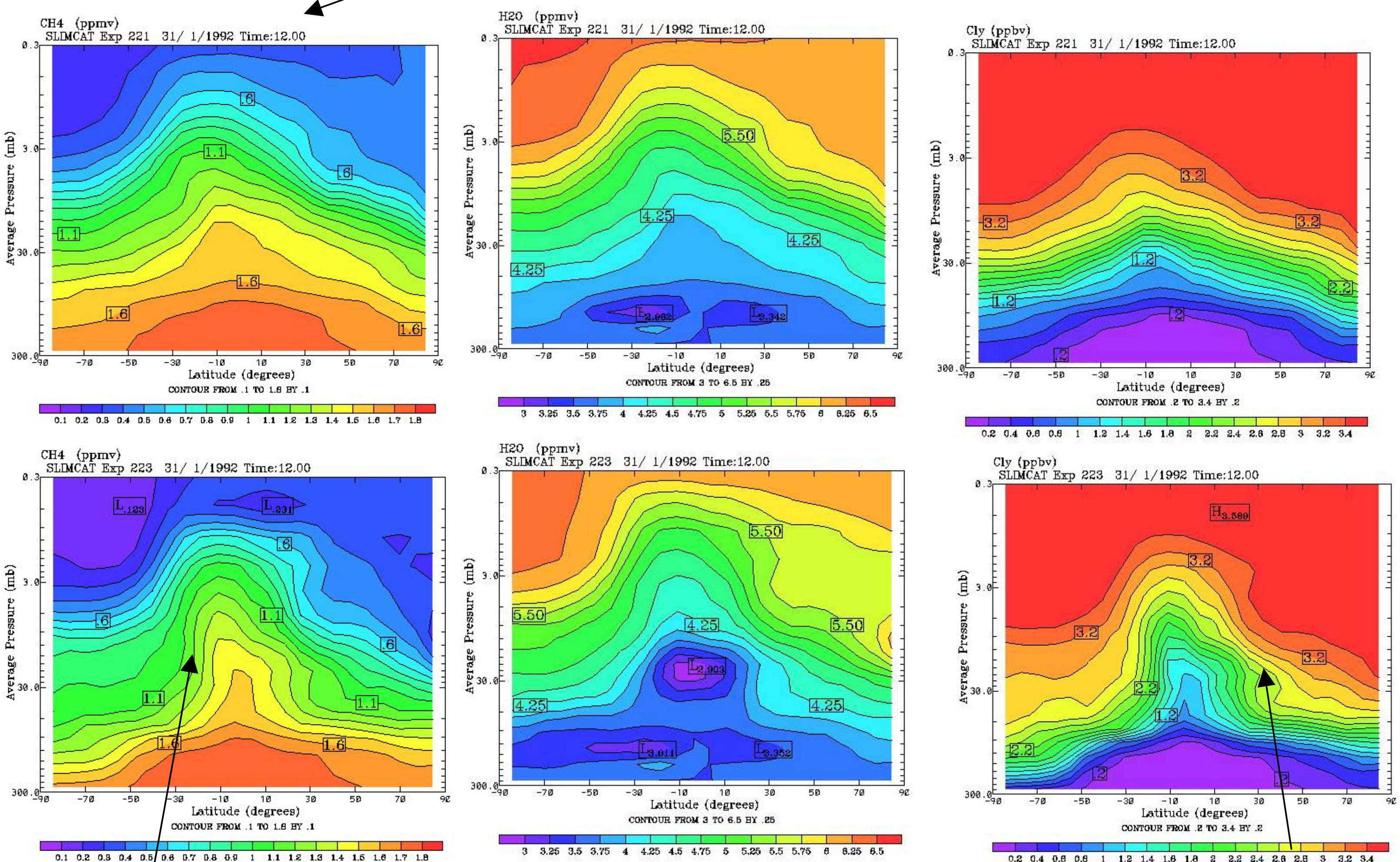
Latitude Progression

Effect of Assimilation: CH_4 , H_2O, Cly (*not observed*)

UKMO winds

No Assim.

Assim.



Large change in subtropics

Zonal mean fields 31/1/1992

Change to Cly occurs through tracer-tracer correlations with CH_4

Suggestions for Analysis Products

Quality

Temperatures in LS: < 1K error?

Horizontal winds in tropics

Vertical winds (BD circulation)?

Products

Diabatic heating rates (LW + SW components, contributions from latent heat release in troposphere)

Convective mass fluxes.

Higher top boundary (transport from mesosphere?)