



Stratospheric ozone: satellite observations, data assimilation and forecasts

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1) Ozone and Numerical Weather Prediction



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

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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:

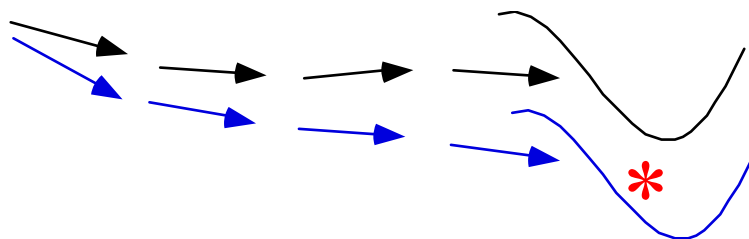
satellite observations 1978-present, TOMS, SBUV



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



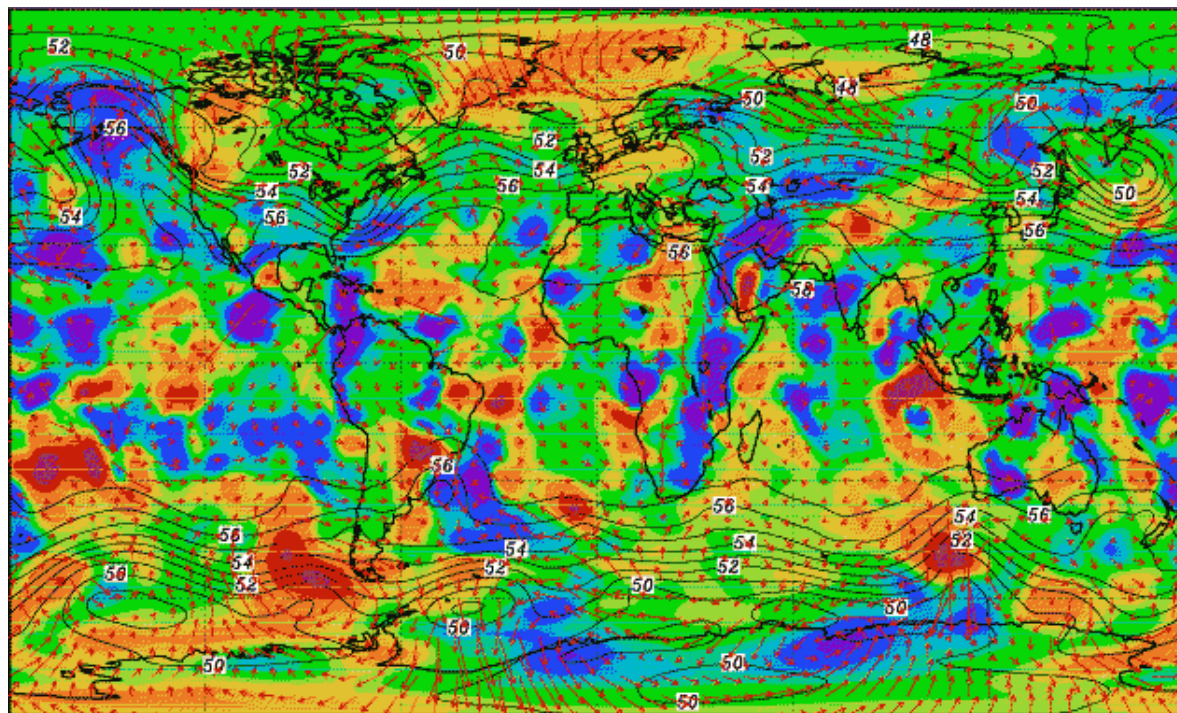


Impact of ozone on NWP

Wind increments
due to
TOVS ozone
observations

ECMWF model

(EU SODA project)

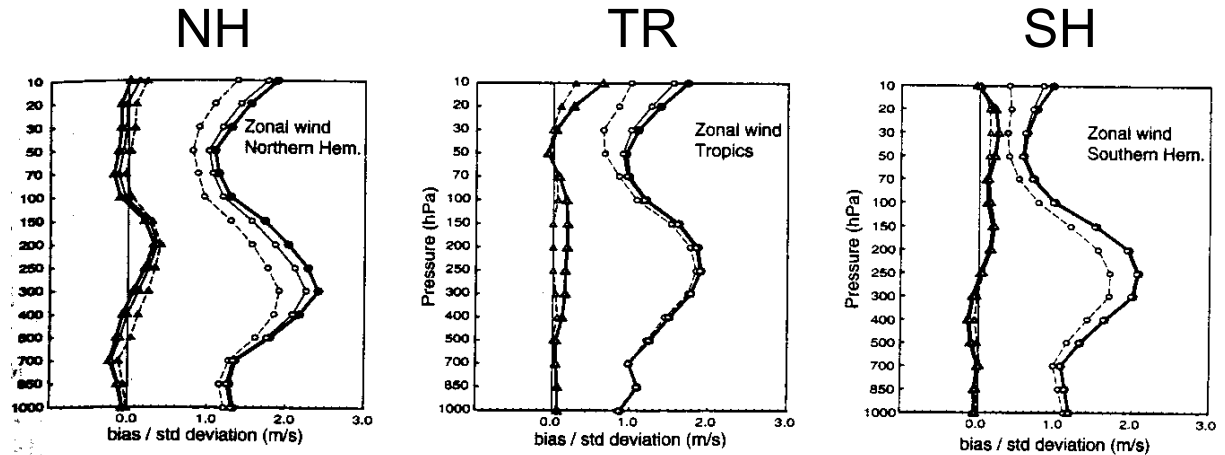


Wind increments ~ 0.5 m/s

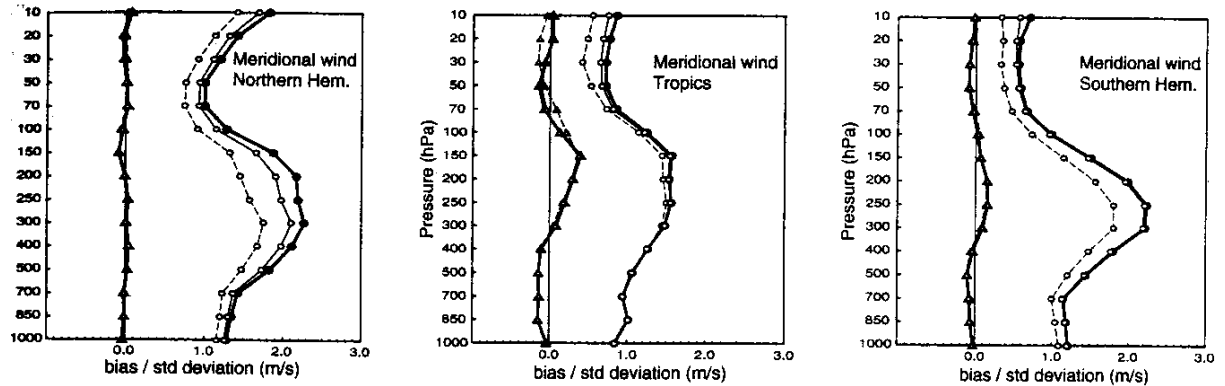


OSSE: Impact of TOVS column retrievals on winds

Zonal wind



Merid. wind



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

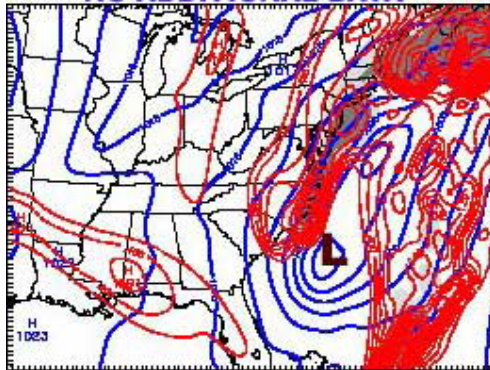
August 07, 2003- (date of web publication)



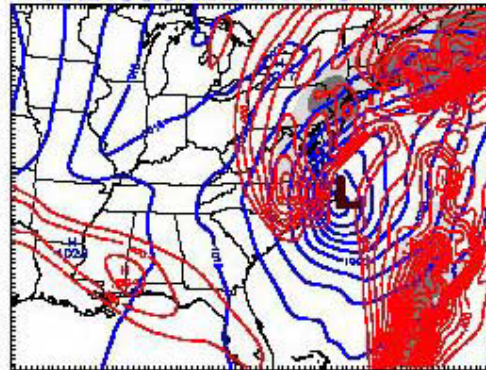
With TOMS data



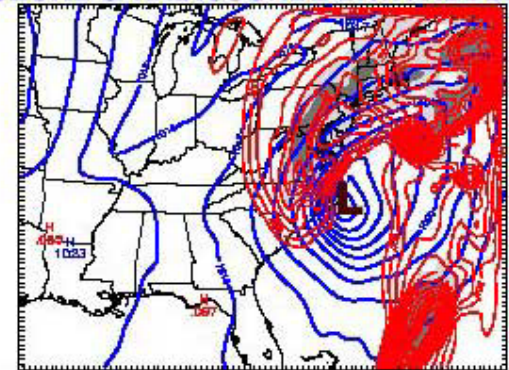
NO ADDITIONAL DATA



RADIOSONDE DATA ONLY



OZONE & RADIOSONDE DATA ADDED



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:

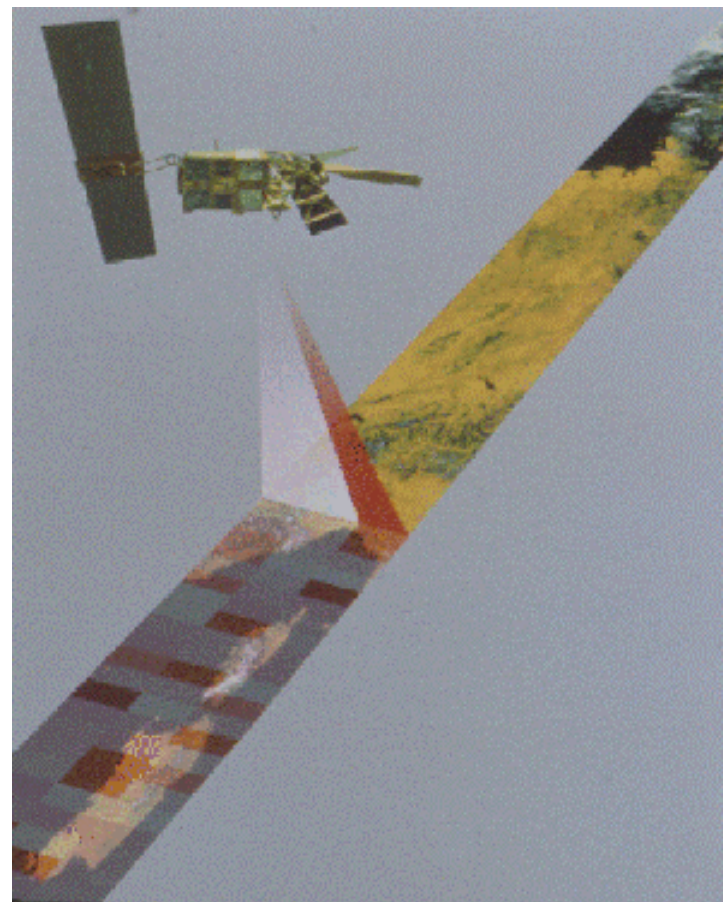
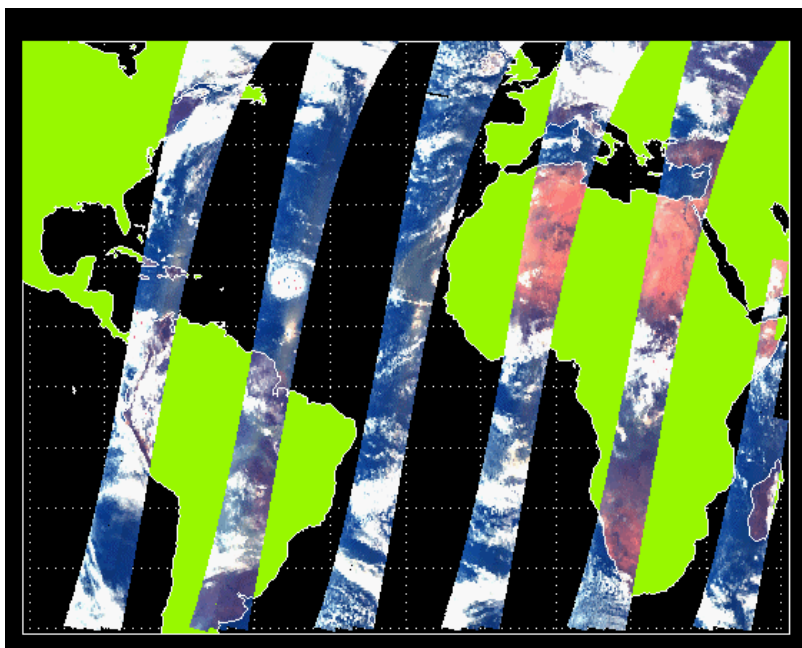
TOMS, GOME, SCIAMACHY

Ground-based observations

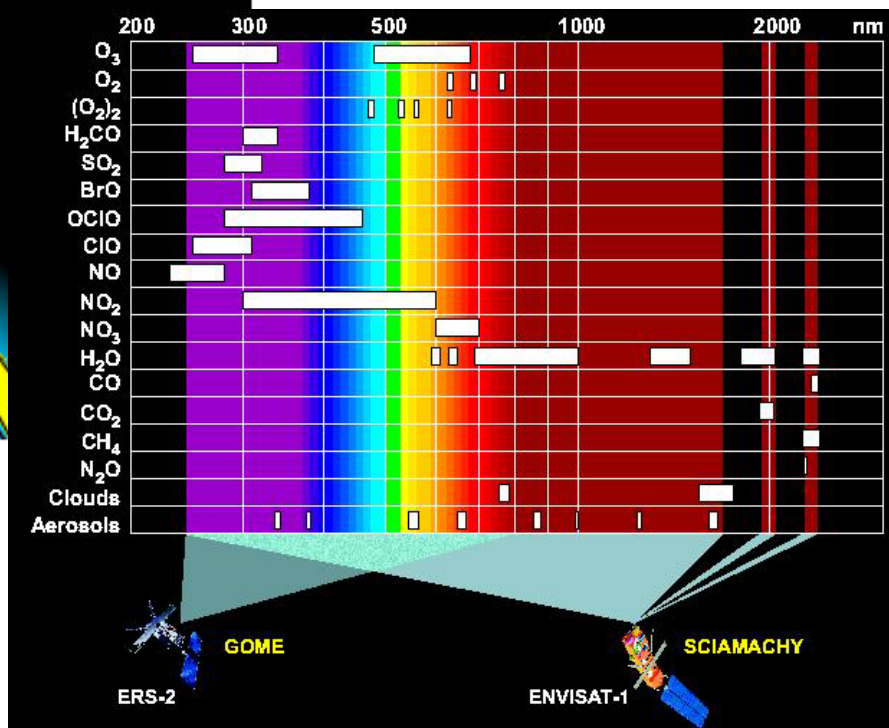
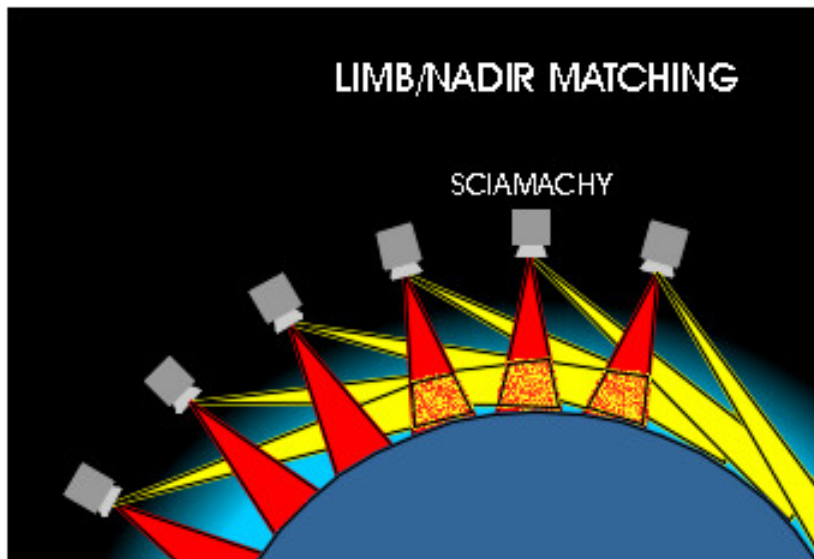




GOME on ERS-2, 1995 -



SCIAMACHY on ENVISAT, 2002 -

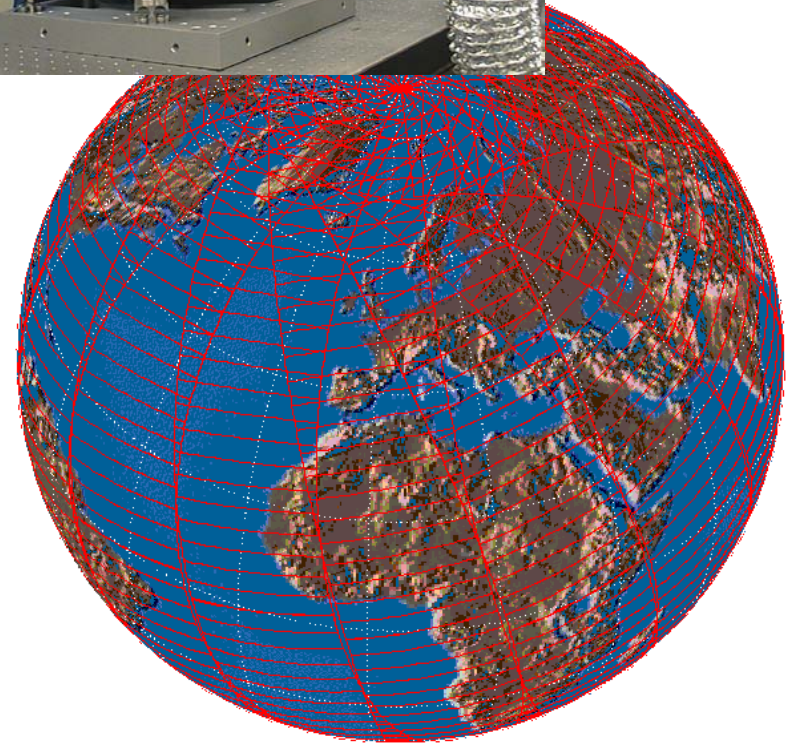
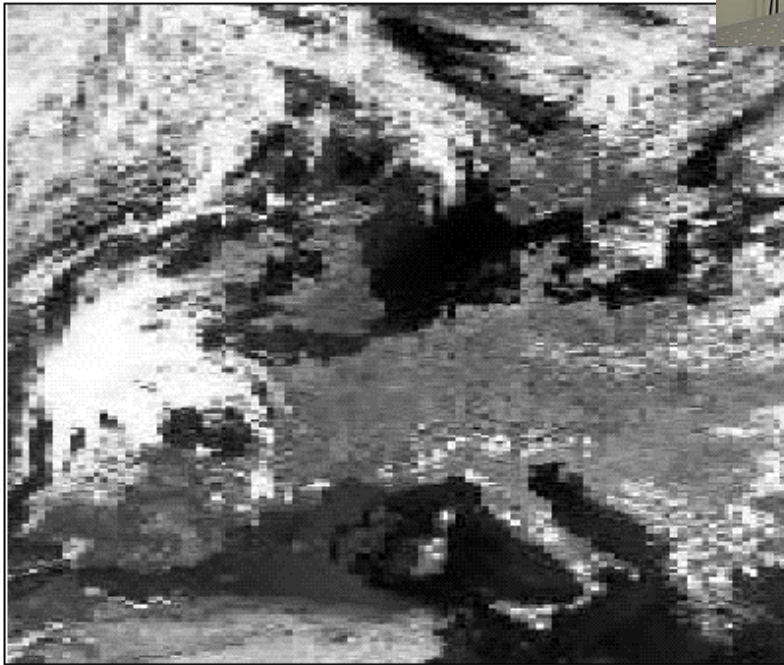
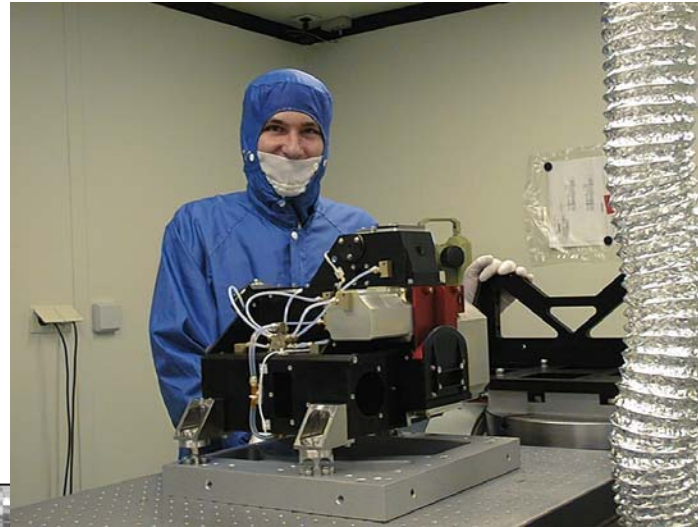


Troposfeer & stratosfeer

- O₃, NO₂, H₂CO, SO₂
- CH₄, CO, CO₂



OMI on EOS-AURA, 2004 -



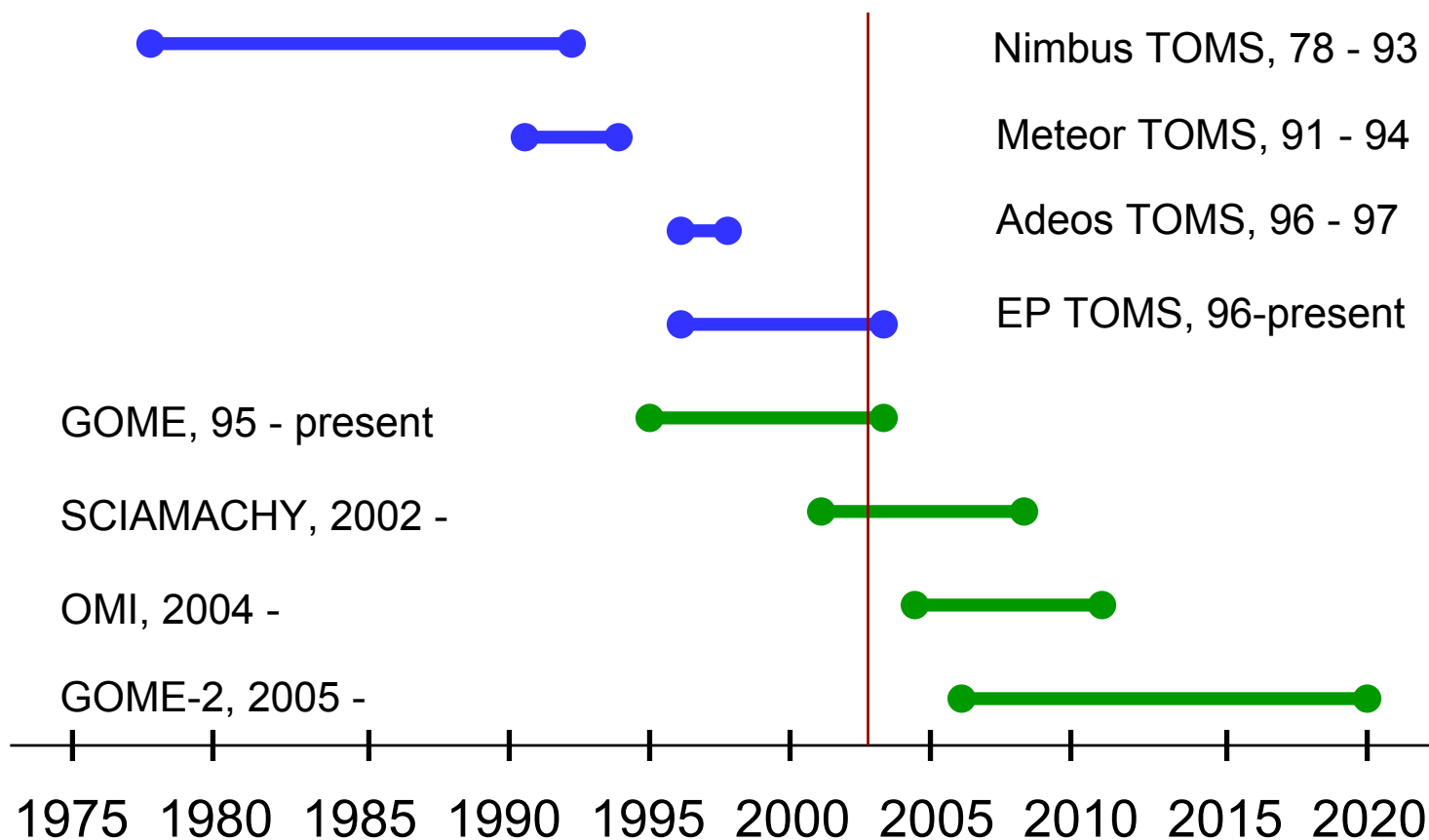


GOME-2 on METOP, 2005-2020





Ozone column measurements, 1978 - 2020



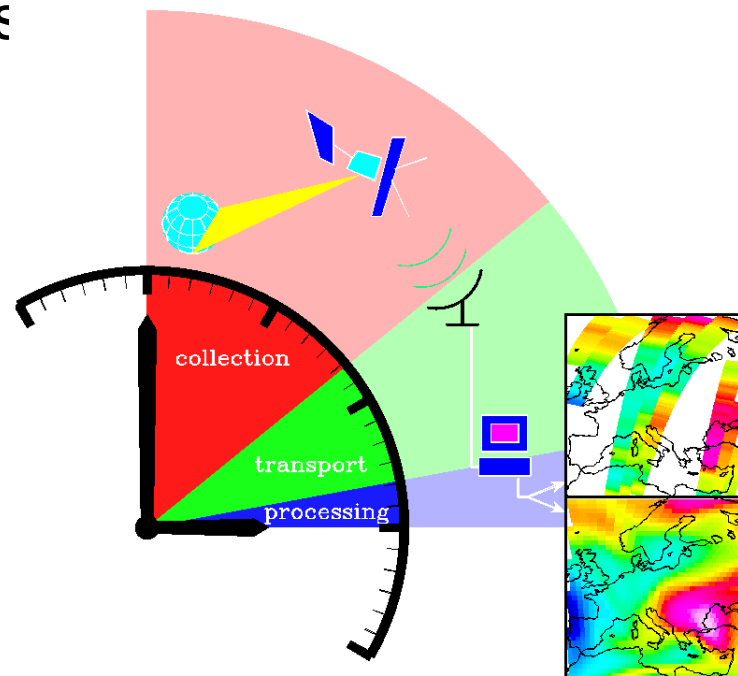


3) Retrieval



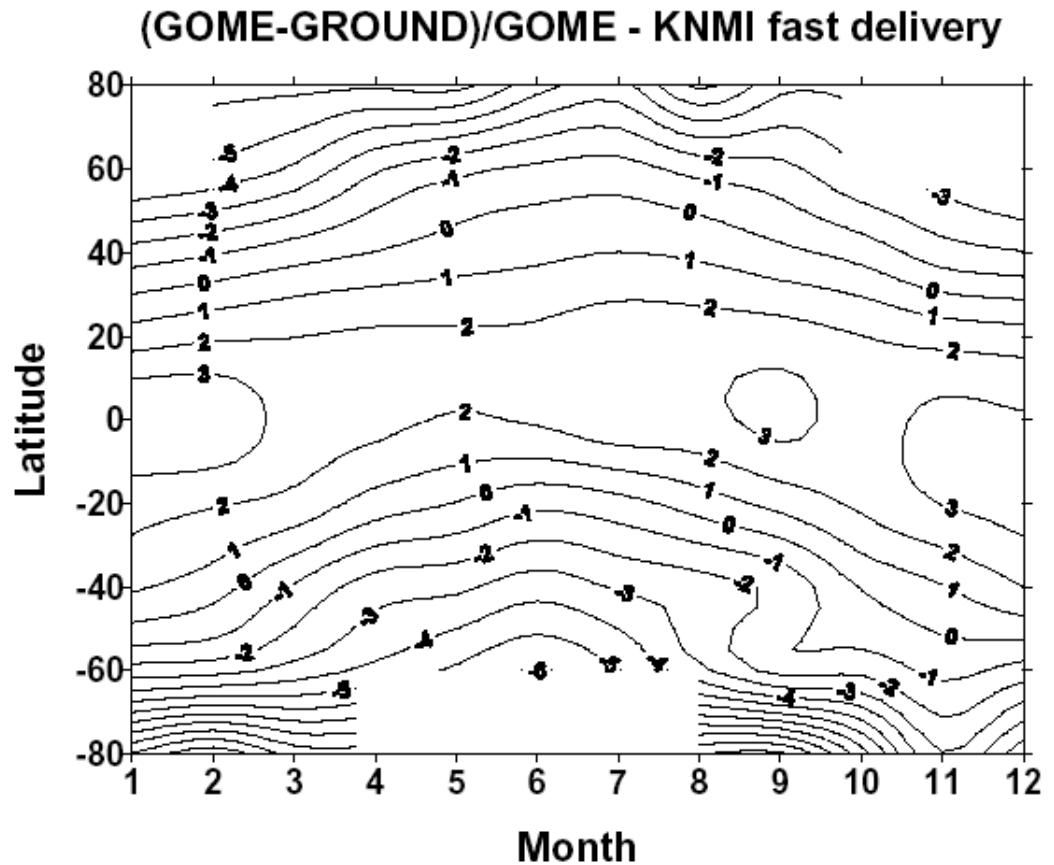
KNMI/ESA GOME Fast Delivery total ozone product

- Availability of ozone observations in less than 3 hours after the measurement (ESA Data User Programme)
- Used in ECMWF operational analyses





KNMI/ESA GOME Fast Delivery total ozone product



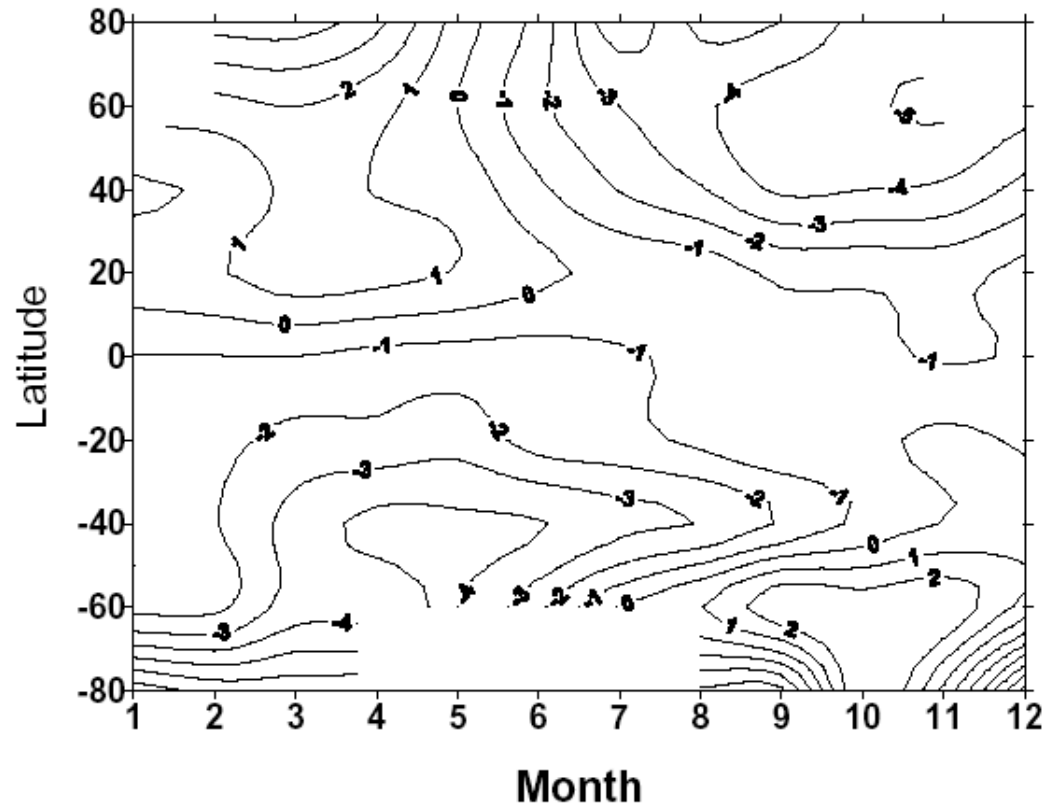
Validation:
Dimitris Balis, LAP
Fast Delivery vs.3
KNMI





ESA/DLR GOME Data Processor

(GOME-GROUND)/GOME - GDP 2.7

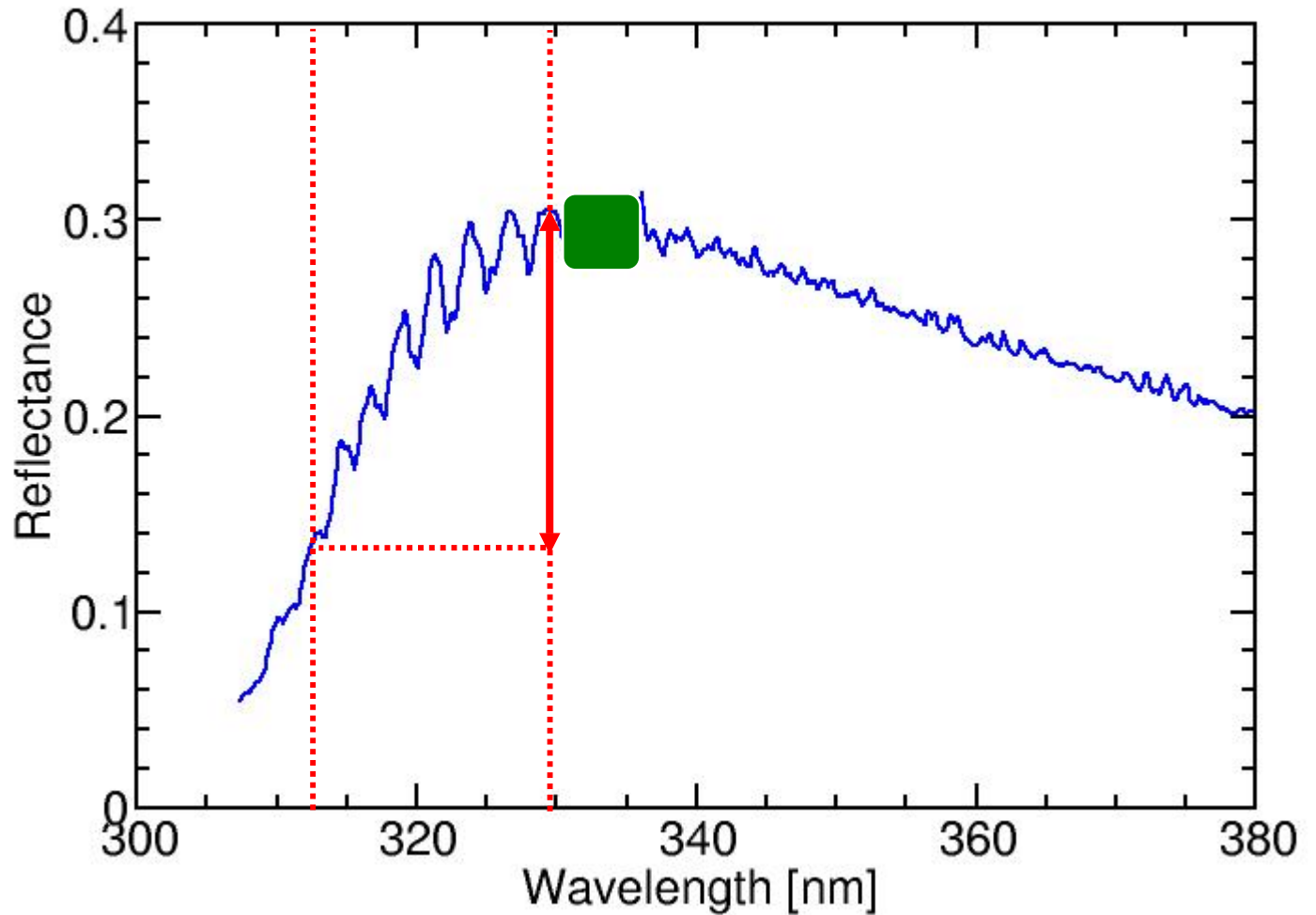


Validation:
Dimitris Balis, LAP
DLR GDP v2.7



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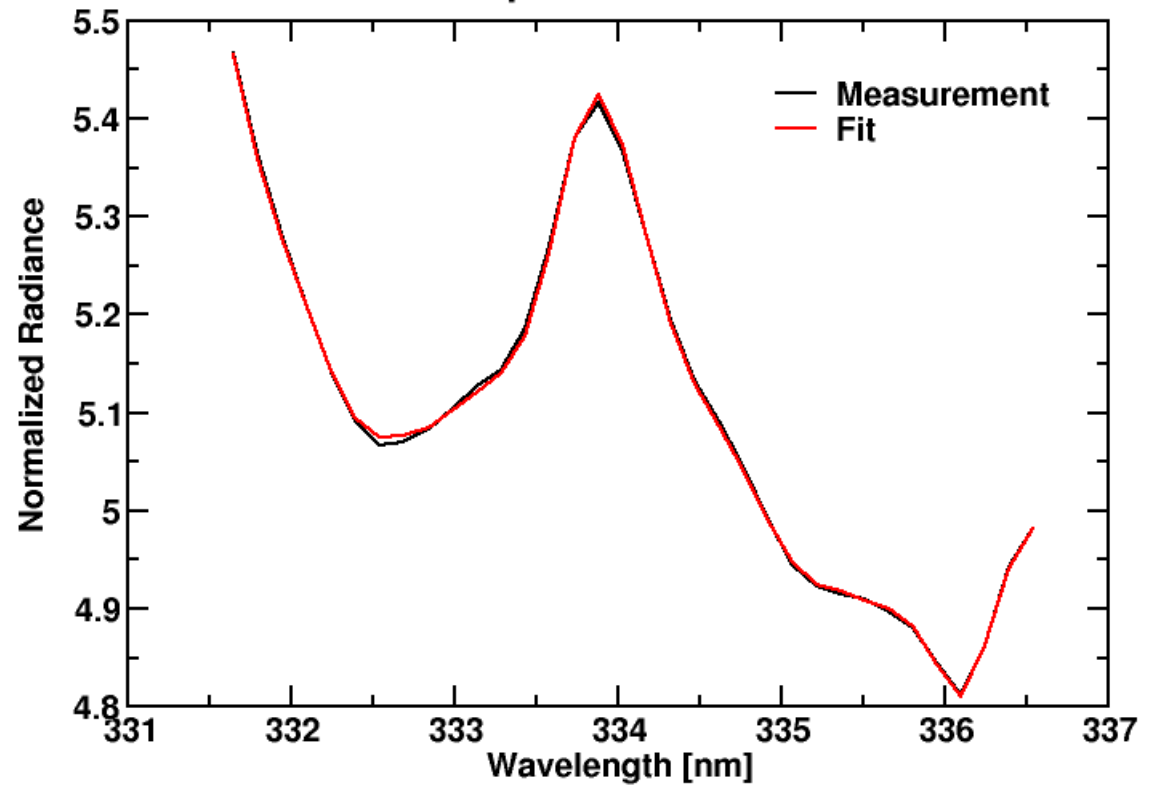
Ozone retrieval: TOMS retrieval vs. DOAS





Ozone retrieval: DOAS

Example of a DOAS Fit



First OMI ozone measurements



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Ozone retrieval: new DOAS algorithm

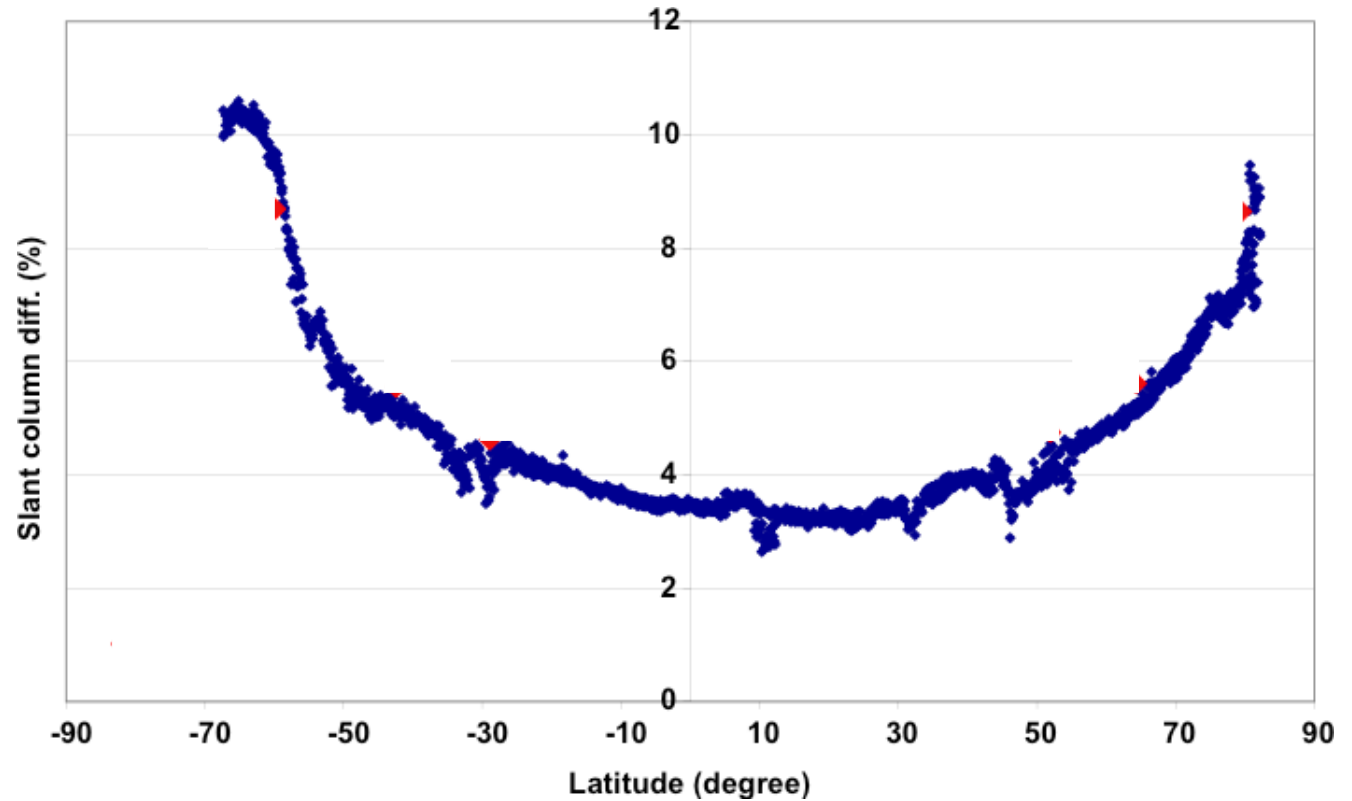
Based on the OMI-DOAS operational algorithm (P. Veefkind)
Implementations for GOME (P. Valks) and Sciamachy

Innovations compared to Fast Delivery, vs 3

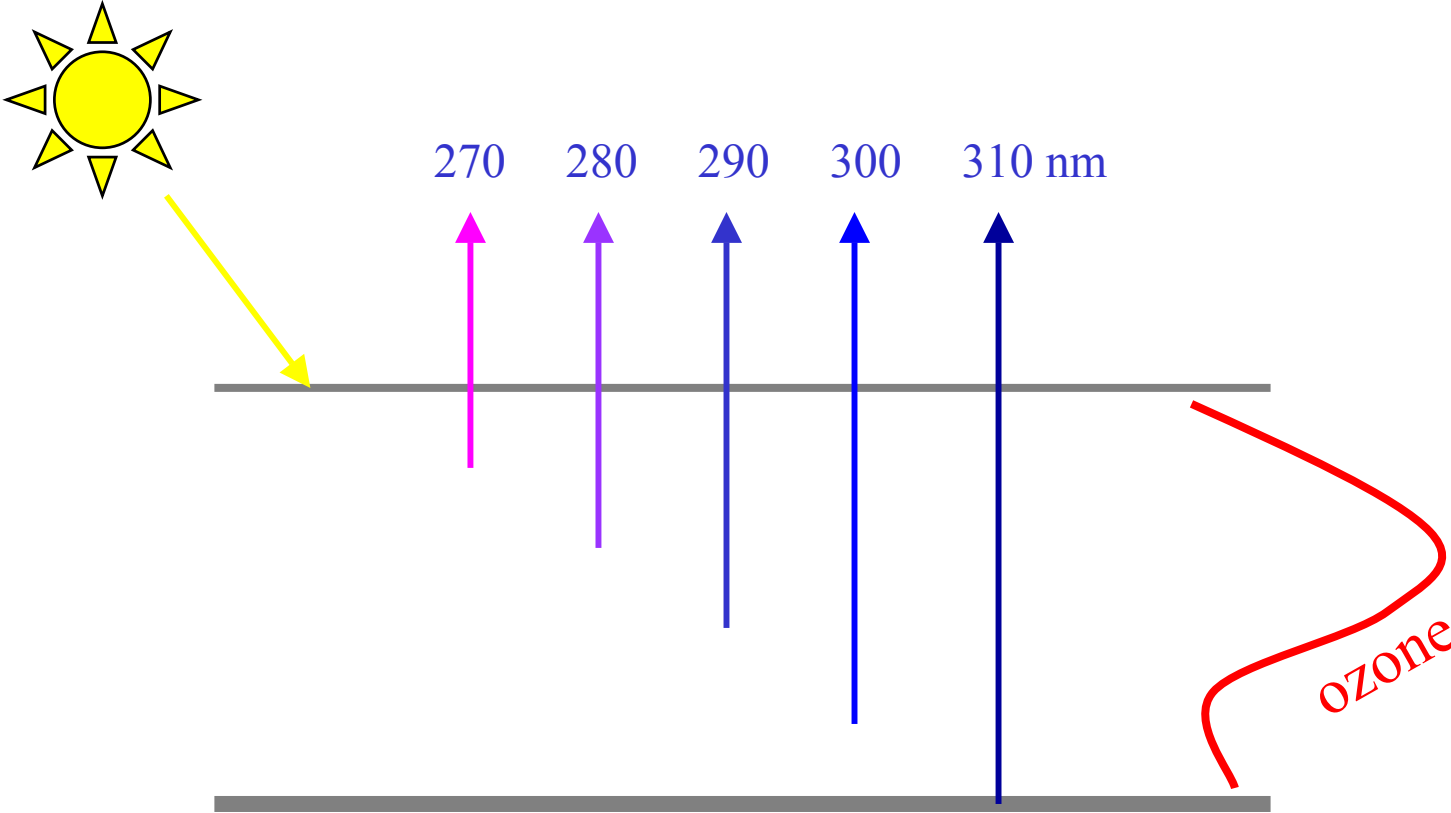
- New treatment of Raman scattering (J. de Haan)
- Empirical air-mass factor approach
- Wavelength window - reduced T dependence
- TOMS v8 ozone profile data base
- Radiative transfer improvement

New approach to Raman scattering

Difference between old and new treatment of Raman



Ozone nadir profile retrieval

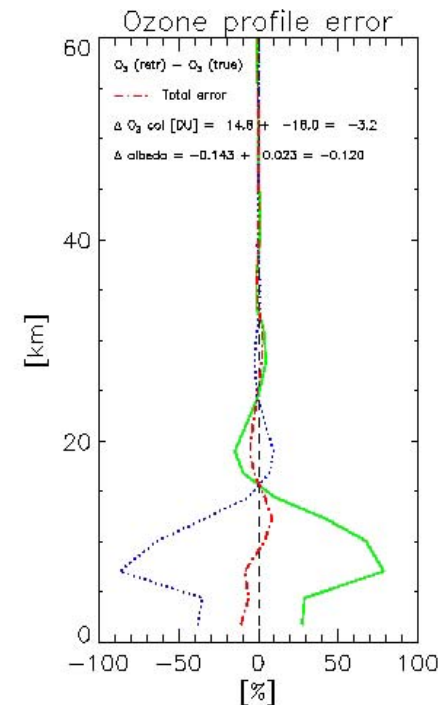
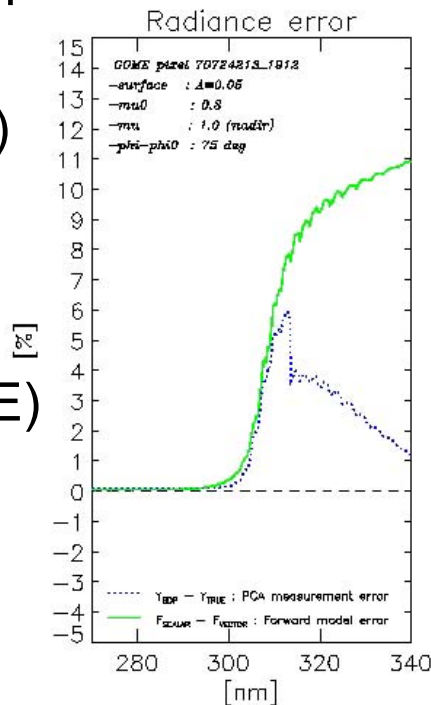


Ozone profile retrieval: challenges

Understanding/ Explaining spectrum

- Radiation modelling:
 - ✓ Raman scattering (*Ring effect*)
 - ✓ Spherical atmosphere
 - ✓ Polarisation

- Instrumental characteristics (GOME)
 - ✓ Degradation
 - ✓ Radiometric calibration
 - ✓ Wavelength calibration
 - ✓ Polarisation correction





4) Ozone assimilation



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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

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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



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Stratospheric chemistry

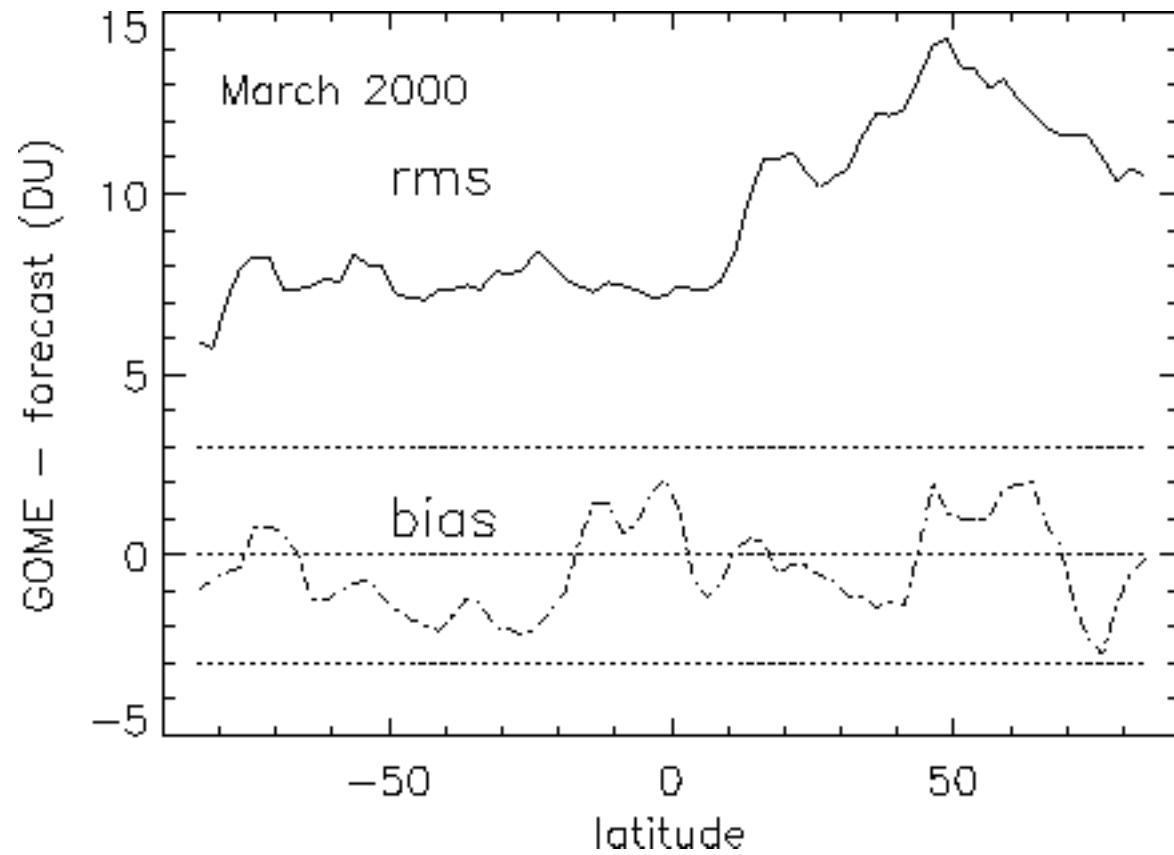
A serious chemistry scheme for the stratosphere involves order 40 transported species - very expensive for NWP

Alternative:

Import ozone production and loss rates from a lower resolution CTM

$$\frac{\partial \chi}{\partial t} = P - \frac{1}{\tau_{loss}} \chi$$

Observation minus forecast statistics



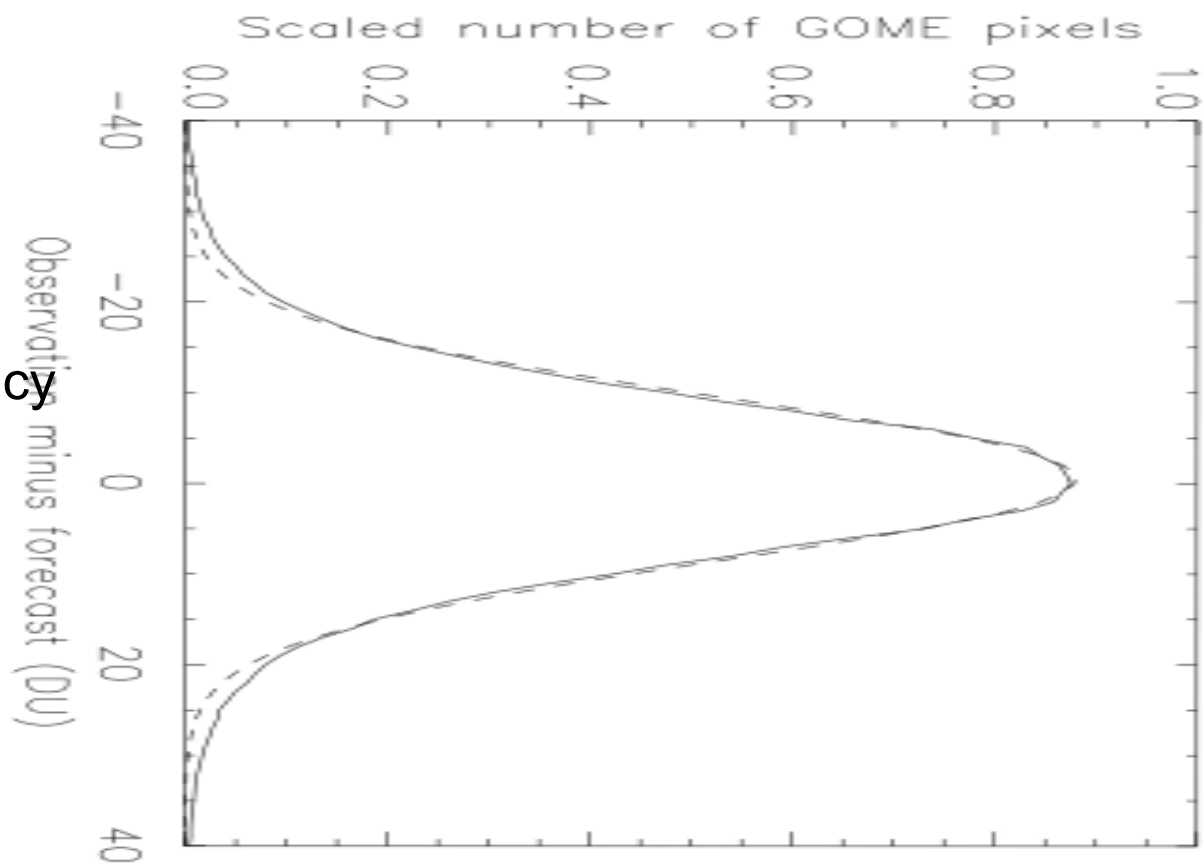


Gaussian statistics

Internal consistency
GOME data

Low noise ($< 2\%$)

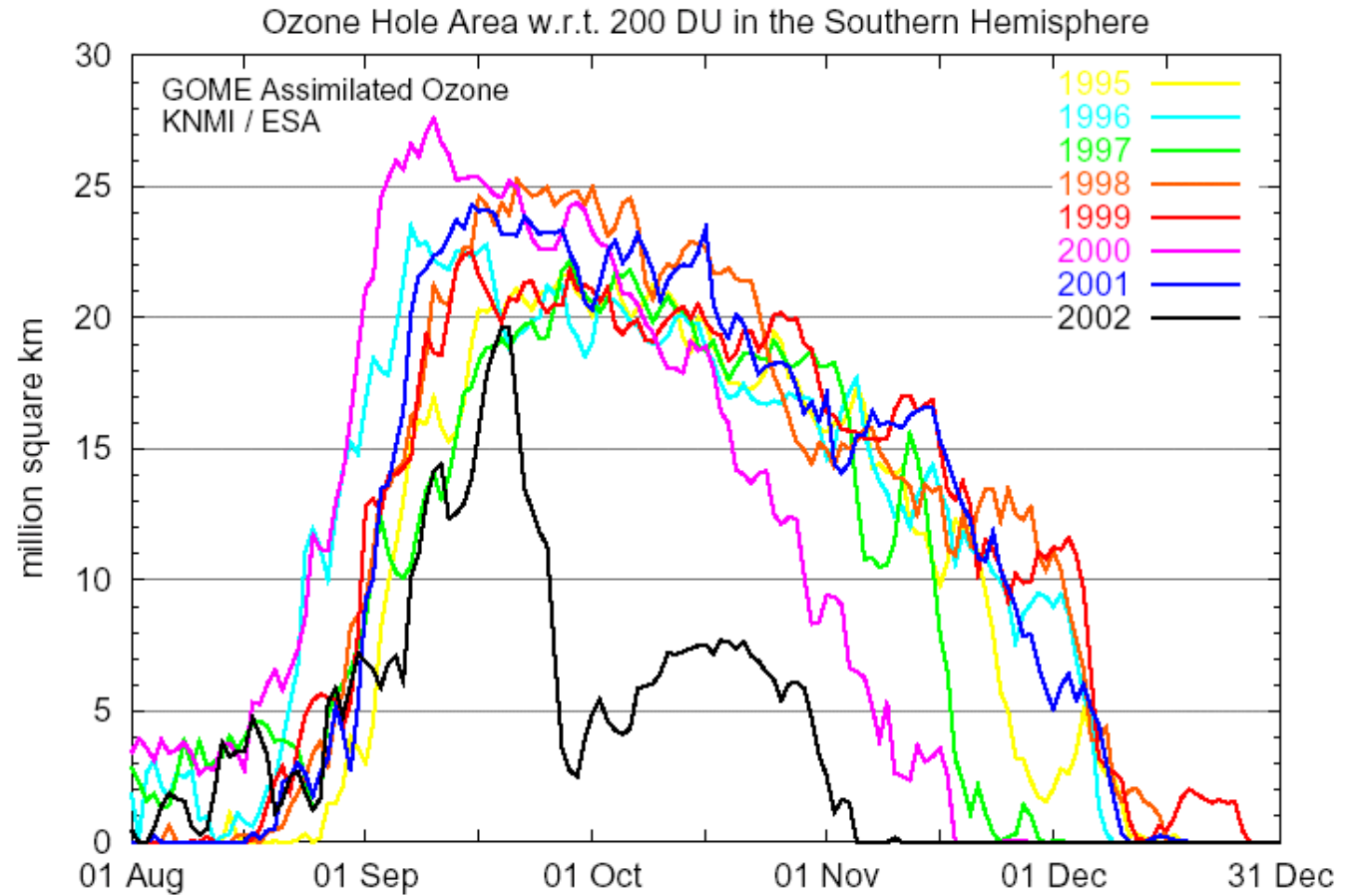
No quality control
needed





7 year GOME data set

<http://www.knmi.nl/goa>





5) Residual circulation and trace gas distributions: Brewer-Dobson, STE



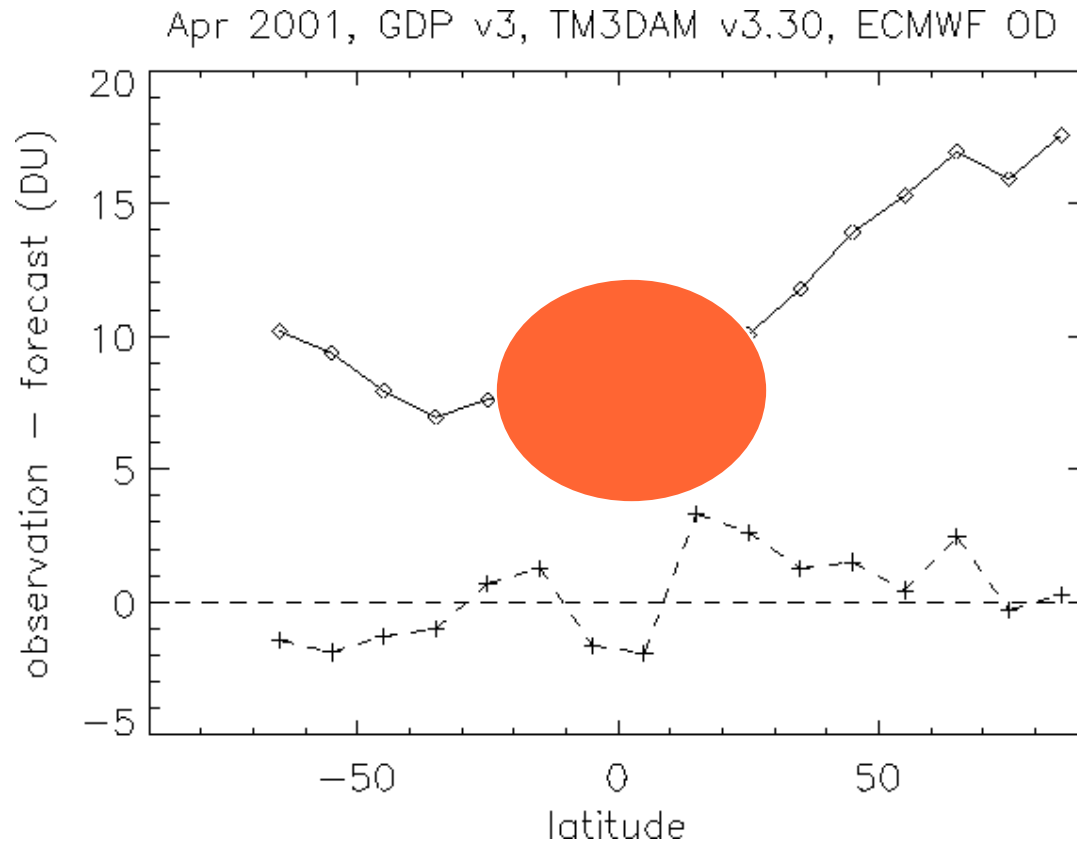


Ozone assimilation: dependence on ECMWF meteorology

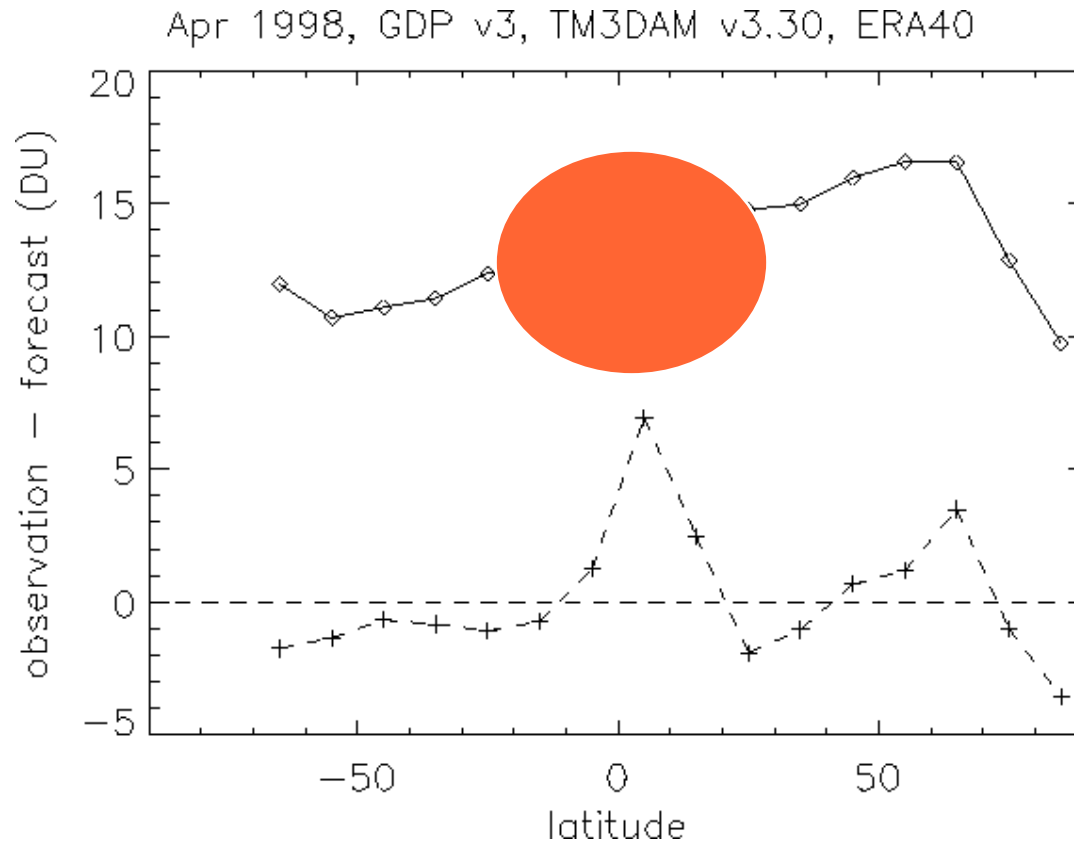
- ERA-40 (1995-1999)
- OD (1999-2002)



Observation minus forecast statistics: ECMWF OD

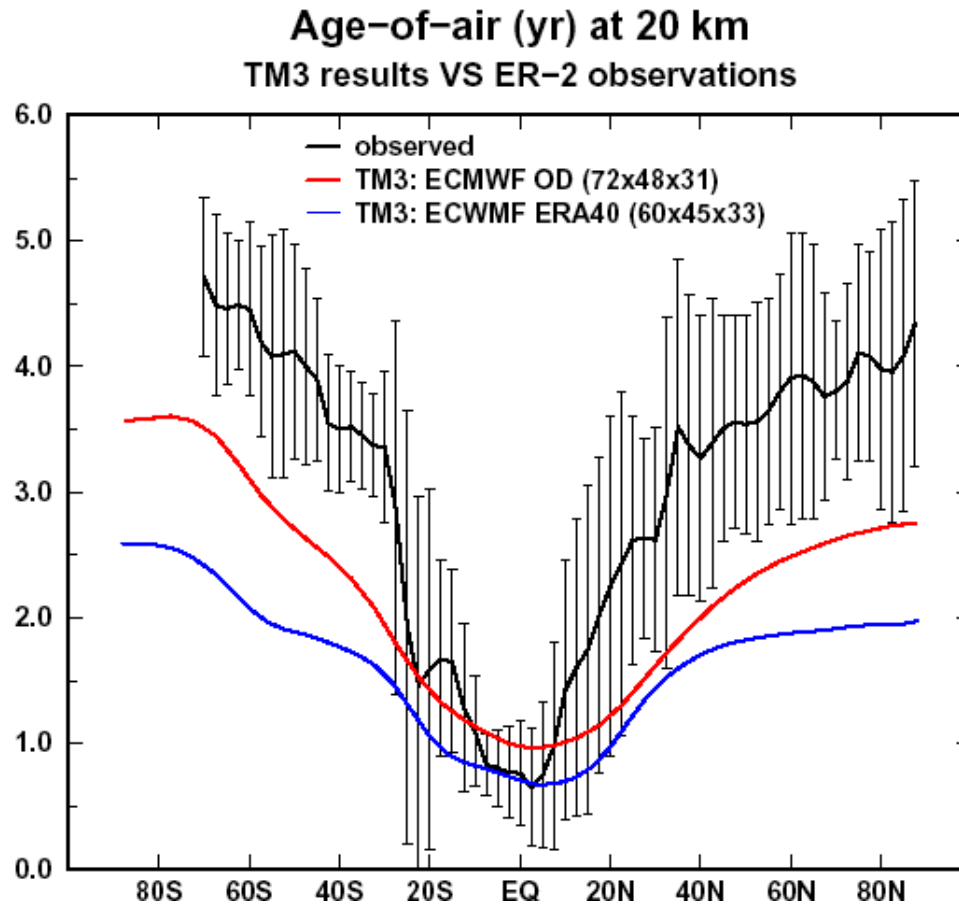


OmF vs latitude, GDP3, ECMWF ERA-40





Age of air



Bram Bregman, proc. ozone symp, Goteborg, 2002

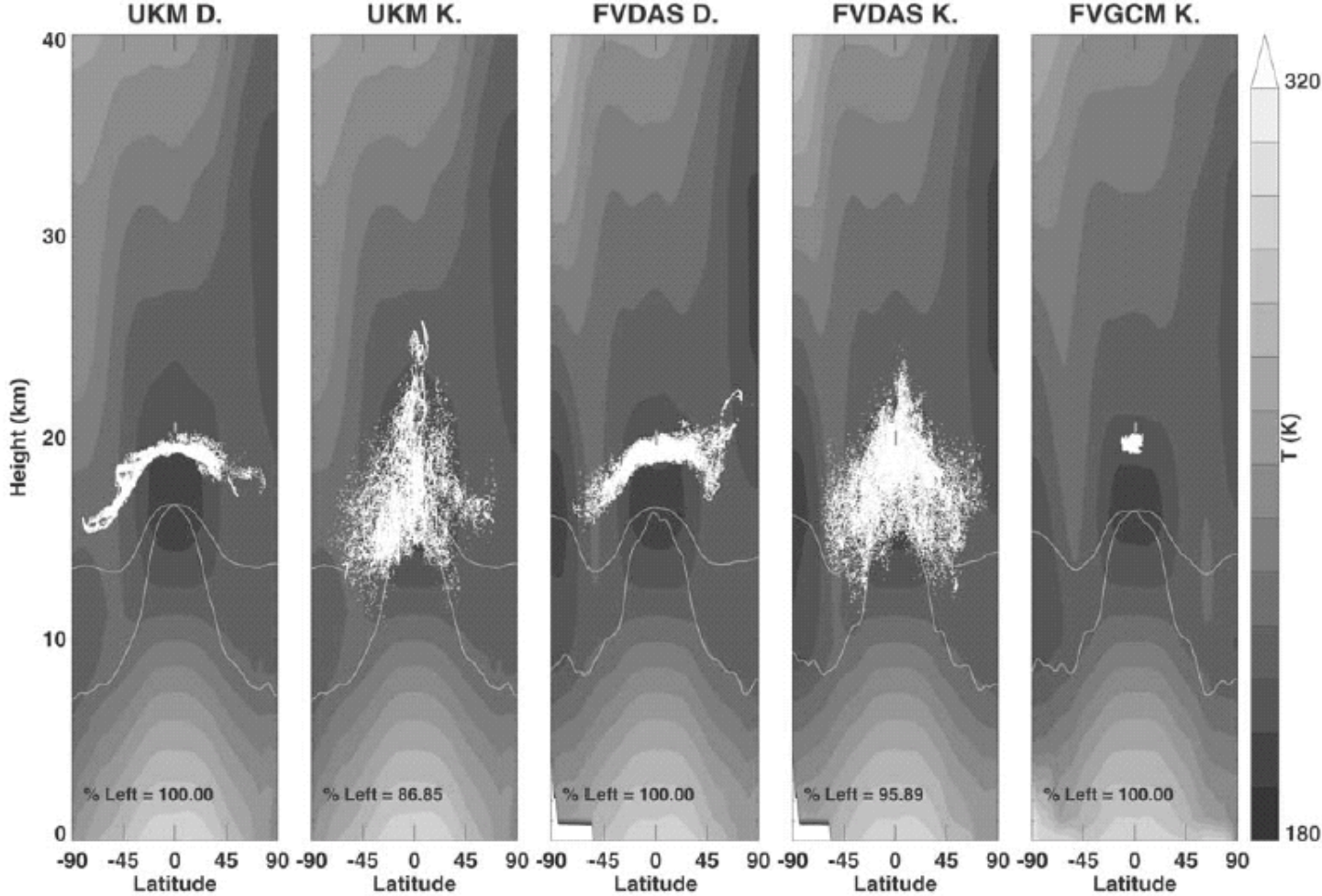


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Ozone flux from the stratosphere (TM3 CTM)

Simulation	Stratospheric influx (Tg/year)
OD 2001	568
OD 2000	611
OD 1996	575
ERA40 1996	1329
ERA40 1993	1155
ERA15 1993	530
ERA40 1991	1168
ERA40 1974	1055

Trajectory study: Schoeberl et al, jgr 108, 2003





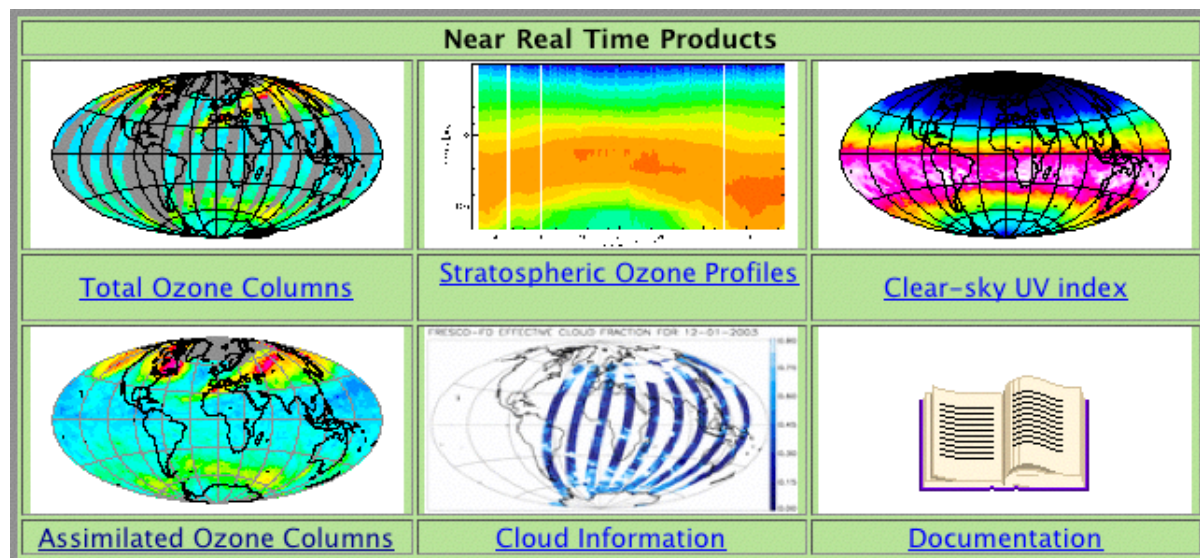
6) Ozone forecasts, based on GOME total ozone

http://www.knmi.nl/gome_fd





GOFAP project (ESA-DUP)



Products:

- ¥ NRT GOME level-2 ozone columns
- ¥ NRT ozone profiles
- ¥ Cloud properties (Fresco)
- ¥ Clear-sky UV index
- ¥ Assimilated ozone fields (level-4)
- ¥ Daily ozone and UV forecasts
- ¥ Data base of assimilated fields, 1999-2002
- ¥ Ozone hole statistics

http://www.knmi.nl/gome_fd
(service discontinued 22 June 2003)





KNMI Ozone analyses and forecasts

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

--> Daily ozone analyses and 5-day forecasts (9-day from 2002)





Anomaly correlation, RMS error

Anomaly correlation

$$C = \langle (f-c)(a-c) \rangle / \sqrt{\langle (f-c)^2 \rangle} \sqrt{\langle (a-c)^2 \rangle}$$

Root mean square error

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

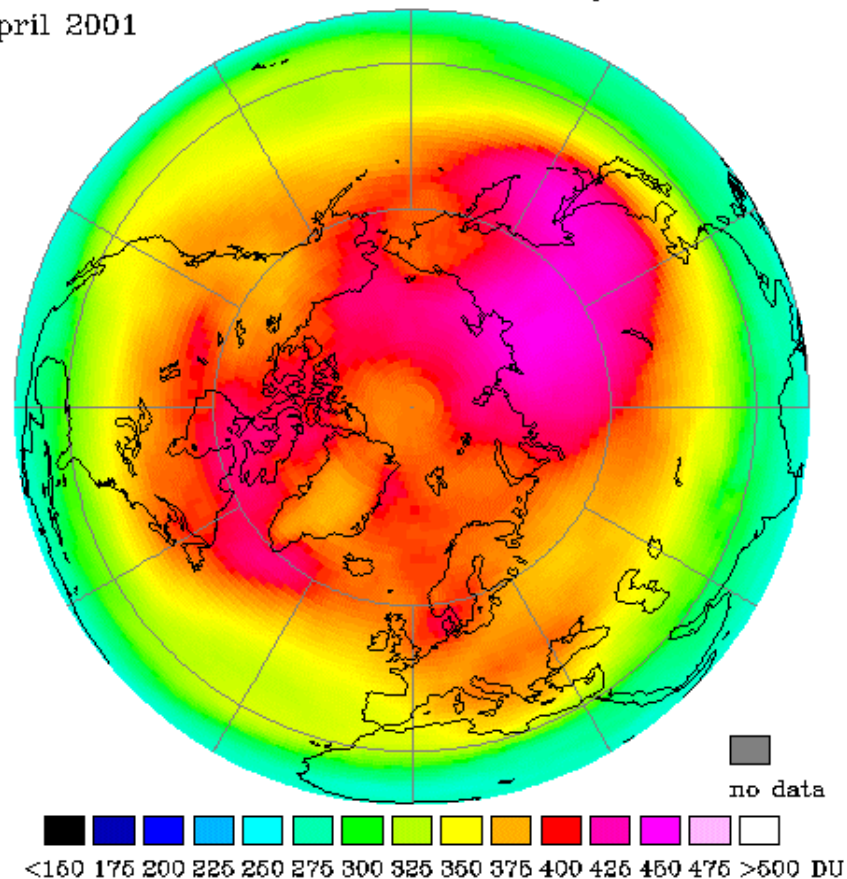
(f = forecast, a = analysis, c = climatology)

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



April 2001
Monthly mean

Assimilated GOME total ozone, monthly mean
April 2001

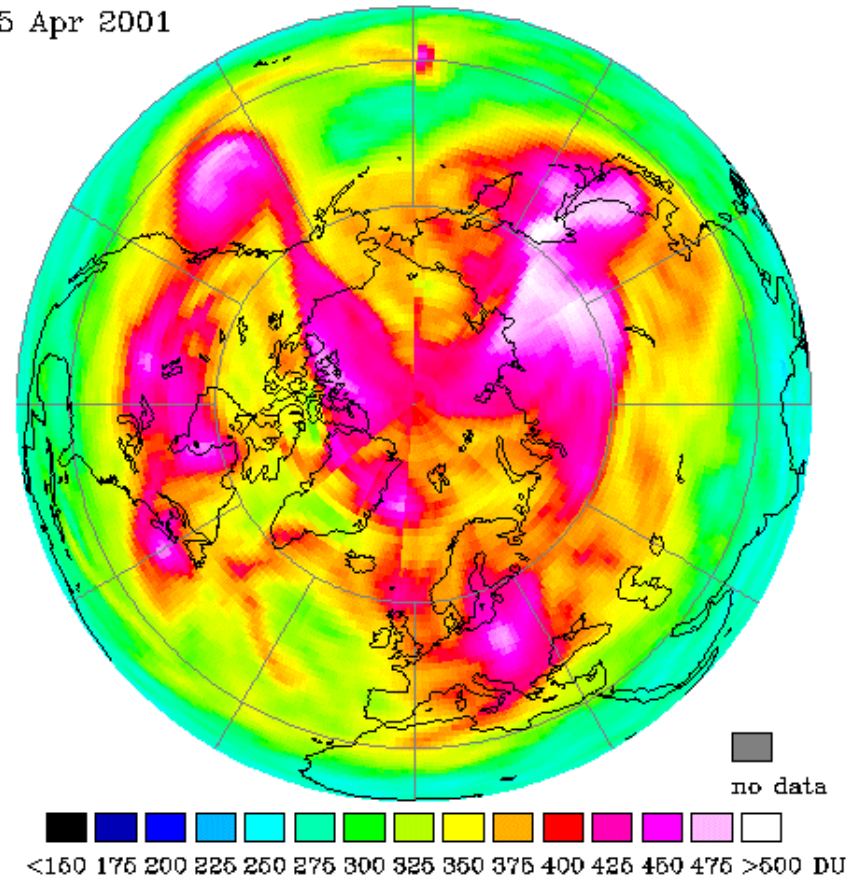


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Analysis

15 April 2001

Assimilated GOME total ozone, 12h local time
15 Apr 2001

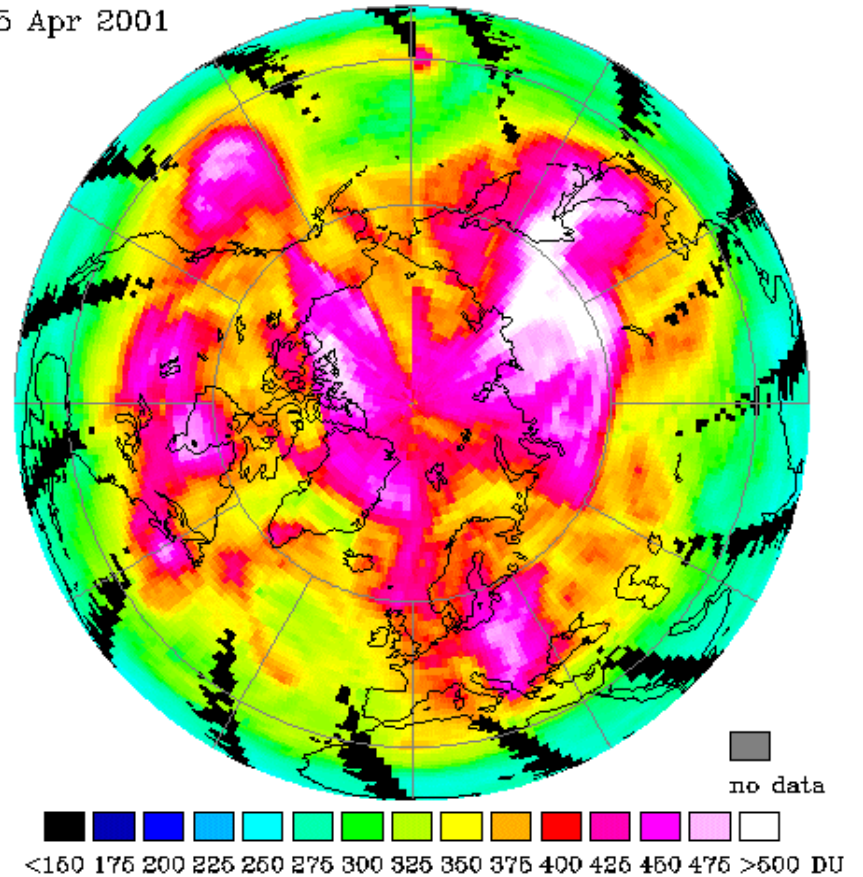




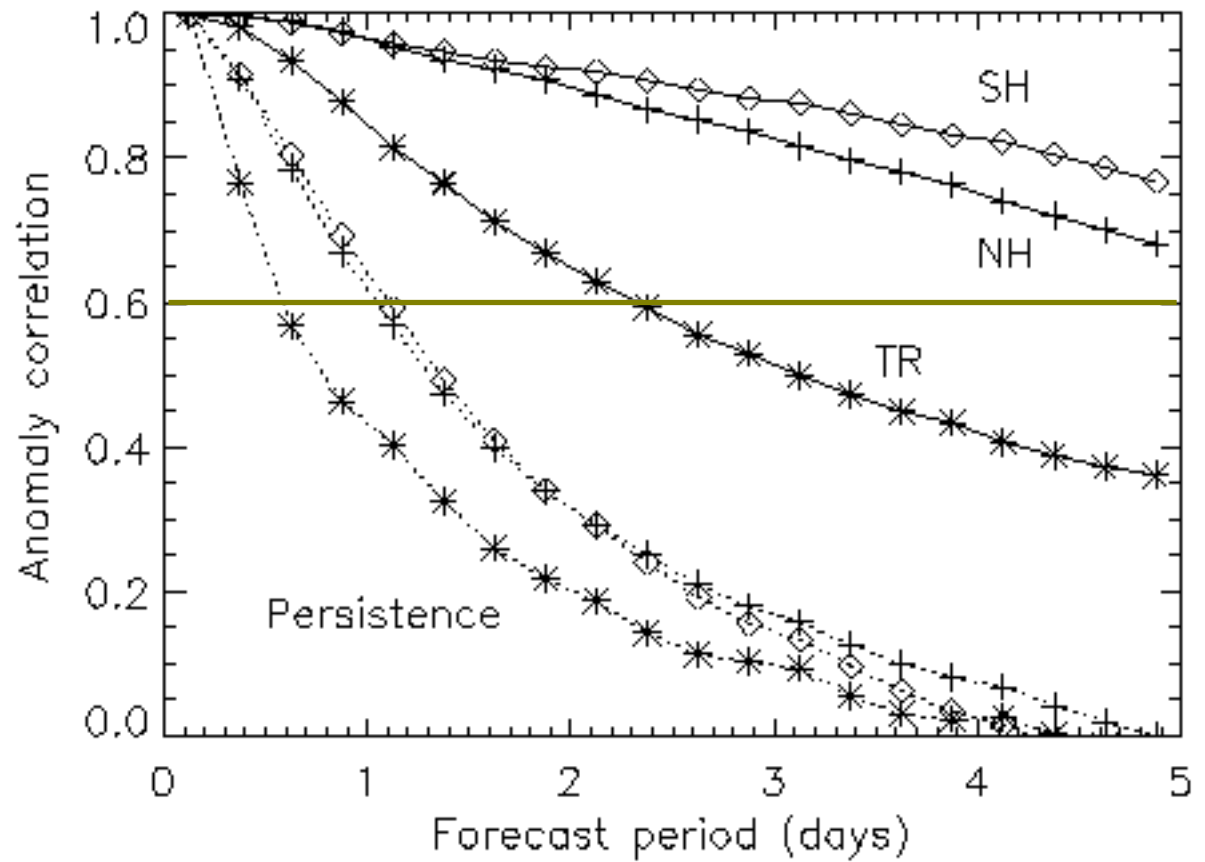
TOMS

15 April 2001

NASA Earth Probe TOMS
15 Apr 2001

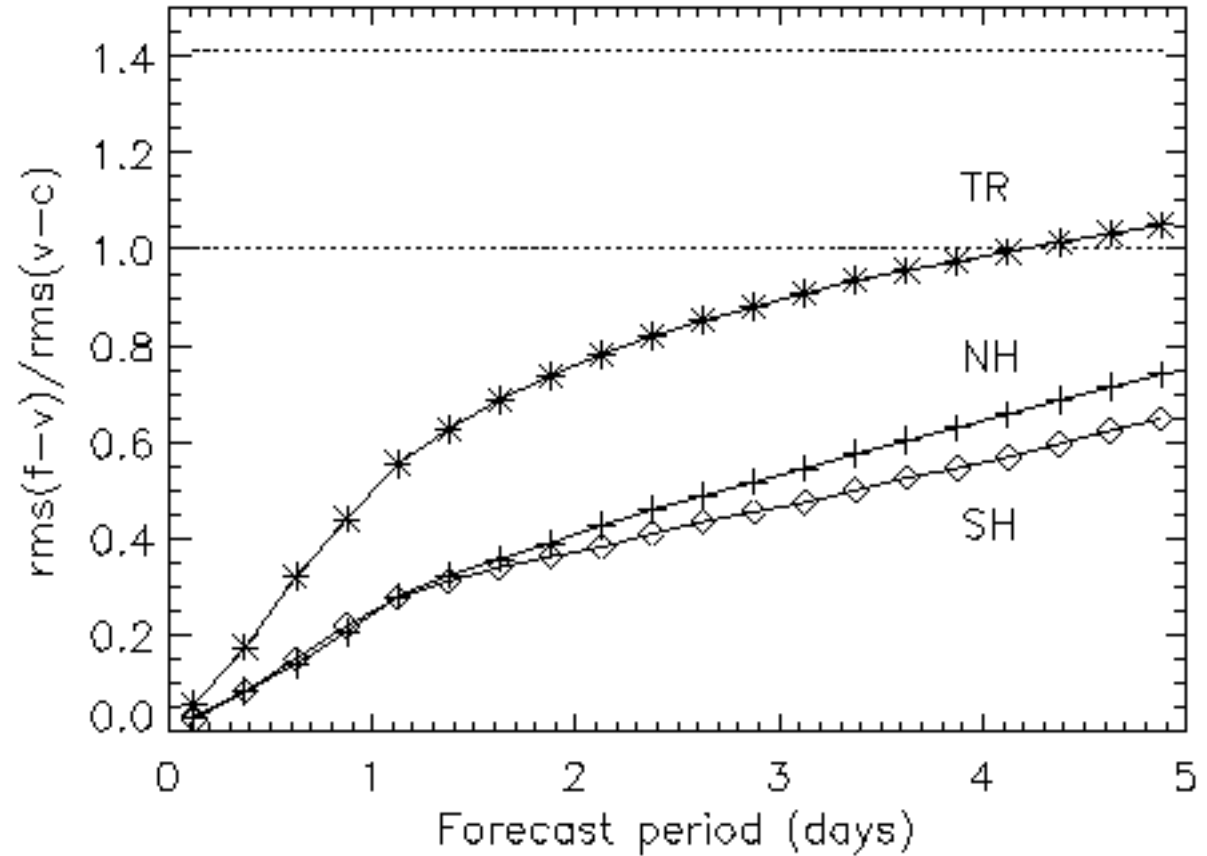


Anomaly correlation





RMS error



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Tropics

In tropics anomaly forecast score lower than in extratropics

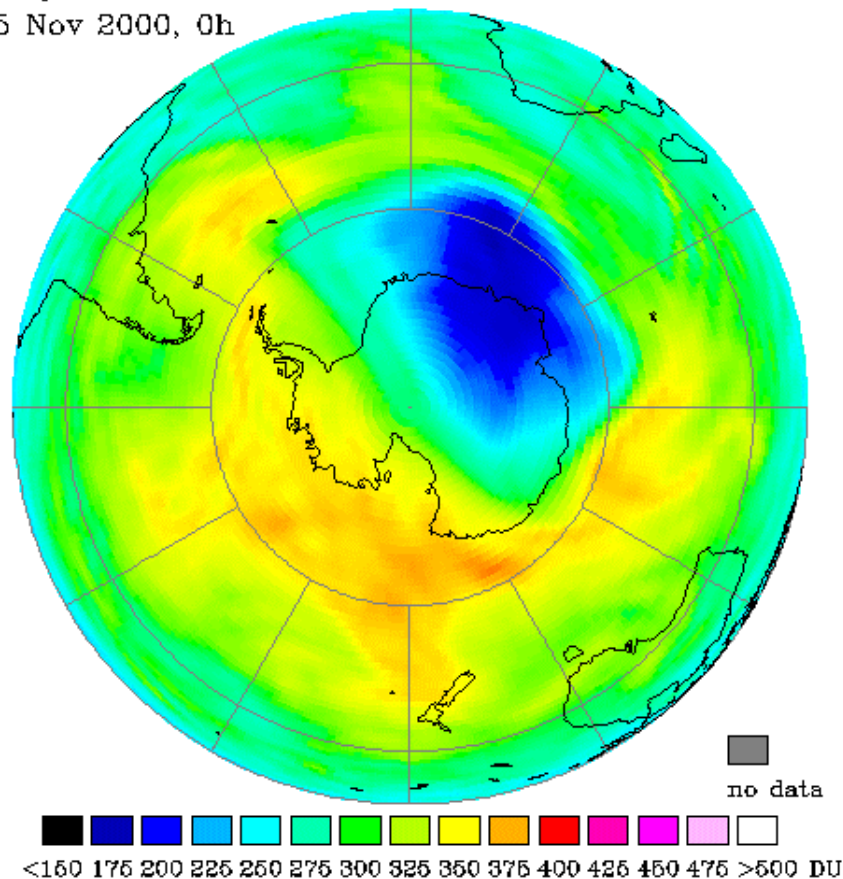
- > Anomaly small (2-3% compared to 5-10%)
 - > More sensitive to observation noise, retrieval errors
 - > Anomaly mainly tropospheric
- No tropospheric ozone chemistry in model



Breakup 2000 ozone hole

15 November 2000
analysis
based on GOME
ozone observations

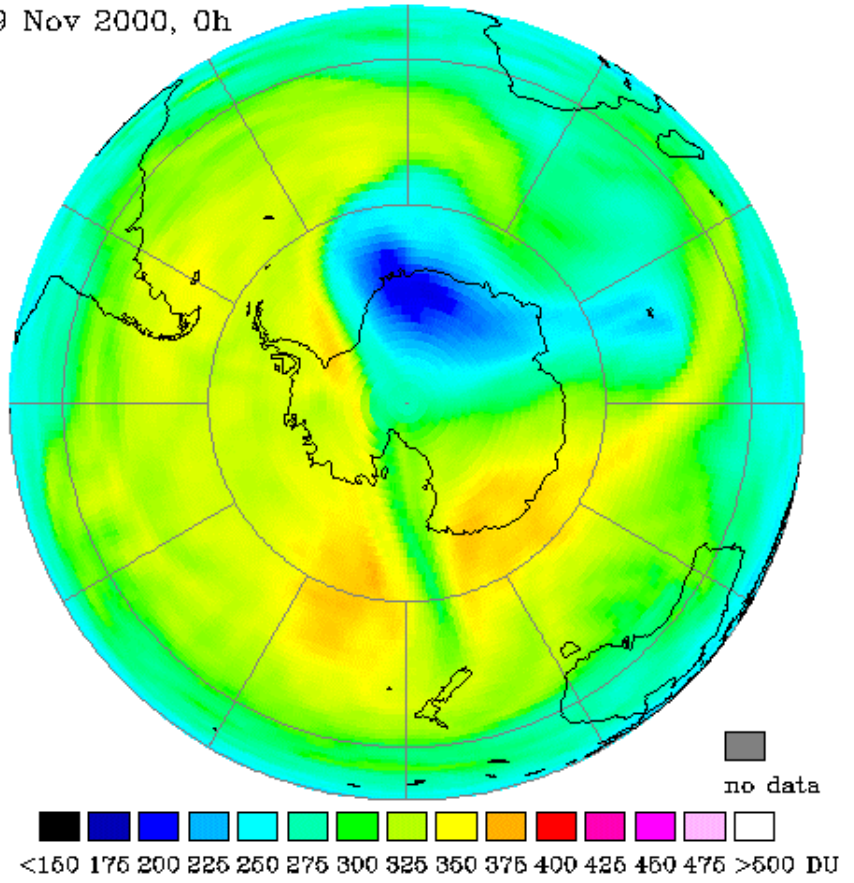
Analysis
15 Nov 2000, 0h



Breakup 2000
ozone hole

19 November 2000
4-day forecast

Forecast (15 Nov + 4)
19 Nov 2000, 0h

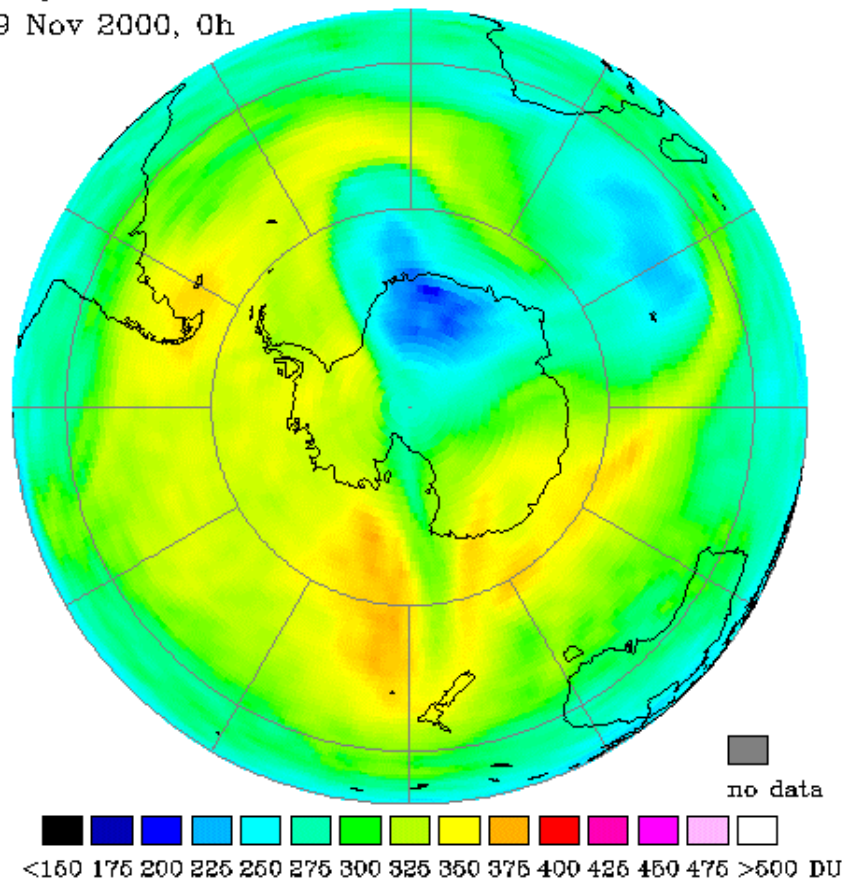




Breakup 2000 ozone hole

19 November 2000
analysis

Analysis
19 Nov 2000, 0h



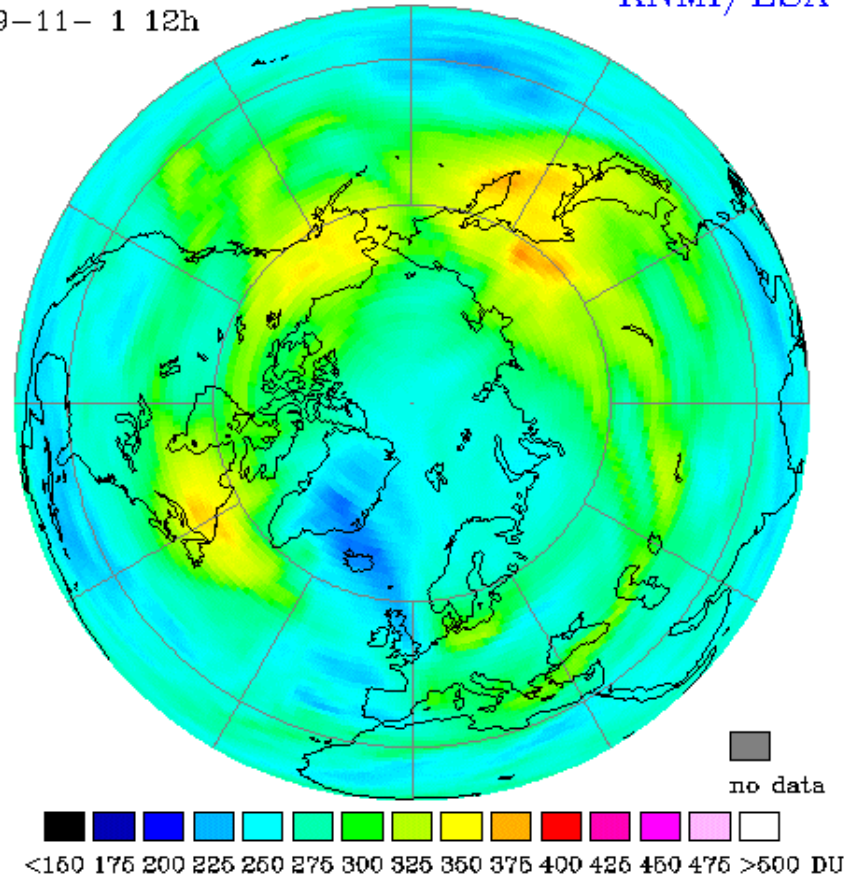
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Low ozone episode

5-day forecast
9 November 2001

Assimilated GOME total ozone
9-11- 1 12h

KNMI/ESA



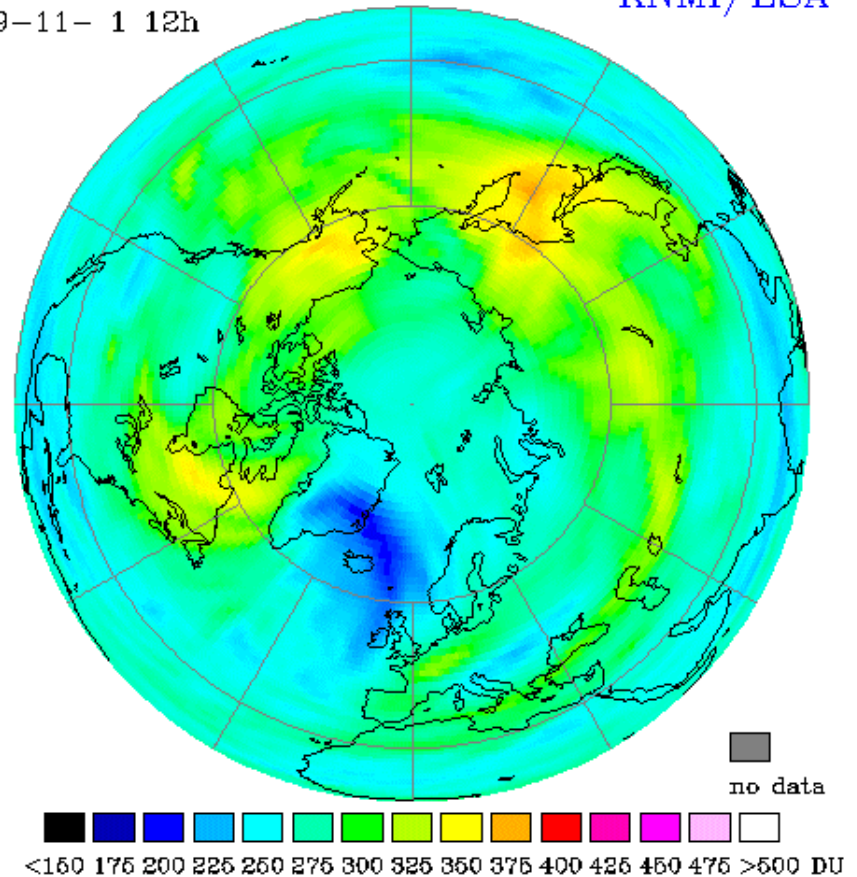
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Low ozone episode

3-day forecast
9 November 2001

Assimilated GOME total ozone
9-11- 1 12h

KNMI/ESA



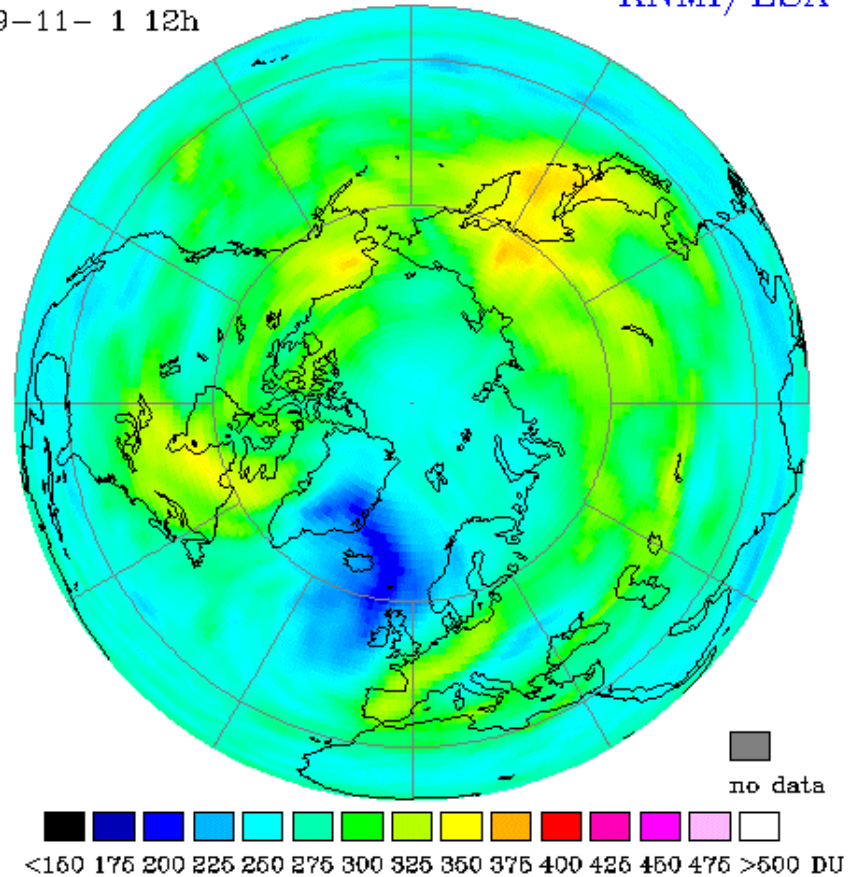


Low ozone episode

analysis
9 November 2001

Assimilated GOME total ozone
9-11- 1 12h

KNMI/ESA



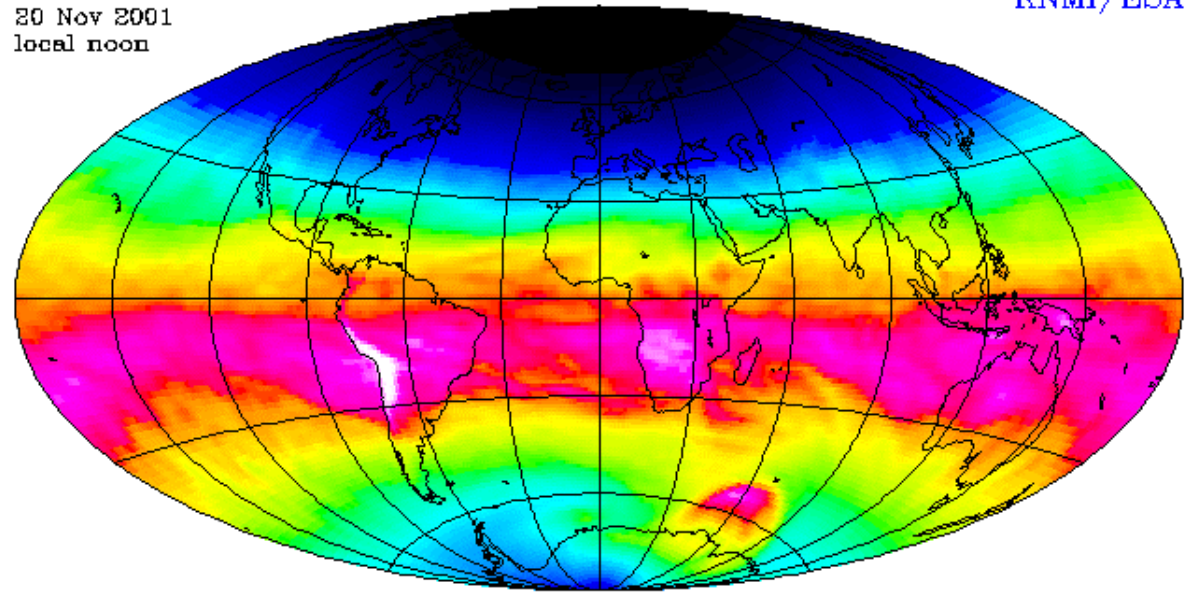


UV forecast

20 November 2001
(5-day forecast)

UV index based on GOME
20 Nov 2001
local noon

KNMI/ESA

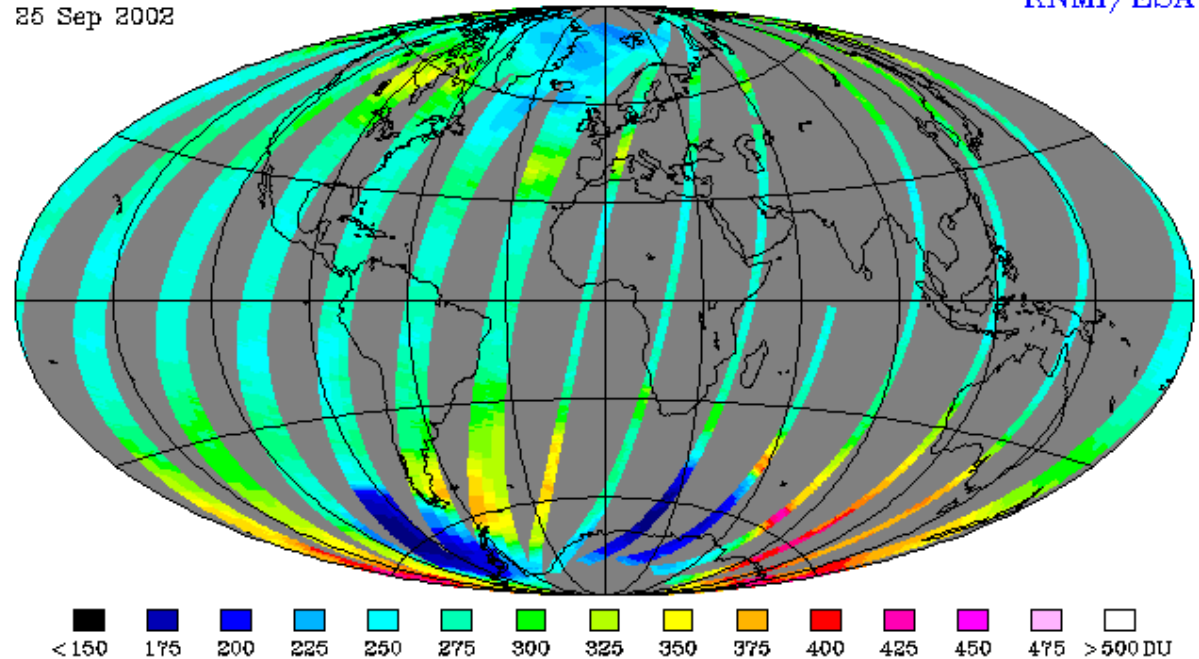




GOME measurements at 25 September 2002

FD TOTAL OZONE VALUES
25 Sep 2002

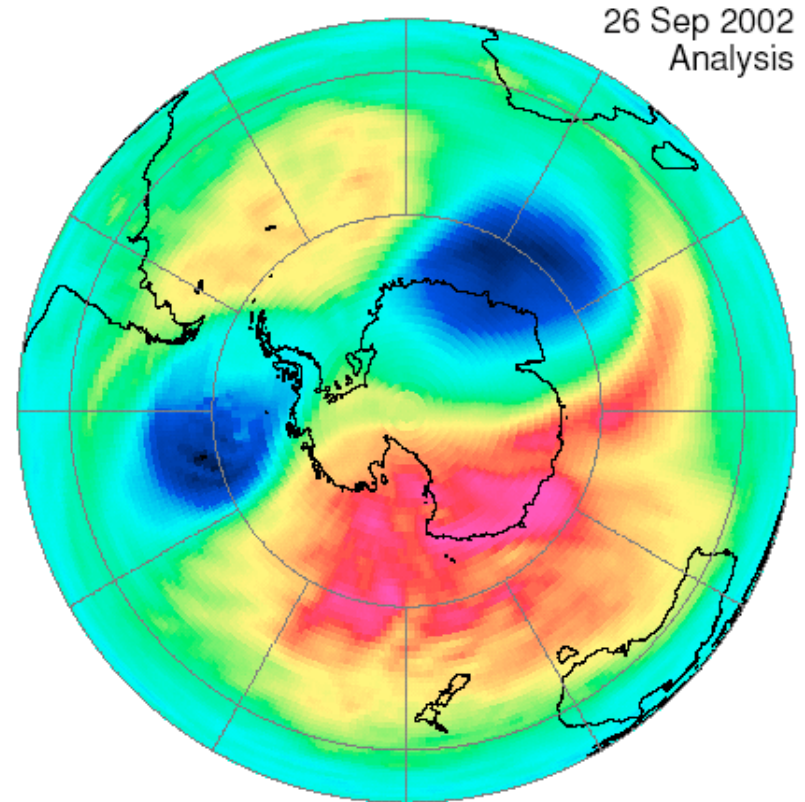
KNMI/ESA





Ozone hole breakup, 2002

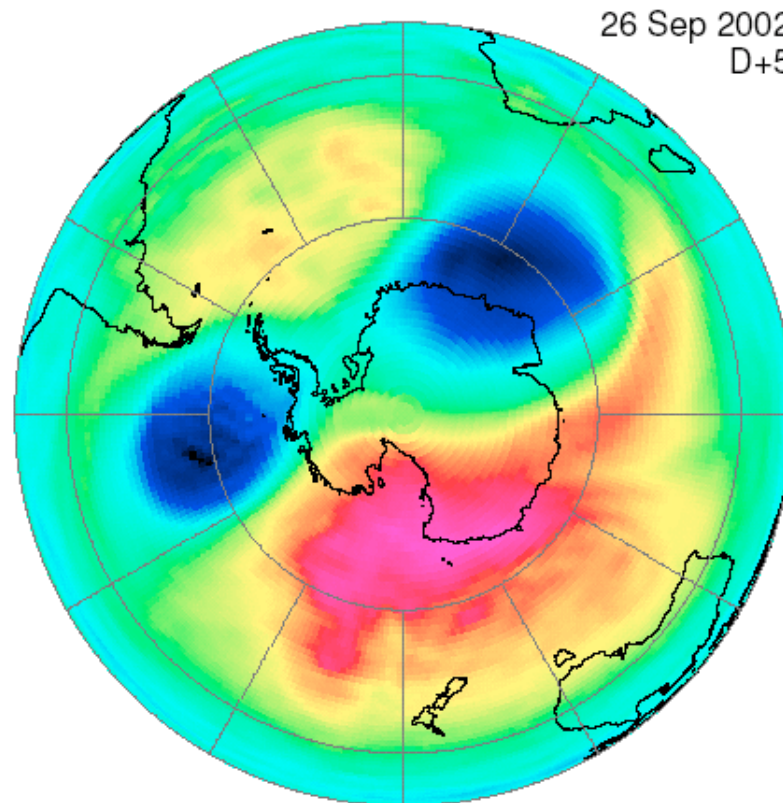
26 September 2002
Analysis based on GOME





Ozone hole breakup, 2002

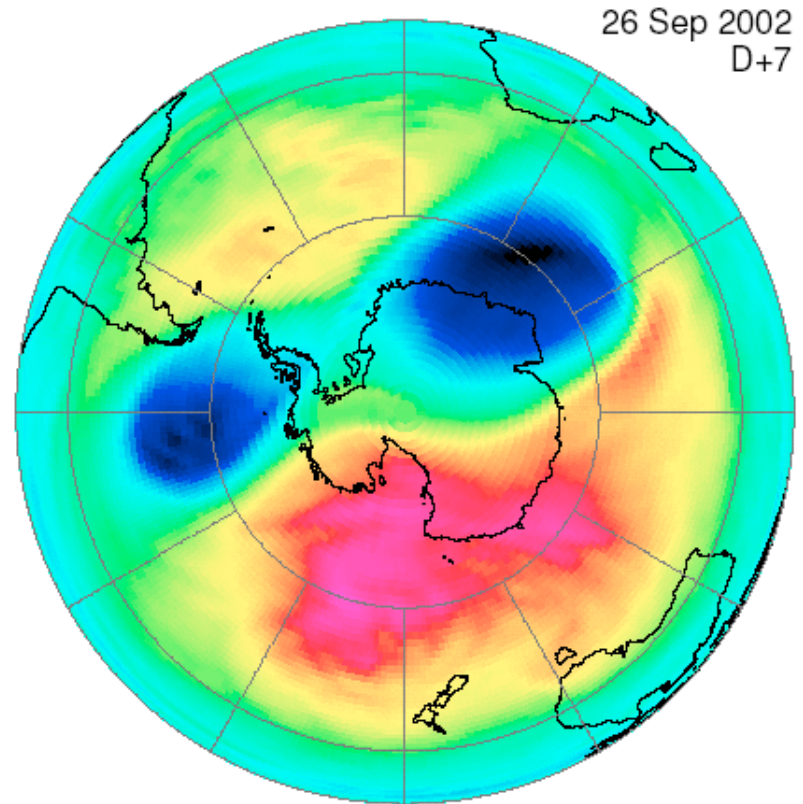
26 September 2002
5-day forecast





Ozone hole breakup, 2002

26 September 2002
7-day forecast

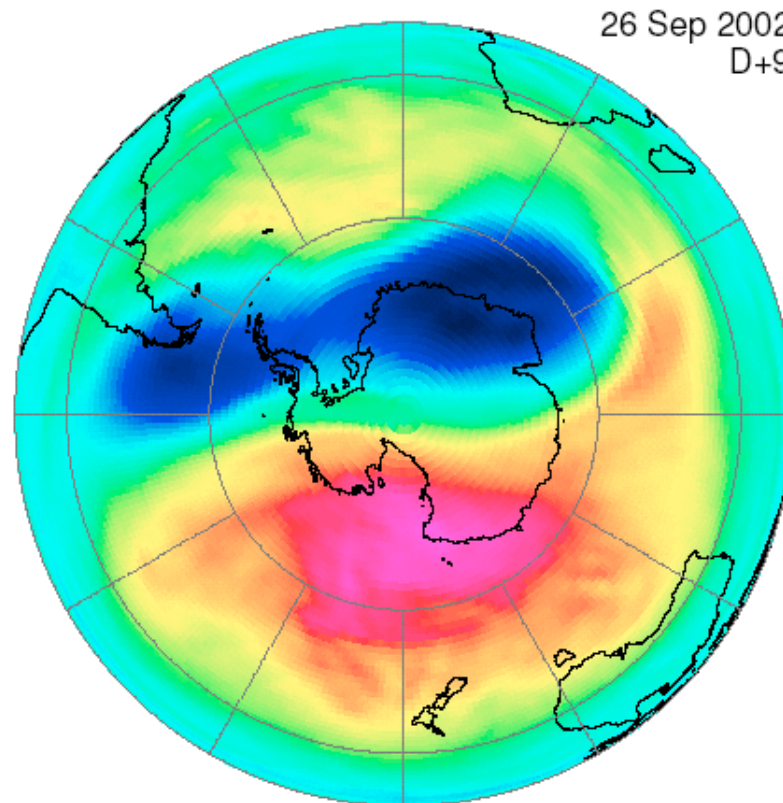




Ozone hole breakup, 2002

26 September 2002

9-day forecast



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Summary (1)

Satellite instruments measuring ozone

- GOME, Sciamachy, OMI, GOME-2 will play important role to continue the TOMS ozone record

Total ozone retrieval

- Total ozone products of GOME can be improved
- New KNMI total ozone algorithm:
applied to GOME, Sciamachy, OMI

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Summary (2)

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 %

Age of air, strat-trop exchange

- Assimilation models: too strong mixing tropics-extratropics (M. Schoeberl)
- ERA-40 compared to OD:
small age of air, large STE

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Summary (3)

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