Stratospheric ozone: satellite observations, data assimilation and forecasts

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1) Ozone and Numerical Weather Prediction

Assimilation of ozone at NWP centres

The major weather centres have programmes on ozone data assimilation
(extension of the models into the stratosphere/mesosphere)

- ECMWF
  - ERA-40 (TOMS, SBUV)
  - Operational (GOME, SBUV, MIPAS)
- NOAA NCEP-CPC (TOVS, SBUV)
- DAO (TOMS, SBUV)
- Meteo France (TOVS)
- UKMO, Univ.Reading (GOME, MLS, ENVISAT)

Ozone assimilation in numerical weather prediction

Benefits for atmospheric chemistry science community:

Multi-year data base of 4D ozone fields,

- consistent with the available (satellite) observations,
- consistent with the dynamical state of the atmosphere

Science questions:

- Recovery ozone layer
- Chemistry - climate interaction

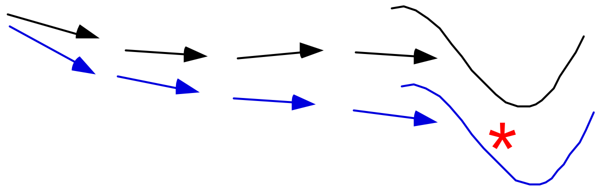
ECMWF ERA-40:

satellite observations 1978-present, TOMS, SBUV

Impact of ozone on NWP

Benefits of accurate ozone observations to numerical weather prediction

- Radiation: ozone has strong influence on temperature (and wind)
- Satellite retrieval: TOVS
- Assimilated ozone observations lead to wind increments
- UV forecast

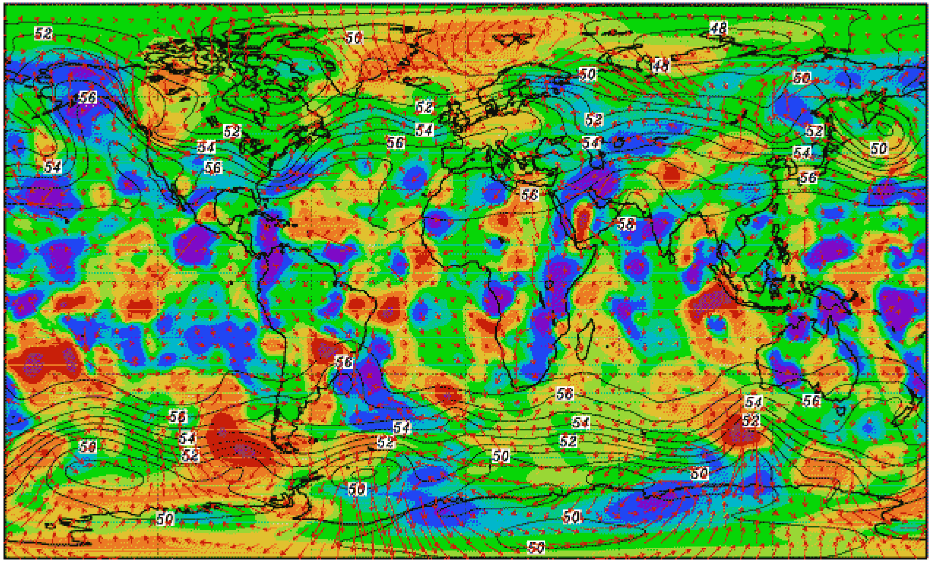


Impact of ozone on NWP

Wind increments
due to
TOVS ozone
observations

ECMWF model

(EU SODA project)

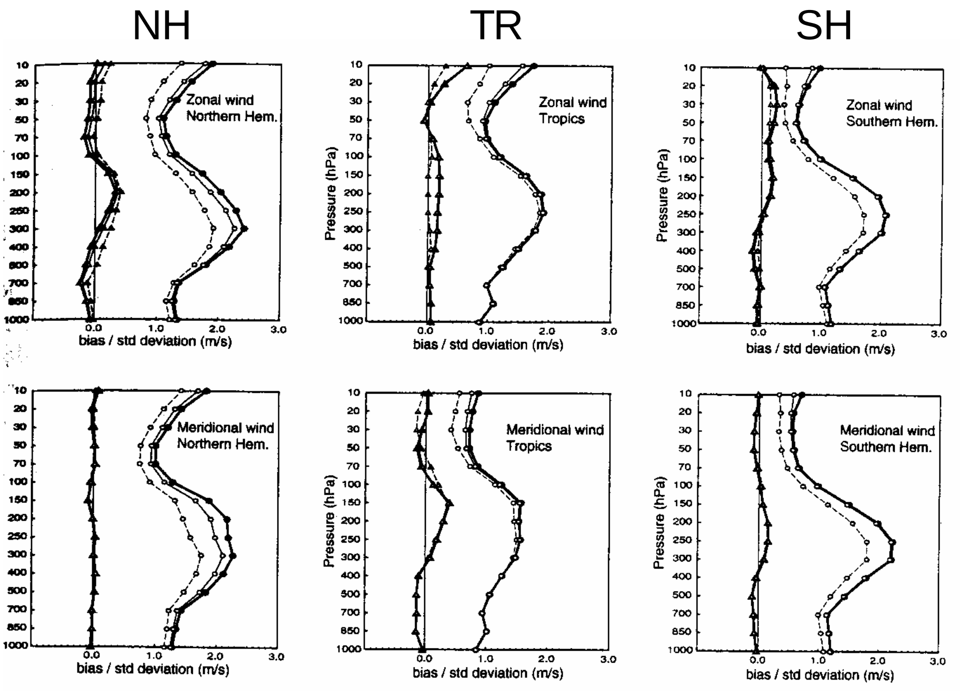


Wind increments ~ 0.5 m/s

OSSE: Impact of TOVS column retrievals on winds

Zonal wind

Merid. wind



A. Peuch et al, QJRMS 126, 1641, 2000

top story Goddard Space Flight Center

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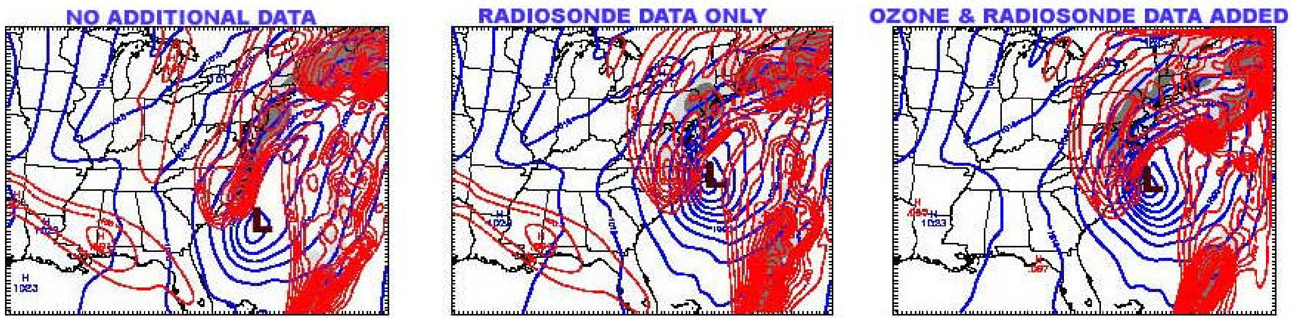
Related Links

August 07, 2003- (date of web publication)

NASA OZONE SATELLITE IMPROVES SNOWSTORM FORECASTS

With TOMS data



Jang et al, J.Appl.Meteorol. 42, 2003

2) Satellite observations of ozone

Satellite instruments

UV-Vis nadir

• TOMS (1978-present), SBUV, SBUV-2, GOME, SCIAMACHY

Occultation

• HALOE, SAGE, POAM, GOMOS

Limb (IR, MW, UV-Vis)

• MLS on UARS, MIPAS, OSIRIS, SMR

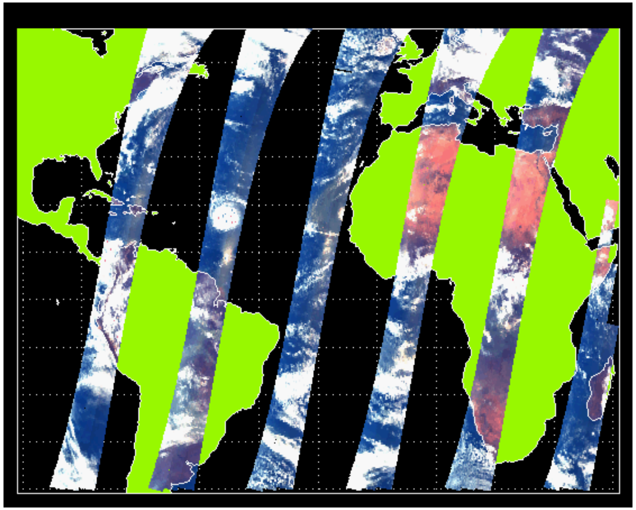
Nadir (IR)

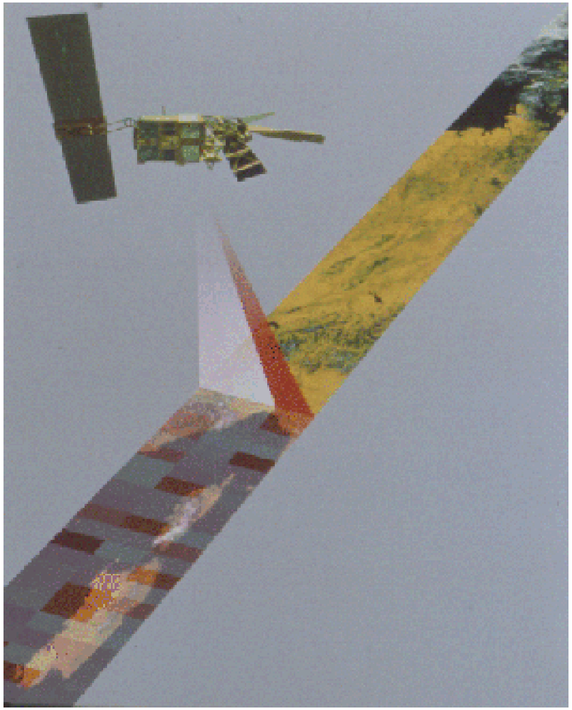
• TOVS, AIRS

Information on the troposphere:
TOMS, GOME, SCIAMACHY

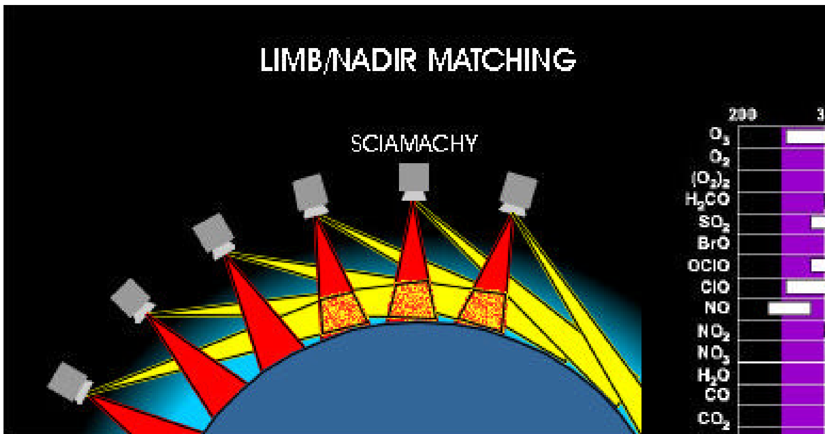
Ground-based observations

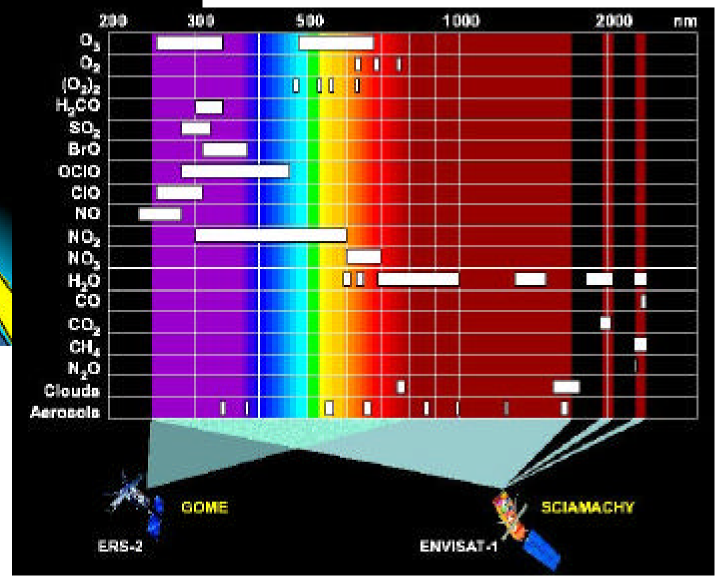
GOME on ERS-2, 1995 -





SCIAMACHY on ENVISAT, 2002 -

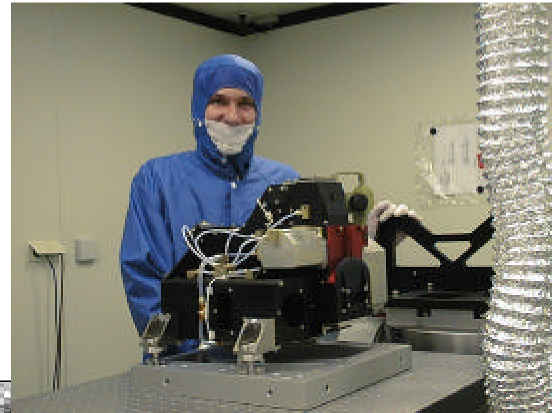


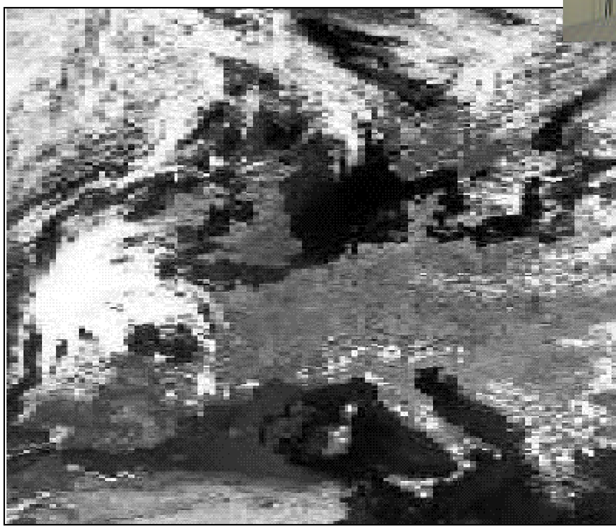


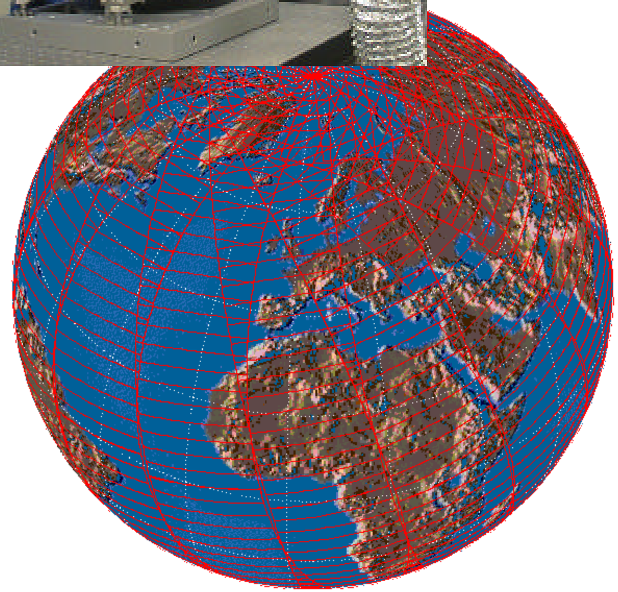
Troposfeer & stratosfeer

- O_3, NO_2, H_2CO, SO_2
- CH_4, CO, CO_2

OMI on EOS-AURA, 2004 -

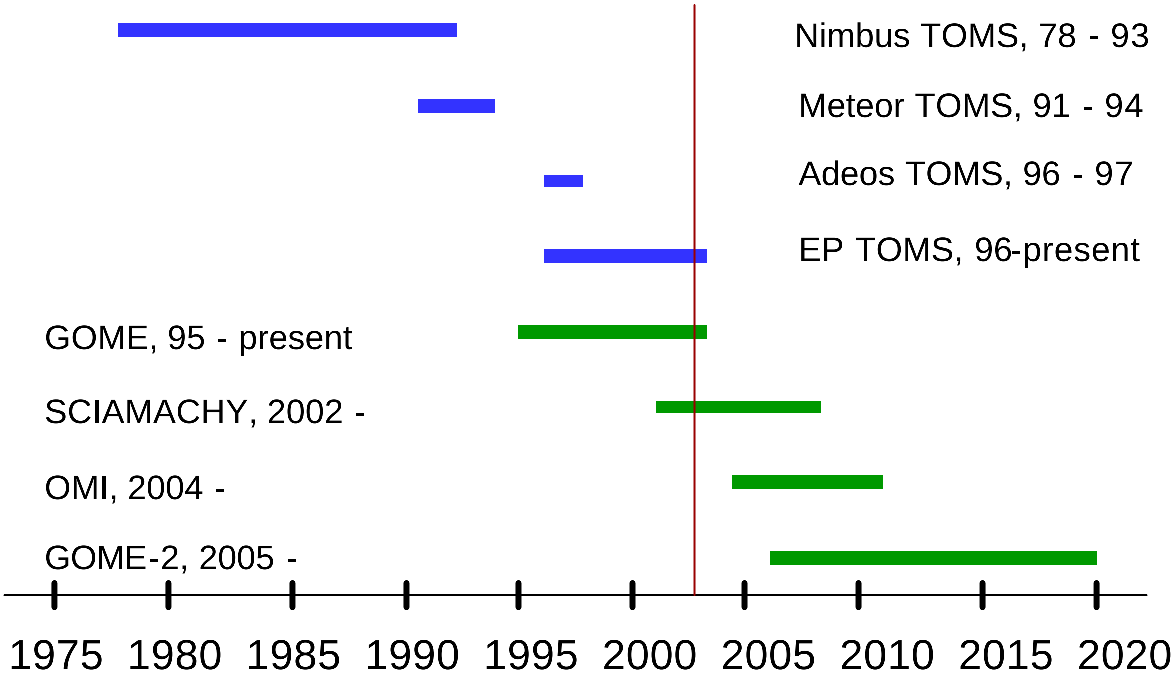






GOME-2 on METOP, 2005-2020

Ozone column measurements, 1978 - 2020



3) Ozone assimilation

GOME ozone assimilation: motivation

- Extend the use of GOME data (level-4 products)
  - 4D ozone data base
  - global synoptic maps every 6 hours
- Feedback on error statistics
  - Quality of observations
  - Quality of model
- Participation in satellite validation
- Ozone forecasts
- Case studies, e.g. mini-holes, 2002 ozone hole break-up

GOME ozone assimilation

Chemistry-transport assimilation model TM3DAM:

- GOME data: KNMI NRT ozone columns
- 2.5 degree resolution, 44 layers
- ECMWF meteo (60 layer)
- Prather second moment advection
- Parameterised stratospheric chemistry
  - Gas-phase
  - Heterogeneous
- Detailed forecast error modelling

Stratospheric chemistry parametrization

Gas-phase chemistry

Cariolle, Déqué, JGR 91, 10825, 1986

$$\frac{d\chi}{dt} = \langle S \rangle + \left\langle \frac{\partial S}{\partial \chi} \right\rangle (\chi - \langle \chi \rangle) + \left\langle \frac{\partial S}{\partial T} \right\rangle (T - \langle T \rangle) + \left\langle \frac{\partial S}{\partial \Phi} \right\rangle (\Phi - \langle \Phi \rangle)$$

χ ozone concentration
S sources - sinks
Φ ozone column above point

Stratospheric chemistry parametrization

Heterogeneous chemistry

(Peter Braesicke, CAS, Cambridge Univ.)

$$\frac{d\chi}{dt} = -\frac{1}{\tau} A \chi$$

$$\frac{dA}{dt} = \frac{1}{\tau_p}(1 - A) - \frac{1}{\tau_l} A$$

χ	ozone concentration
A	activation tracer field (cold tracer)
τ	ozone depletion time scale
τ_p	activation time scale
τ_l	cold tracer life time

Forecast error modelling

Sub-optimal Kalman filter approach:

Several fundamental Kalman filter properties can be maintained by expressing the covariance as a product of a time-dependent diagonal matrix and a time-independent correlation matrix.

$$\mathbf{B} = \mathbf{D}^{1/2}\mathbf{C}\mathbf{D}^{1/2}$$

$$\mathbf{D}^f(t_{i+1}) = N\left[\mathbf{D}^a(t_i)\right]$$

$$\mathbf{B}^a(t_i) = \mathbf{B}^f(t_i) - \mathbf{B}^f(t_i)\mathbf{H}_i^T\left[\mathbf{H}_i\mathbf{B}^f(t_i)\mathbf{H}_i^T + \mathbf{R}_i\right]^{-1}\mathbf{H}_i\mathbf{B}^f(t_i)$$

$$\mathbf{D}^a(t_i) = \mathrm{diag}\left[\mathbf{B}^a(t_i)\right]$$

A variance propagation model has been introduced here

Forecast error modelling

Sub-optimal Kalman filter approach:

Forecast covariance = time-dependent variance * fixed correlations

Correlation matrix:

function of the distance only

functional form determined from OmF statistics

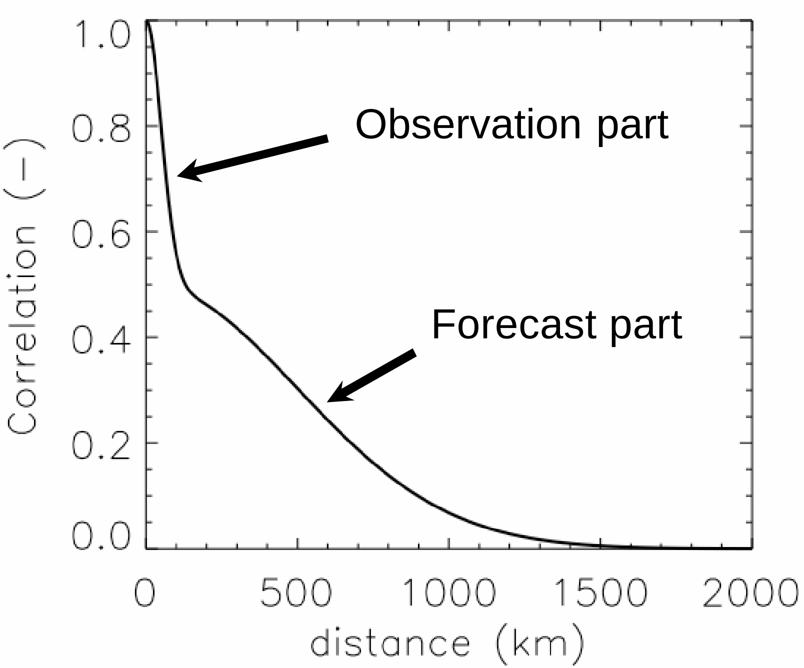
Variance:

- Model error, growth of the forecast variance with time
- Advection of the forecast variance
- Analysis equation for forecast variance

Correlations

OmF error covariance is sum of observation and forecast covariance

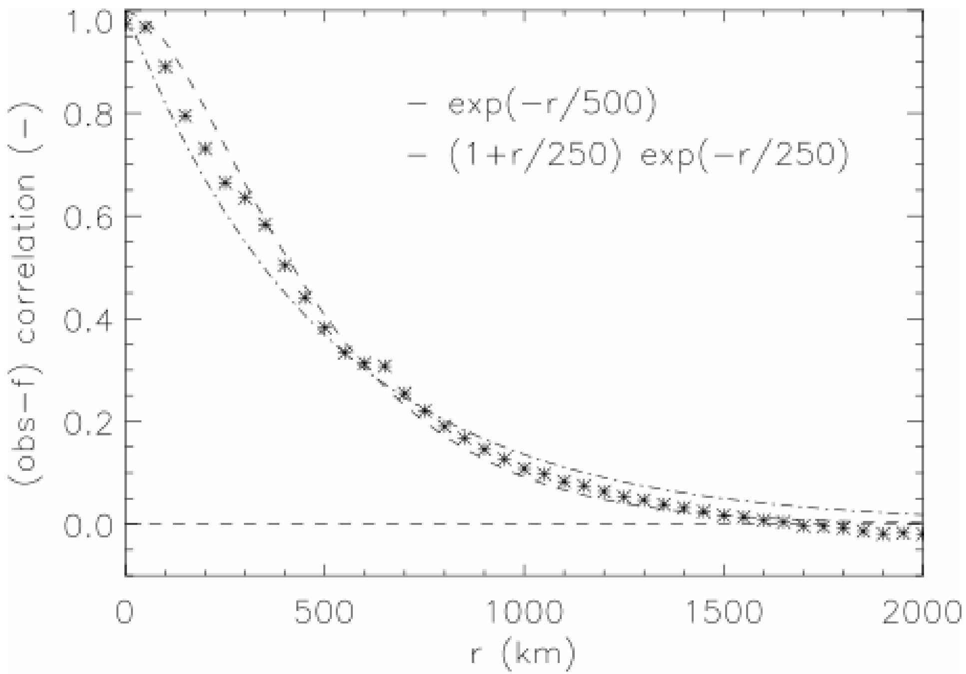
E.g. Hollingsworth and Lonnberg Meteorol. Atmos. Phys. 40, 3, 1989.



$$\langle(\mathbf{y}^o - H[\mathbf{x}^f])(\mathbf{y}^o - H[\mathbf{x}^f])^T\rangle = \mathbf{B} + \mathbf{R}$$

Correlations

Distance dependence descibed by 2nd order autoregressive function

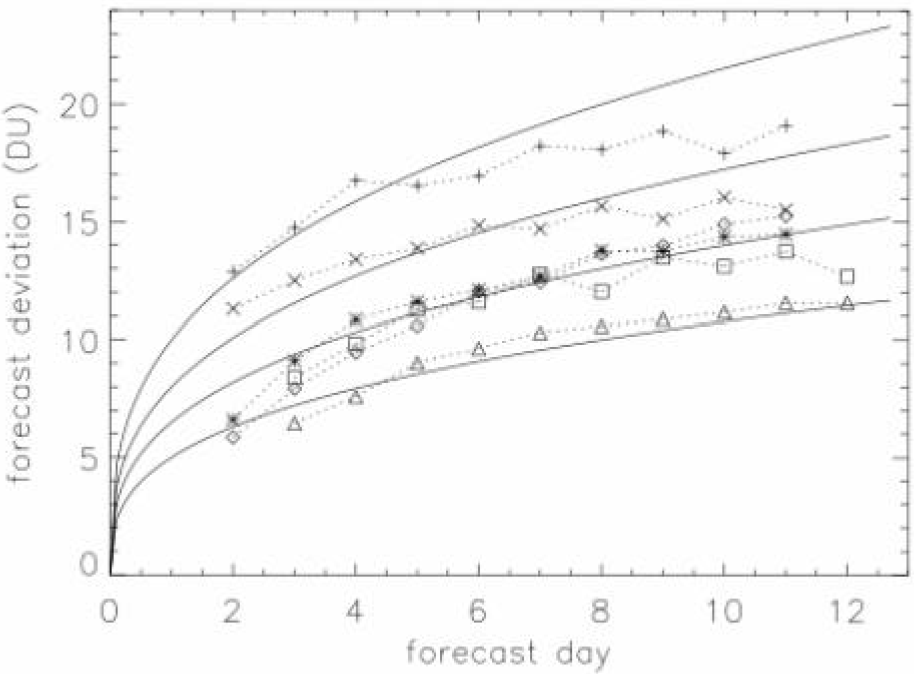


Model error

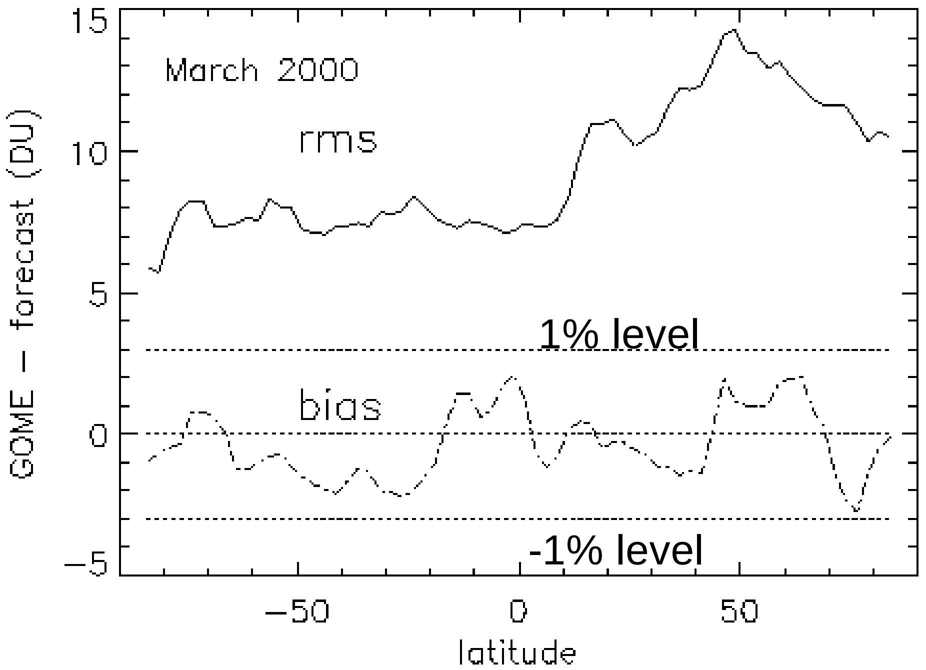
One-coefficient fit function to the observed ozone total column OmF as a function of the forecast period

Coefficient:
Function of latitude and month

Model error:
Derivative of curve



Observation minus forecast statistics

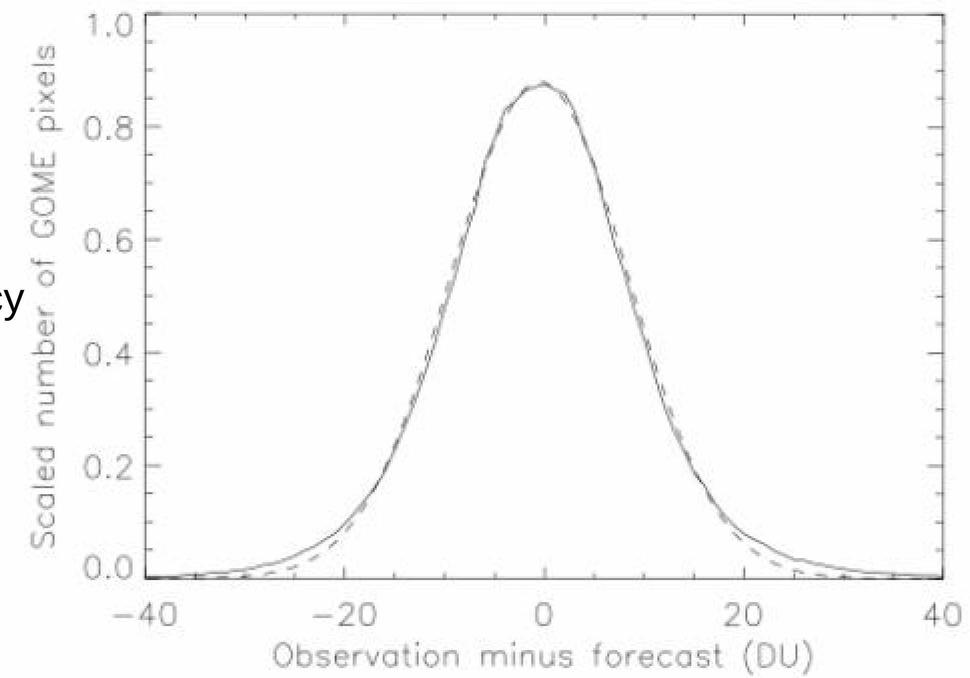


Gaussian statistics

Internal consistency GOME data

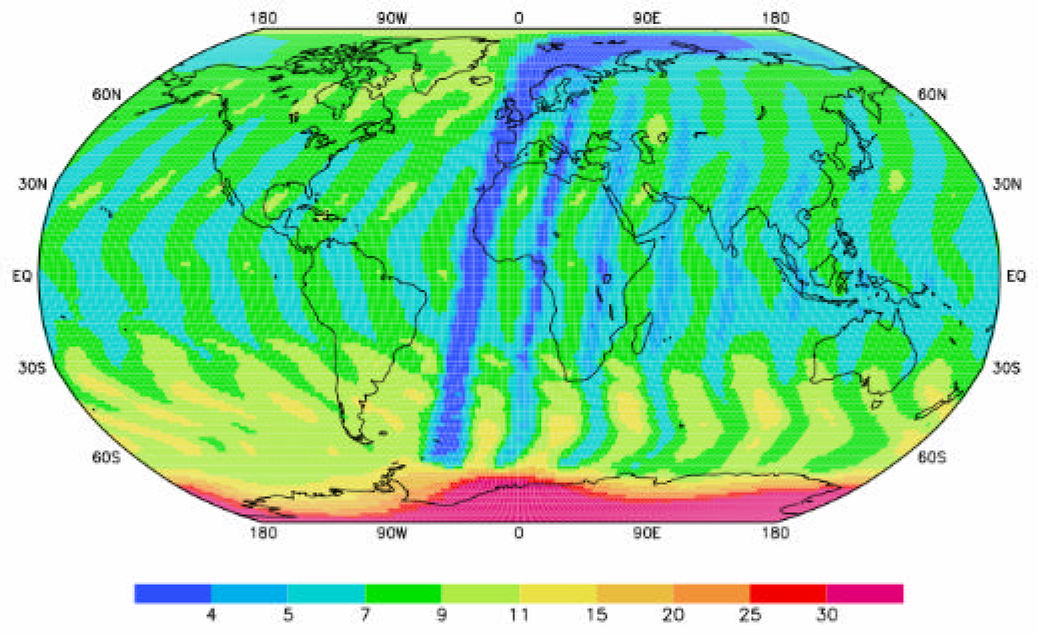
Low noise (< 2%)

No quality control needed



Forecast error

- Analysis
- Advection
- Model error



Forecast error verification

χ^2 test (E.g. Menard, 2000)

$$\left\langle \left(\mathbf{y}_i^o - H_i[\mathbf{x}^f(t_i)]\right)^T \left[\mathbf{H}_i\mathbf{P}^f(t_i)\mathbf{H}_i^T + \mathbf{R}_i\right]^{-1} \left(\mathbf{y}_i^o - H_i[\mathbf{x}^f(t_i)]\right) \right\rangle \approx 1$$

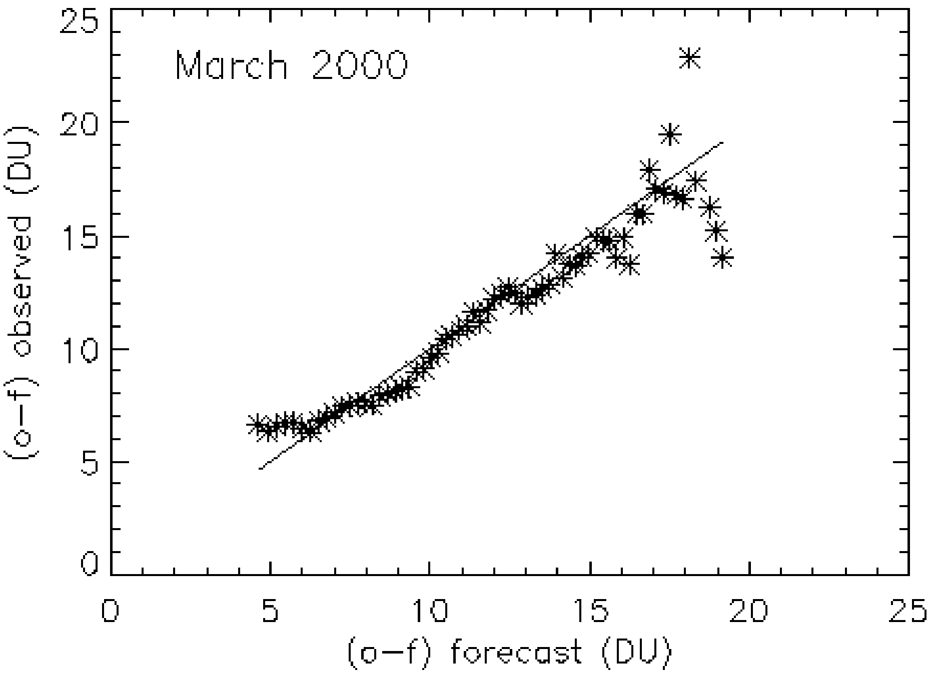
or

$$\mathrm{cov}(\mathbf{y} - H[\mathbf{x}]) \approx \mathbf{HPH}^T + \mathbf{R}$$

Forecast error verification

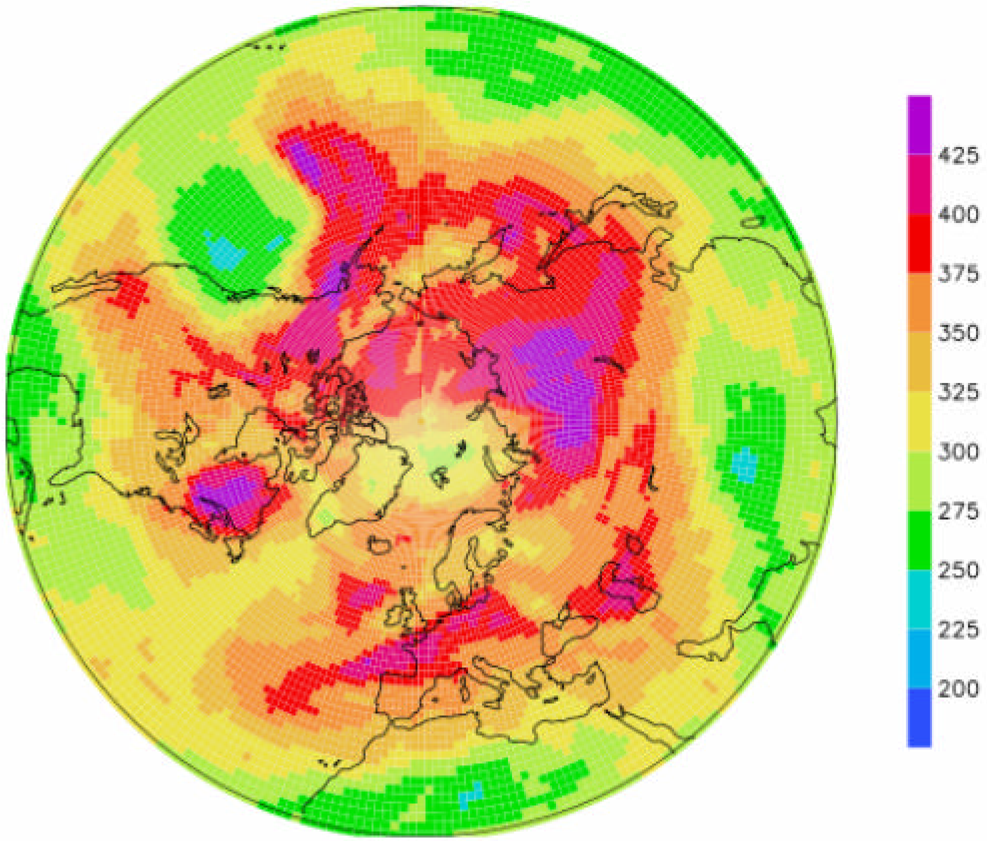
Note:

χ^2 test checks consistency of the average (o-f)



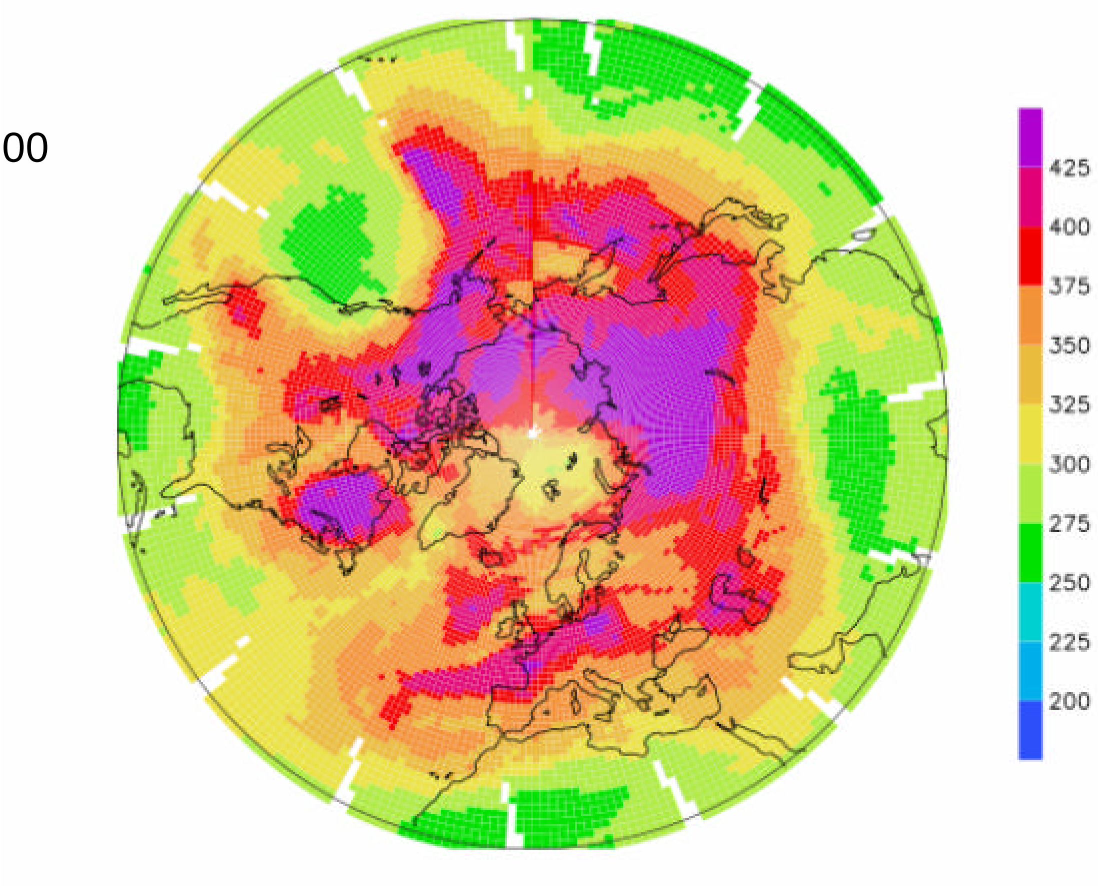
Comparison with TOMS total ozone

GOME / TM3DAM
31 March 2000
12h local time

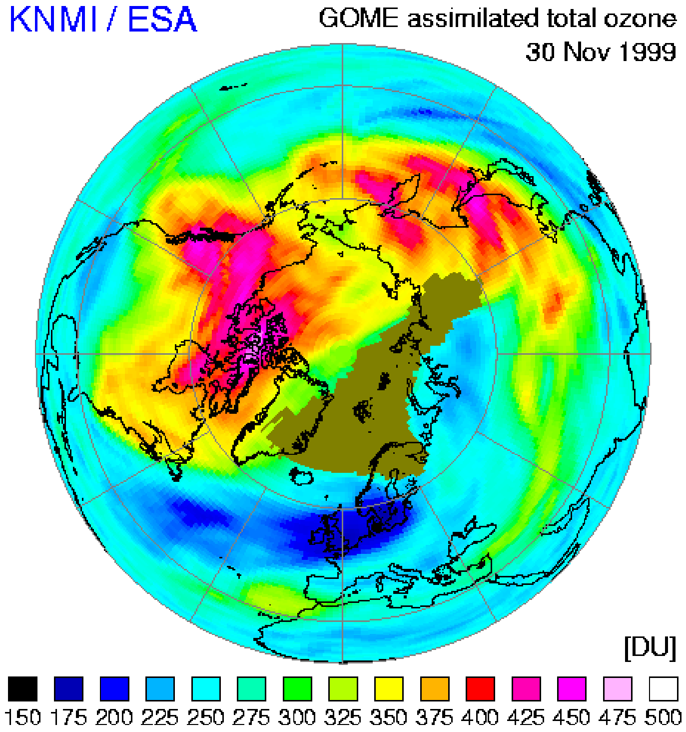


Comparison with TOMS total ozone

TOMS
31 March 2000

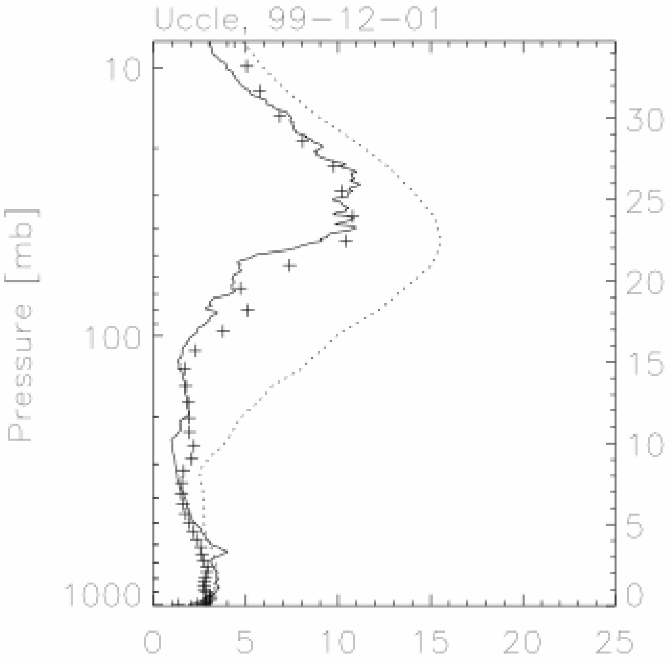


Low-ozone events



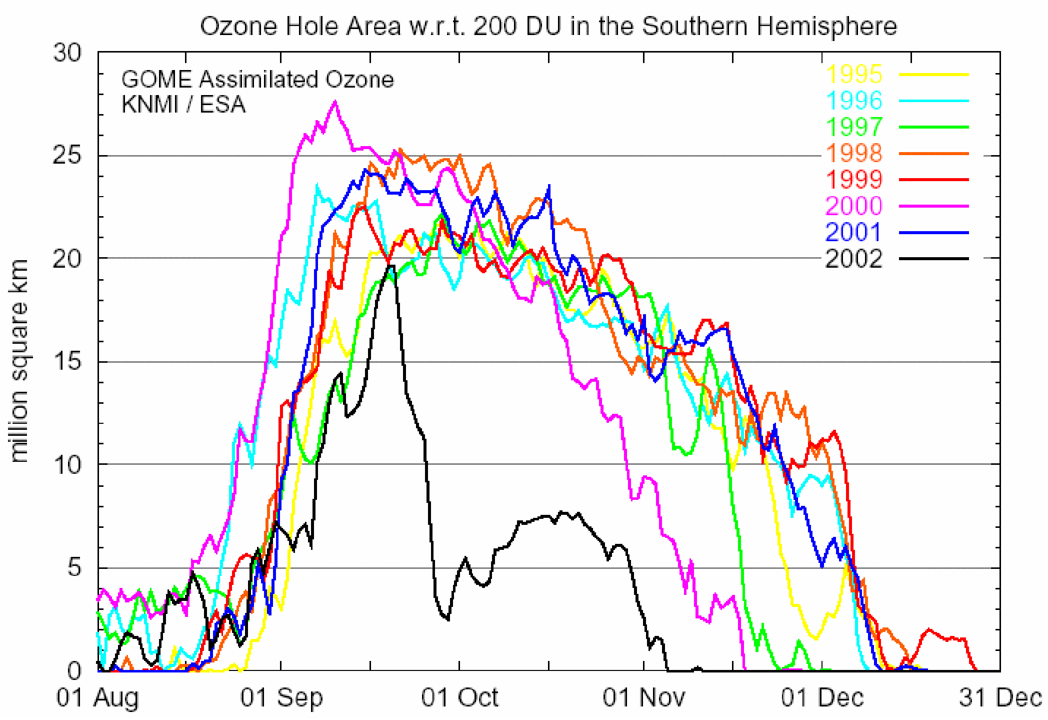
30 Nov 1999:
Lowest ozone value since beginning TOMS series

Low-ozone event: profile



30 Nov 1999:
Lowest ozone value since beginning TOMS series

7 year GOME data set http://www.knmi.nl/goa



4) Ozone forecasts, based on GOME and SCIAMACHY total ozone

http://www.temis.nl/

What determines quality of (chemical) weather forecasts ?

Ingredients

- Accurate analysis of the present state of the atmosphere
  based on available observations
  and short-range model forecast
  combined with data assimilation
- Model of the evolution of dynamics and chemistry in the atmosphere

Observations

- Meteorology:
  temperature, pressure, wind, moisture
- Chemical concentrations
  Ozone, NO_x, CO ...

KNMI ozone analyses and forecasts

• Transport-chemistry model for ozone
    driven by ECMWF meteorlogical analyses and forecasts
• GOME / SCIAMACHY ozone data
    near-real time
• Data assimilation scheme
    sub-optimal Kalman filter

--> Daily ozone analyses and 9-day forecasts
--> Operational since early 2000

Anomaly correlation, RMS error

Anomaly correlation

$C = < (f-c)(a-c) > \;/\; v<(f-c)^2> v<(a-c)^2>$

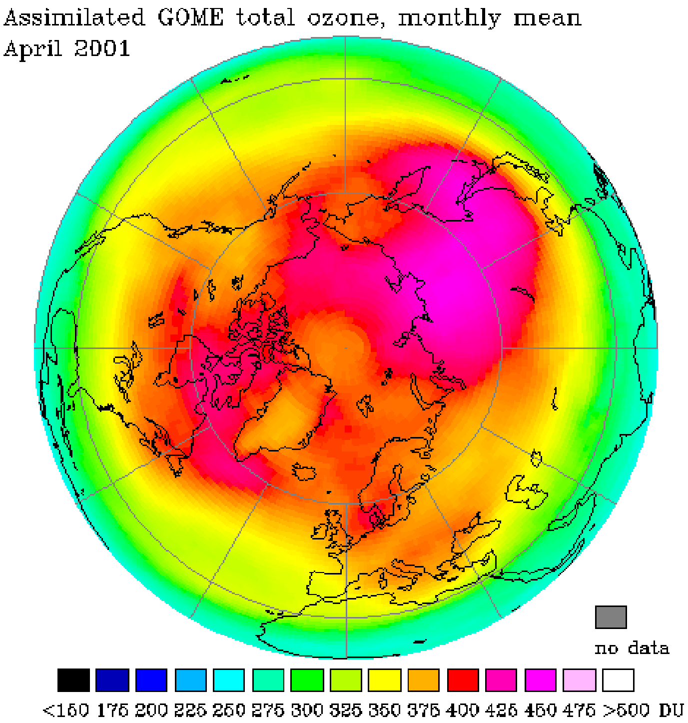
Root mean square error

$E = v<(f-a)^2>$

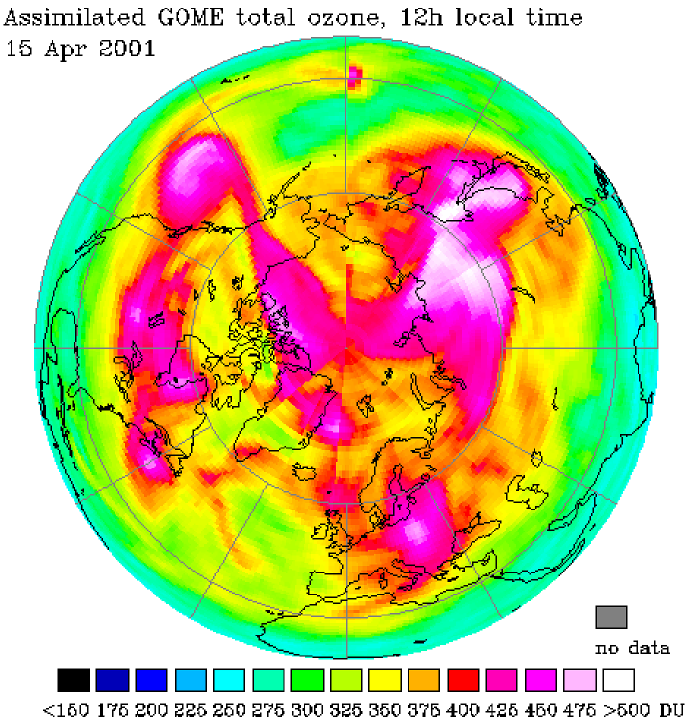
(f = forecast, a = analysis, c = climatology)

- Anomaly defined w.r.t. climatology "c" :
  Not useful for ozone - artificially high scores
- Alternative: "c" = running monthly mean

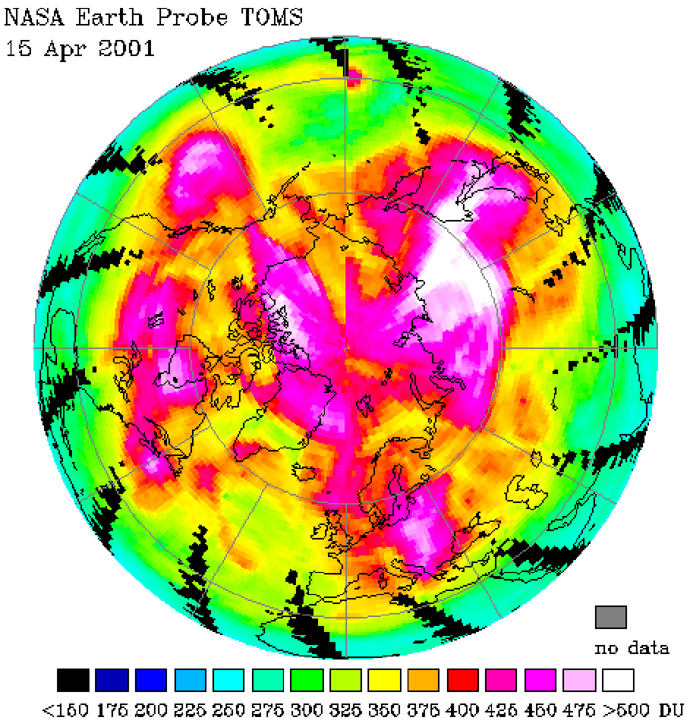
April 2001
Monthly mean



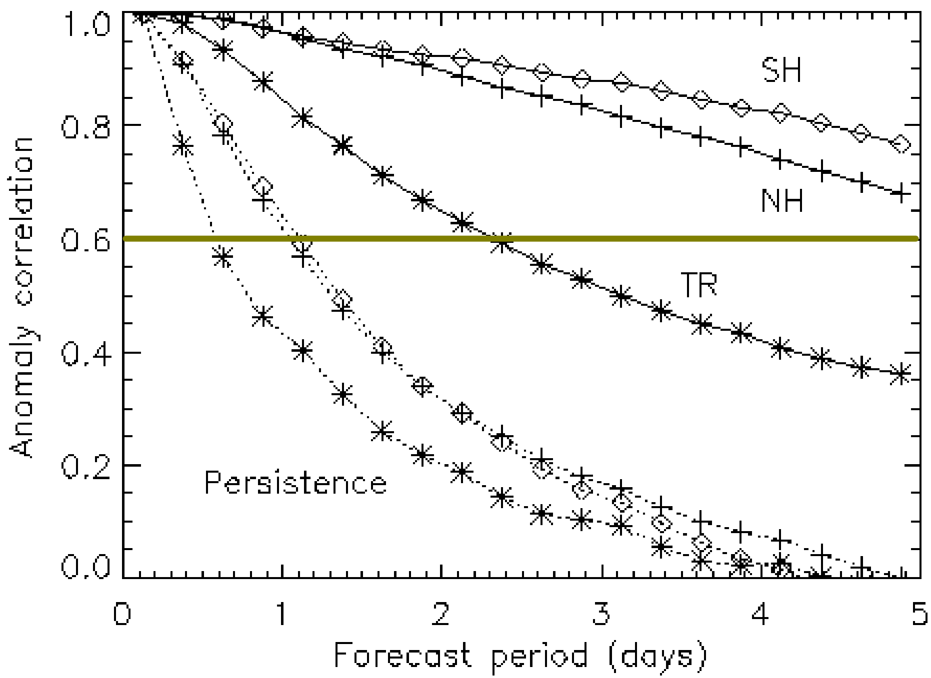
Analysis
15 April 2001



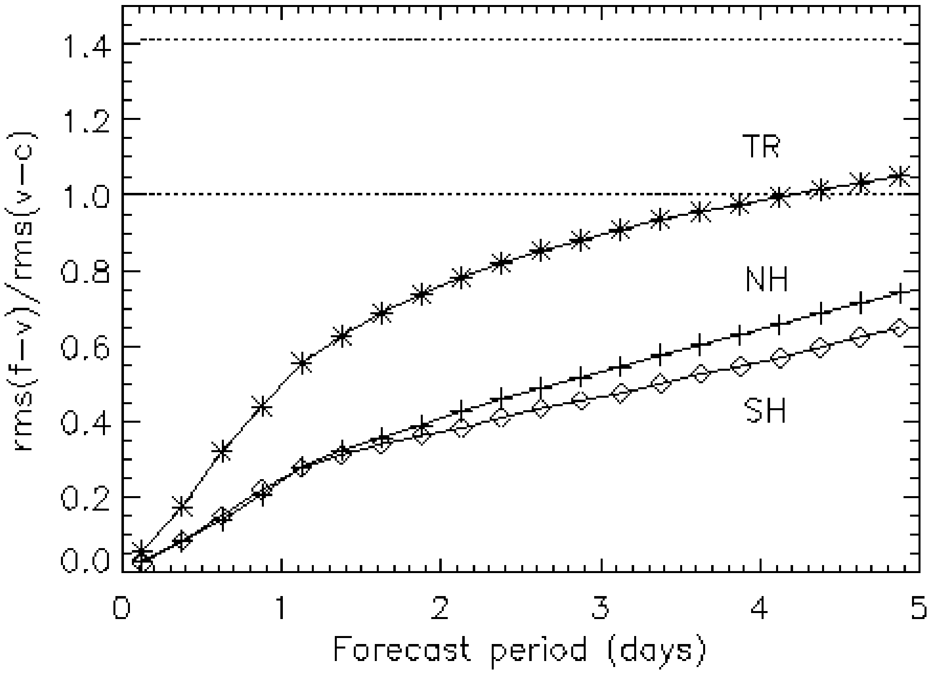
TOMS
15 April 2001



Anomaly correlation



RMS error



rms(f−v)/rms(v−c)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
3
4
5
Forecast period (days)
TR
NH
SH

Tropics

In tropics anomaly forecast score lower than in extratropics

-> Anomaly small (2-3% compared to 5-10%)

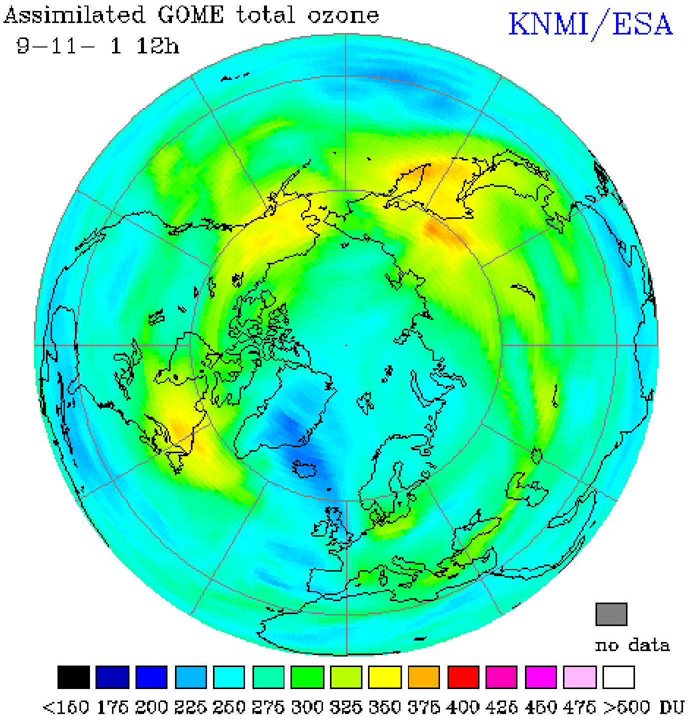
-> More sensitive to observation noise, retrieval errors

-> Anomaly mainly tropospheric

No tropospheric ozone chemistry in model

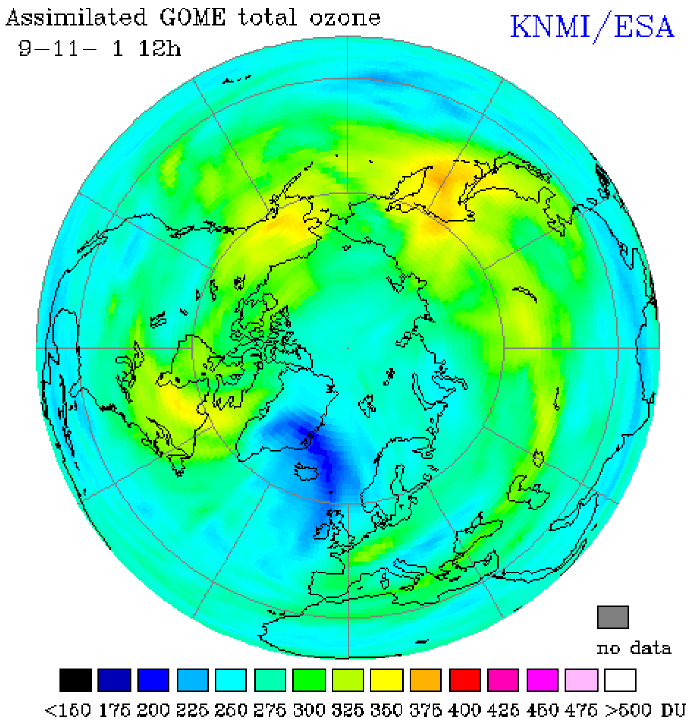
Low ozone episode

5-day forecast
9 November 2001



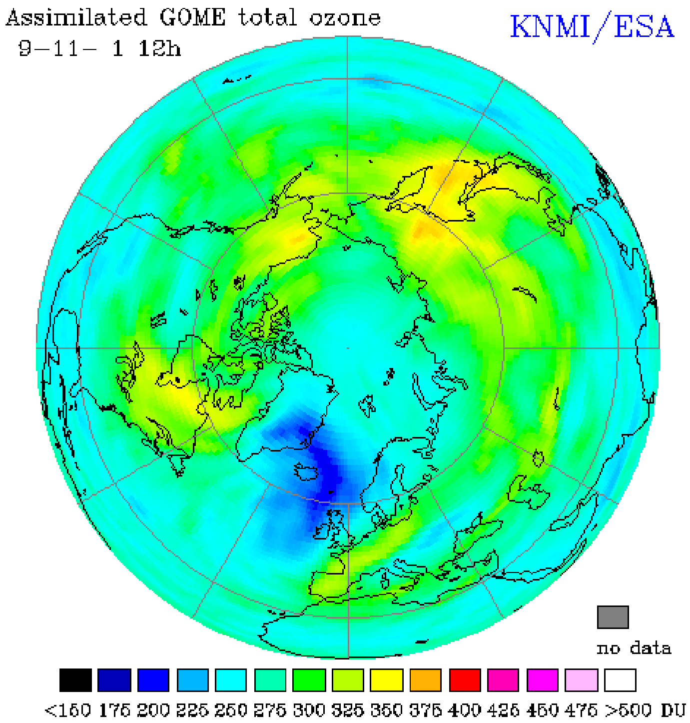
Low ozone episode

3-day forecast
9 November 2001



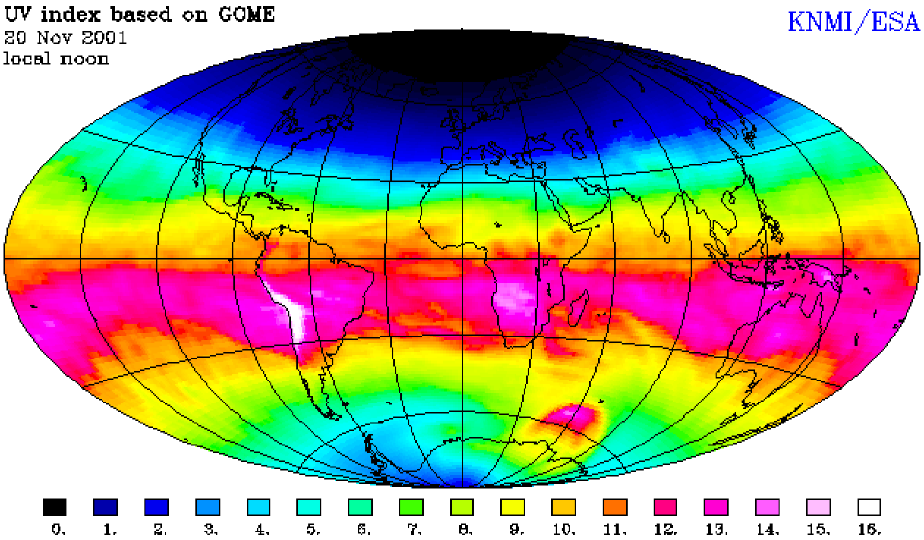
Low ozone episode

analysis
9 November 2001

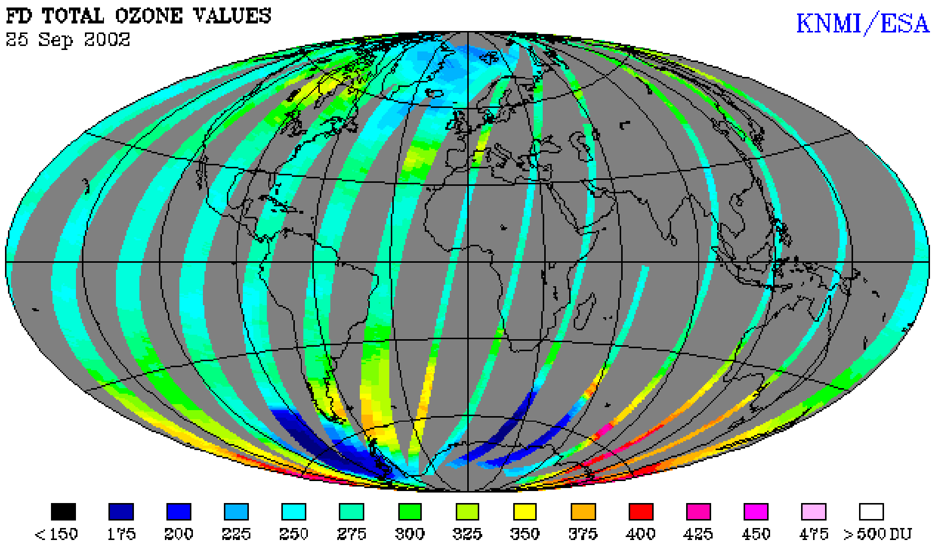


UV forecast

20 November 2001
(5-day forecast)

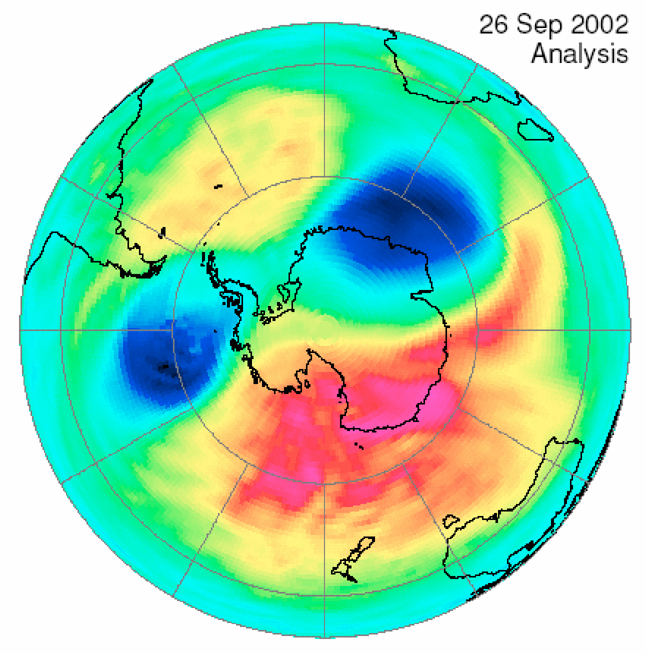


GOME measurements at 25 September 2002



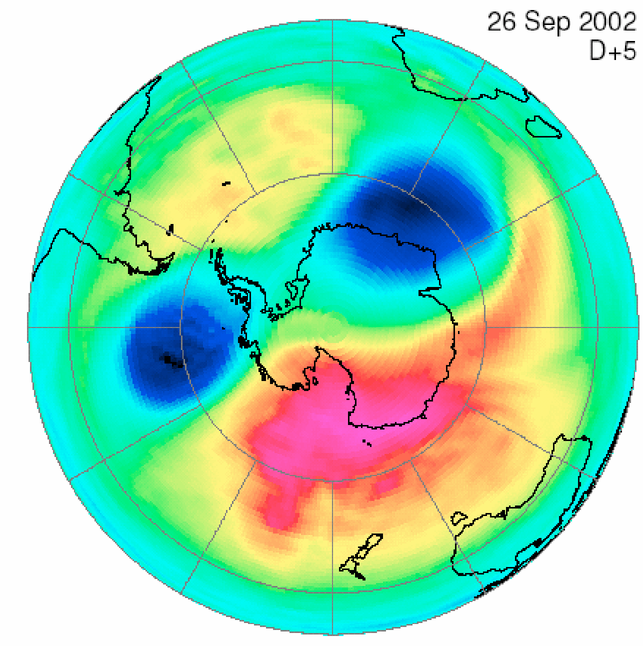
Ozone hole breakup, 2002

26 September 2002
Analysis based on GOME



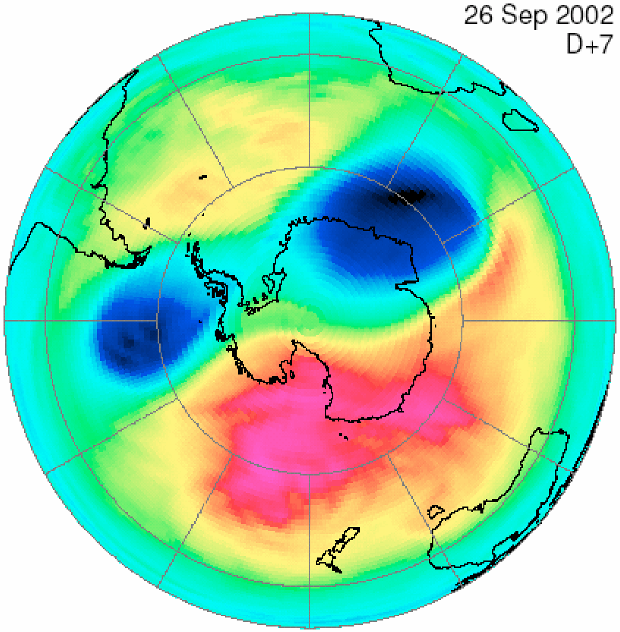
Ozone hole breakup, 2002

26 September 2002
5-day forecast



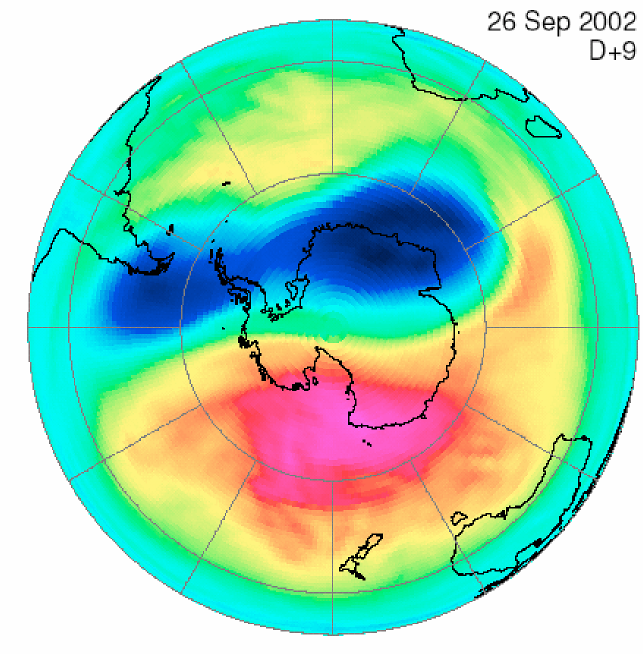
Ozone hole breakup, 2002

26 September 2002
7-day forecast



Ozone hole breakup, 2002

26 September 2002
9-day forecast



Summary

Ozone assimilation

- CTM driven by ECMWF winds describes features of stratospheric ozone in fair detail
- (O-F) total ozone typically 3-4 %
- Noise level GOME total ozone small: < 2 %

Ozone forecasting

- Meaningful forecast up to one week in extratropics
- Tropics: forecast up to 2 days
  (small anomaly, measurement noise, no tropospheric chemistry)
- Examples
  * Breakup 2002 ozone hole
  * Ozone "mini-holes" over Europe
  * UV - excursions of the ozone hole

Further reading

KNMI ozone assimilation

Eskes et al, QJRMS 129, 1663, 2003: GOME ozone assimilation
Eskes et al, ACP 2, 271, 2002: Ozone forecasts

GOME, SCIA and ozone assimilation

Burrows et al, JAS 56, 151, 1999: GOME overview
Bovensmann et al, J. Atmos. Sci. 56, 127, 1999: SCIA overview
Stajner et al, QJRMS 127, 1069, 2001: GEOS O3 data assimilation
Dethof, tech.memo.377, ECMWF, 2002: Ozone in ERA40
Struthers, JGR 107, doi:10.1029/2001JD000957: O3 assim with UKMO
Riishojgaard, QJRMS 122, 1545, 1996: impact O3 assimilation on winds
Khattatov et al, JGR 105, 29135, 2000: assimilation of long-lived tracers
Menard, MWR 128, 2654, 2000: tracer assimilation with Kalman filter