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)
- 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

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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

A. Peuch et al, QJRMS 126, 1641, 2000
With TOMS data

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

Nimbus TOMS, 78 - 93
Meteor TOMS, 91 - 94
Adeos TOMS, 96 - 97
EP TOMS, 96-present

GOME, 95 - present
SCIAMACHY, 2002 -
OMI, 2004 -
GOME-2, 2005 -
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

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Validation:
Dimitris Balis, LAP
DLR GDP v2.7
Ozone retrieval: TOMS retrieval vs. DOAS
Ozone retrieval: DOAS

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

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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
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

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

\(\chi\)  
ozone concentration

\(S\)  
 sources - sinks

\(\Phi\)  
ozone column above point
Stratospheric chemistry parametrization

Heterogeneous chemistry
(Peter Braesicke, CAS, Cambridge Univ.)

\[
\frac{d\chi}{dt} = -\frac{1}{\tau} A \chi
\]
\[
\frac{dA}{dt} = \frac{1}{\tau_p} (1 - A) - \frac{1}{\tau_l} A
\]

\[\chi\] ozone concentration
\[A\] activation tracer field (cold tracer)
\[\tau\] ozone depletion time scale
\[\tau_p\] activation time scale
\[\tau_l\] cold tracer life time
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

\[
\frac{\partial \chi}{\partial t} = P - \frac{1}{\tau_{\text{loss}}} \chi
\]
Observation minus forecast statistics

![Graph showing the comparison of observation and forecast statistics with latitude. The graph displays the root mean square (rms) and bias for different latitudes. The x-axis represents latitude, ranging from -50 to 50 degrees, and the y-axis shows the difference between GOME and forecast (DU). The graph indicates a trend of increasing rms values and fluctuating bias with latitude.]

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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

- OD (1999-2002)
Observation minus forecast statistics: ECMWF OD

Apr 2001, GDP v3, TM3DAM v3.30, ECMWF OD

observation - forecast (DU)

observation

-50 0 50

latitude

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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)

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Stratospheric influx (Tg/year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OD 2001</td>
<td>568</td>
</tr>
<tr>
<td>OD 2000</td>
<td>611</td>
</tr>
<tr>
<td>OD 1996</td>
<td>575</td>
</tr>
<tr>
<td>ERA40 1996</td>
<td>1329</td>
</tr>
<tr>
<td>ERA40 1993</td>
<td>1155</td>
</tr>
<tr>
<td>ERA15 1993</td>
<td>530</td>
</tr>
<tr>
<td>ERA40 1991</td>
<td>1168</td>
</tr>
<tr>
<td>ERA40 1974</td>
<td>1055</td>
</tr>
</tbody>
</table>
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)

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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
\[ C = \frac{\langle (f-c)(a-c) \rangle}{\sqrt{\langle (f-c)^2 \rangle} \sqrt{\langle (a-c)^2 \rangle}} \]

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

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TOMS
15 April 2001
Anomaly correlation
RMS error
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

Forecast (15 Nov + 4)
19 Nov 2000, Oh
Breakup 2000 ozone hole

19 November 2000 analysis
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 (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
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
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