Ozone data assimilation and forecasts

Application of the sub-optimal Kalman filter to ozone assimilation

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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

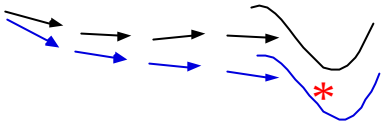
Science questions:
- Recovery ozone layer
- Chemistry - climate interaction

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

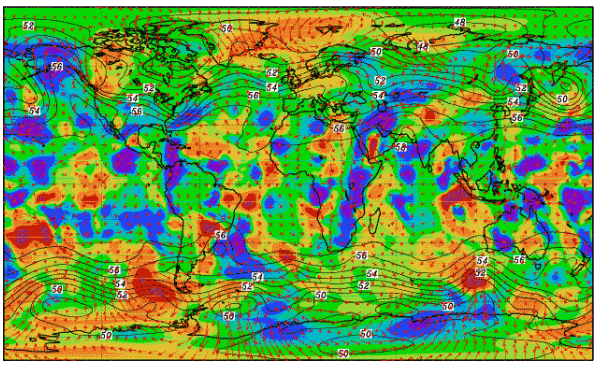


Impact of ozone on NWP

Wind increments due to TOVS ozone observations

ECMWF model

(SODA project)



Wind increments ~ 0.5 m/s

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)
- NOAA/NCEP (SBUV)
- DAO (TOMS, SBUV)
- Meteo France (TOVS)
- UKMO, Univ.Reading (GOME, MLS)

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:

Forecast covariance = time-dependent variance * fixed correlations

Correlation matrix:

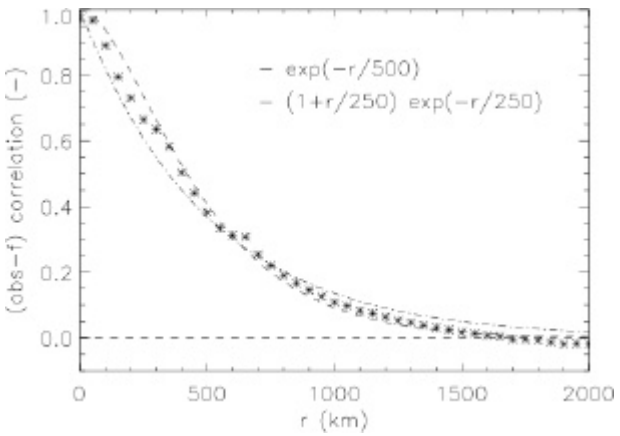
function of the distance only
functional form determined from OmF statistics

Variance:

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

Correlations

Distance dependence descibed by 2nd order autoregressive function

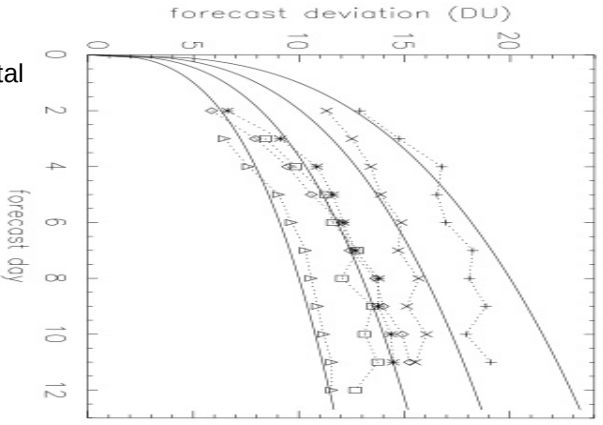


Model error

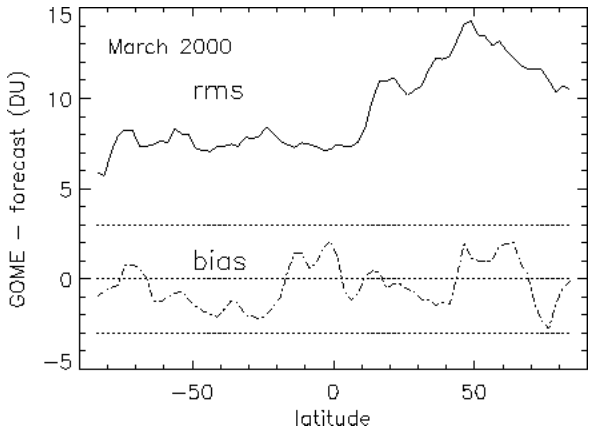
One-coefficient fit function to the observed ozone total column OmF as a function of the forecast period

Coefficient: Function of latitude and month

Model error: Derivative of curve



Observation minus forecast statistics



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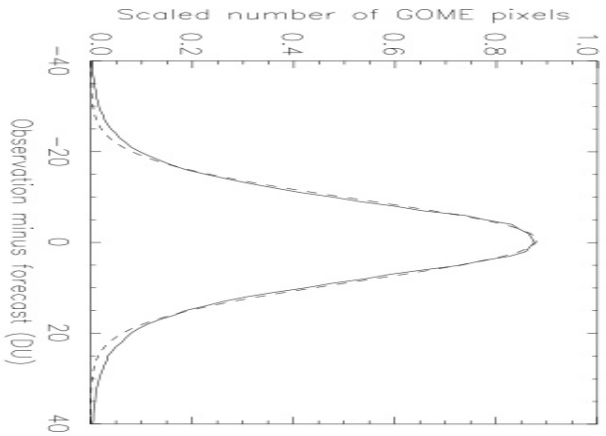
Gaussian statistics



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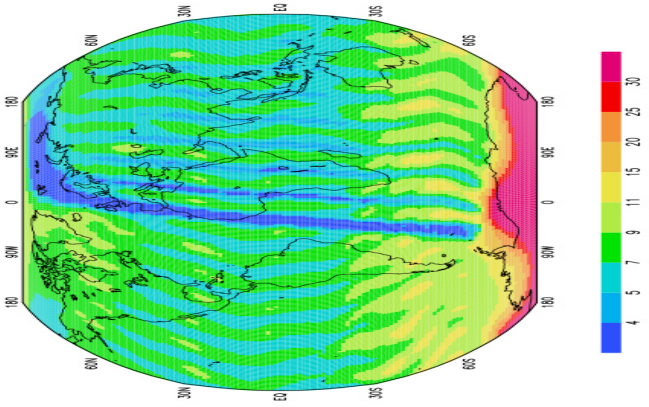
Forecast error

- Analysis
- Advection
- Model error



Forecast error verification

χ^2 test (E.g. Menard, 2000)

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

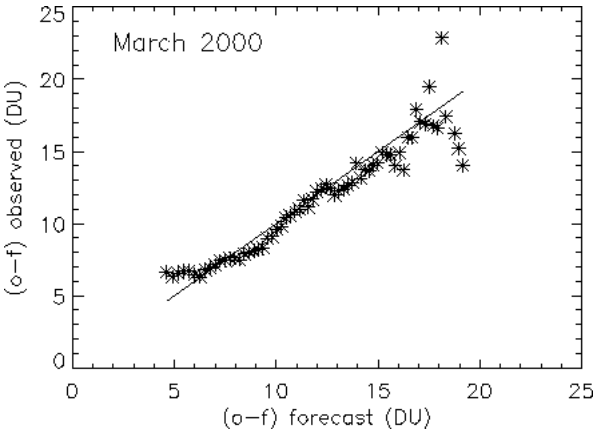
or

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

Forecast error verification

Note:

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



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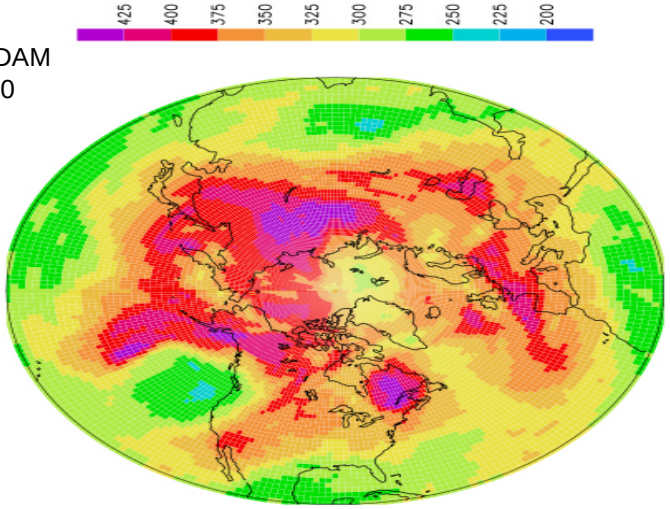
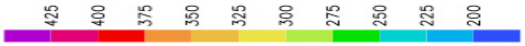
Comparison with TOMS total ozone

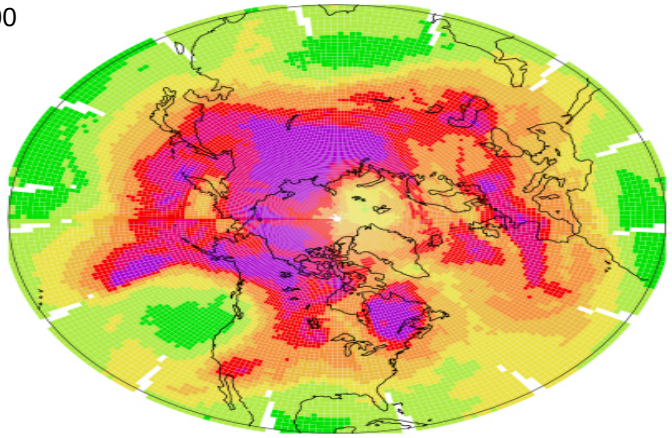
GOME / TM3DAM
31 March 2000
12h local time



Comparison with TOMS total ozone



TOMS
31 March 2000



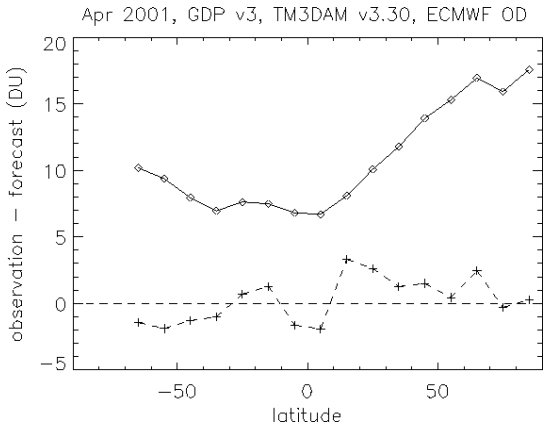
Dependence on GOME retrieval

- Version 3 GDP ozone columns
- KNMI fast delivery, v3

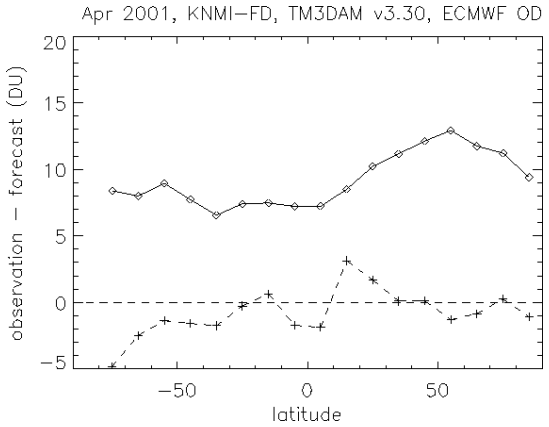
Validation results:
- J.C. Lambert: http://www.oma.be/GOME
- D. Balis: GOA first annual report

Validation studies focus on bias
(rms much more difficult to estimate with ground-based observations)

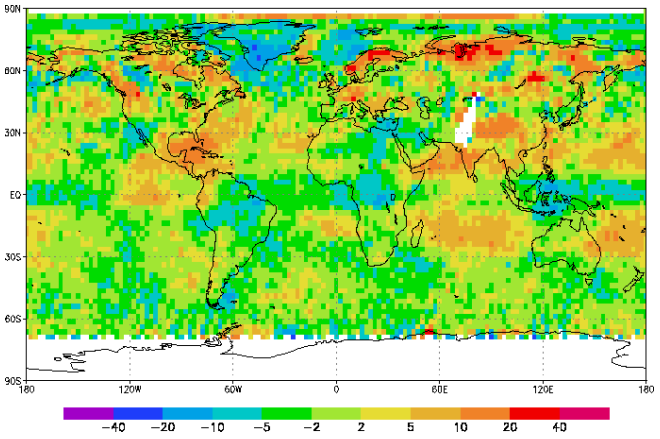
Observation minus forecast statistics: ECMWF OD



OmF vs latitude, KNMI FD, ECMWF OD



OmF distribution, GDP3, ECMWF OD Apr 2001



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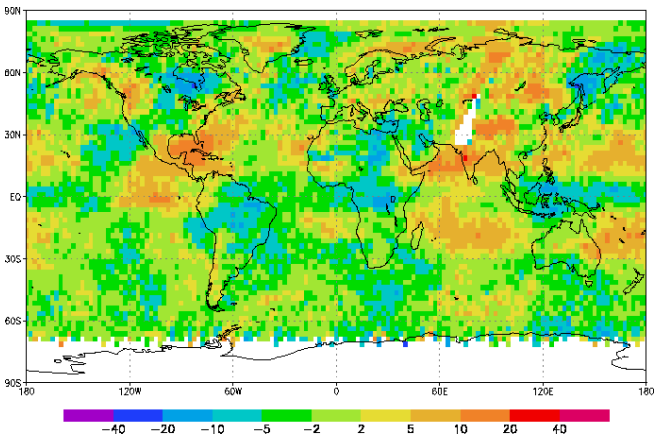
OmF distribution, KNMI FD, ECMWF OD Apr 2001



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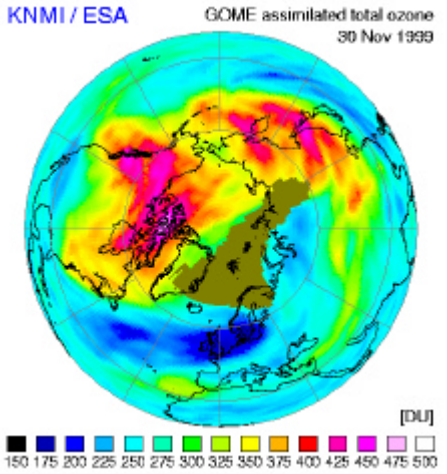
Break

Seven year GOME ozone data set: examples

http://www.knmi.nl/goa

Low-ozone events



30 Nov 1999:
Lowest ozone value since beginning TOMS series

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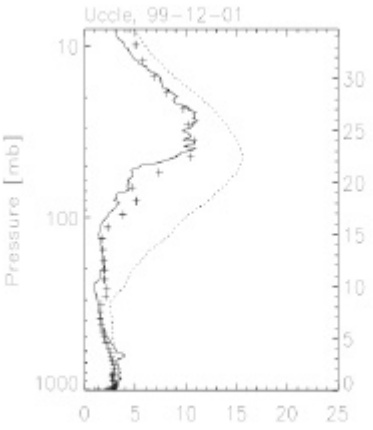
Low-ozone event: profile



30 Nov 1999:
Lowest ozone value since beginning TOMS series

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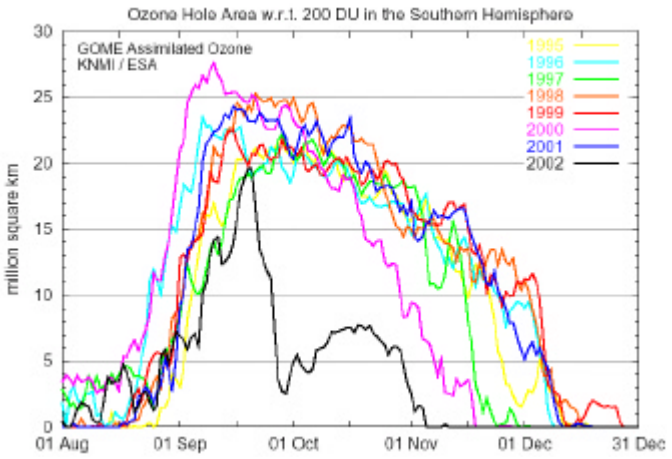
GOME: Ozone hole 1995-2002

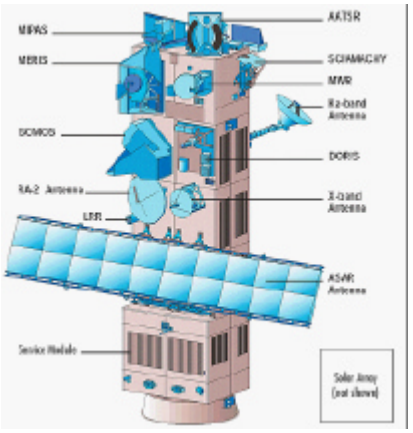


New observations: ENVISAT

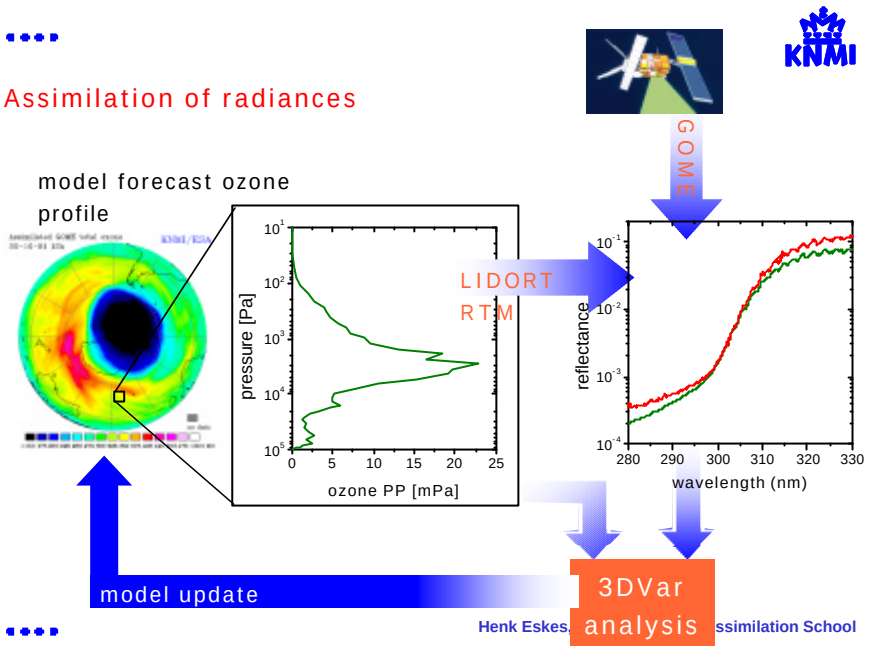
Atmospheric chemistry instruments
- MIPAS
- GOMOS
- SCIAMACHY

Stratosphere
- O_3, Cl, Br, N, H

Troposphere (Sciamachy)
- O_3, NO_2, H_2CO, SO_2
- CH_4, CO, CO_2



Assimilation of radiances



Ozone forecasts, based on GOME observations

Henk Eskes, Peter van Velthoven,
Pieter Valks, Mark Allaart, Ronald van der A,
Hennie Kelder

http://www.knmi.nl/gome_fd

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 ozone data
  - near-real time
- Data assimilation scheme
  - parametrized Kalman filter

--> Daily ozone analyses and 5-day forecasts

Anomaly correlation, RMS error

Anomaly correlation

$C = \langle (f-c)(a-c) \rangle \; / \; \langle (f-c)^2 \rangle \; \langle (a-c)^2 \rangle$

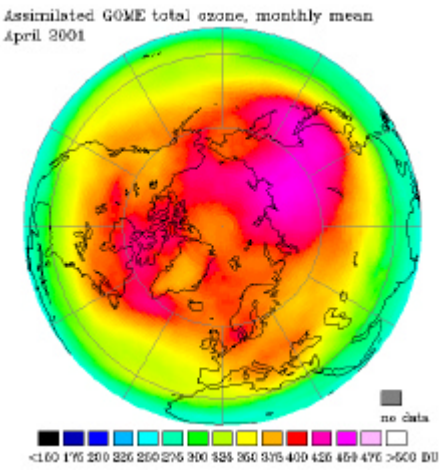
Root mean square error

$E = \langle (f-a)^2 \rangle$

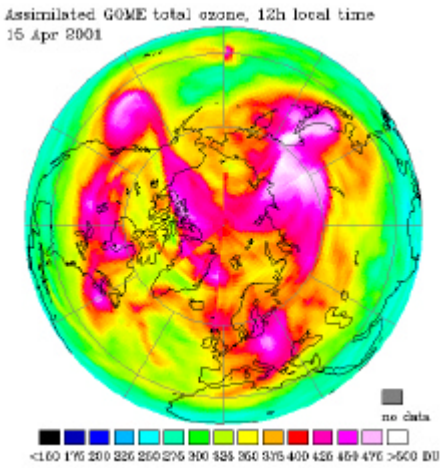
(f = forecast, a = analysis, c = climatology)

- 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



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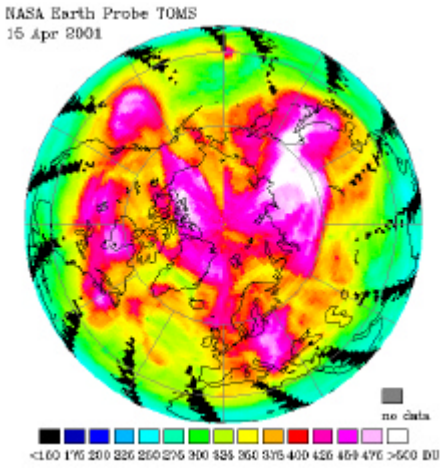
TOMS
15 April 2001



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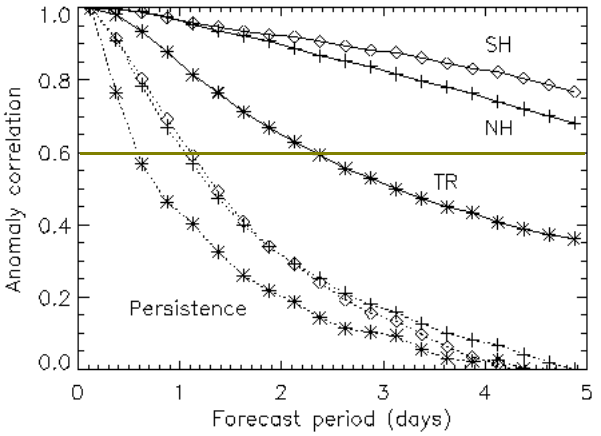
Anomaly correlation



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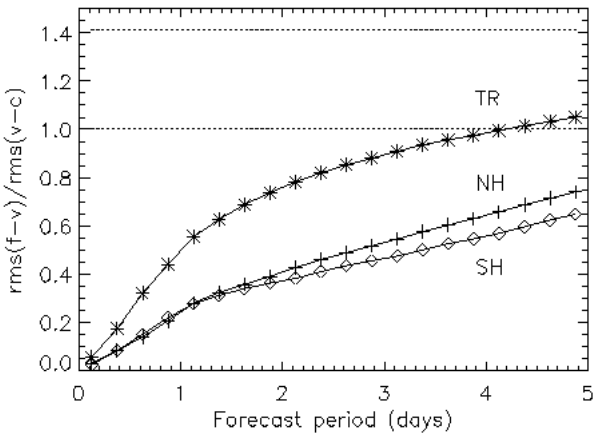
RMS error



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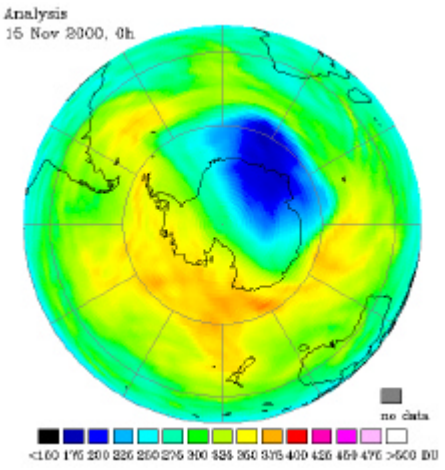
Tropics

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

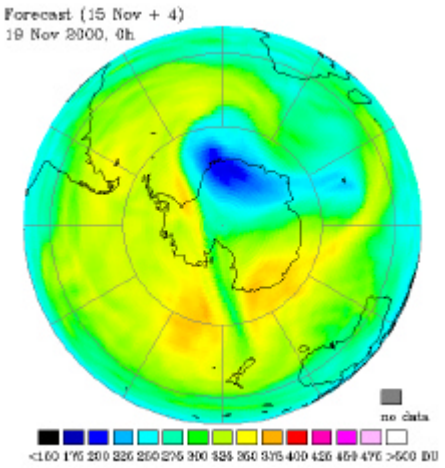
Breakup 2000 ozone hole

15 November 2000 analysis based on GOME ozone observations



Breakup 2000
ozone hole

19 November 2000
4-day forecast



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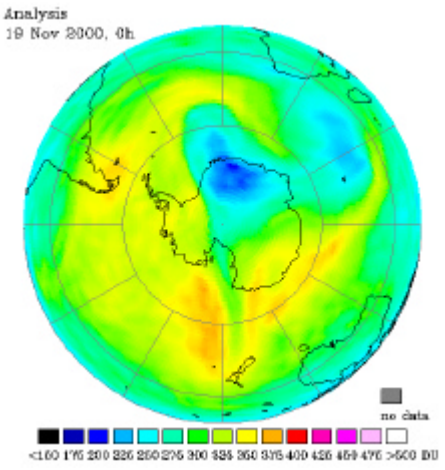
Breakup 2000
ozone hole

19 November 2000
analysis



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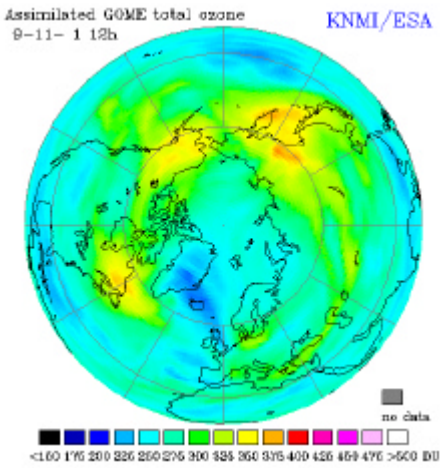
Low ozone episode

5-day forecast
9 November 2001



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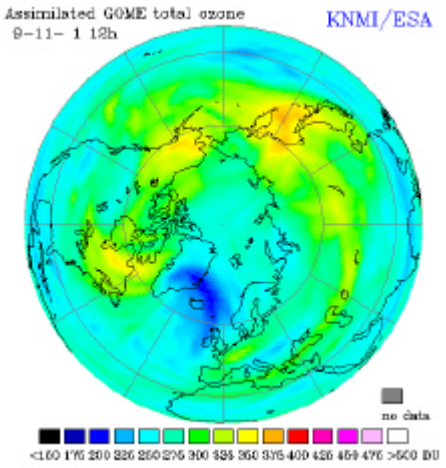
Low ozone episode

3-day forecast
9 November 2001



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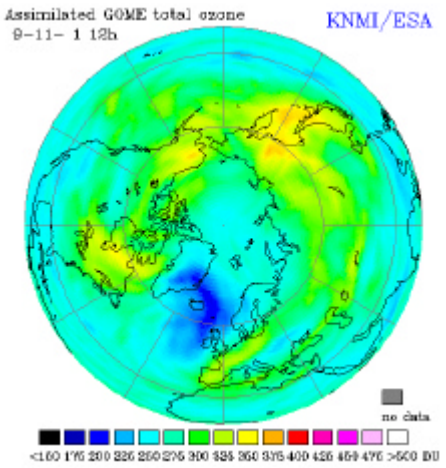
Low ozone episode

analysis
9 November 2001



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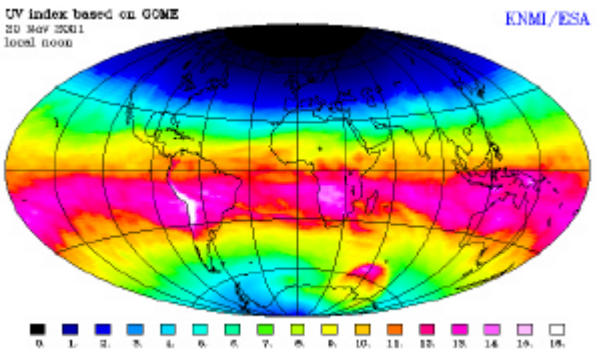
UV forecast

20 November 2001
(5-day forecast)



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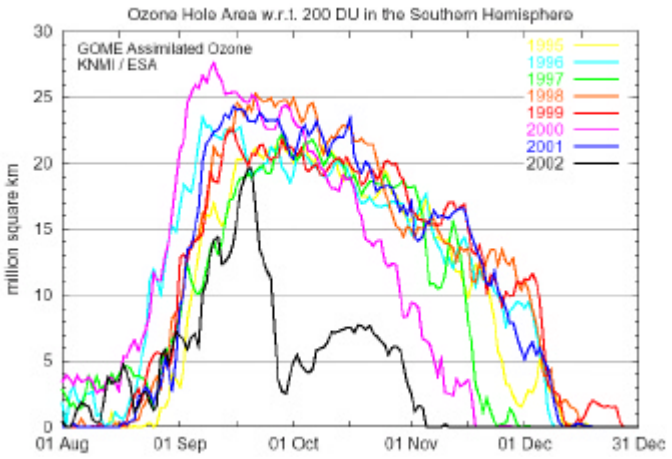
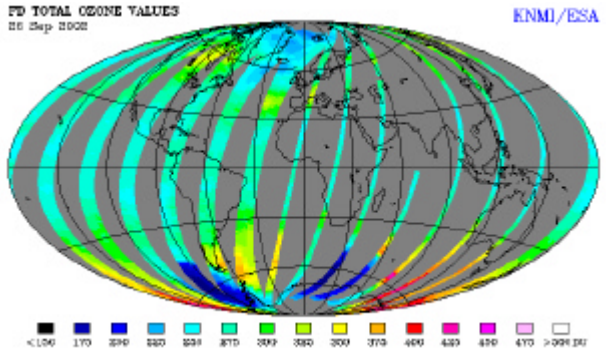
GOME: Ozone hole 1995-2002

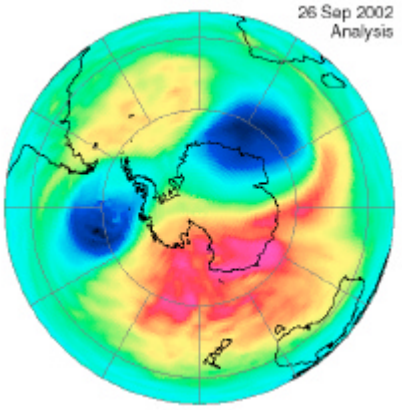


GOME measurements at 25 September 2002



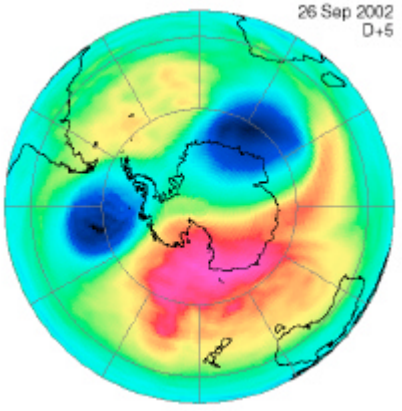
Ozone hole breakup, 2002

26 September 2002
Analysis based on GOME



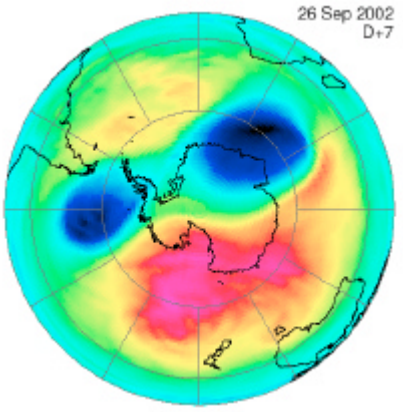
Ozone hole breakup, 2002

26 September 2002
5-day forecast



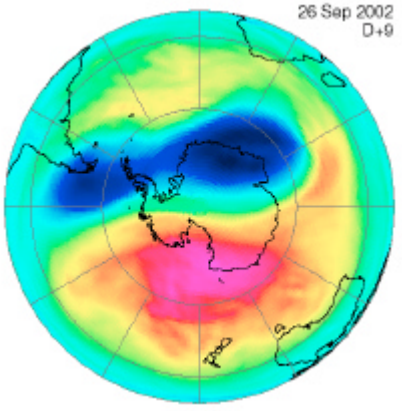
Ozone hole breakup, 2002

26 September 2002
7-day forecast



Ozone hole breakup, 2002

26 September 2002
9-day forecast



Summary

Ozone forecasting

- Meaningful forecast up to one week in extratropics
- Tropics: forecast up to 2 days
  - (small anomaly, measurement noise, no tropospheric chemistry)

Examples

- Breakup 2000/2002 ozone hole
- Ozone "mini-holes" over Europe
- UV: excursion 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 and ozone assimilation

Burrows et al, JAS 56, 151, 1999: GOME 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