Part I

Weighting Function DOAS (WF-DOAS)

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GOME Total Ozone Column Retrieval Development,
Final Presentation, 3 Dec 2003, Frascati

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Topics

Part 1: Weighting Function DOAS

- Intoduction/Motivation
- Foreword: John Burrows
- **WF-DOAS Algorithm**
- Auxilliary Retrieval
  - → Effective albedo
  - → Clouds
  - → Effective scene height
- Ring effect (ozone filling-in)
- Sensitivity study
  - → A-priori ozone climatology
  - → Tropical clouds
  - → Mountains
  - → Aerosol
- Error Budget
- Performance

Weighting-Function-DOAS Equation

$$\ln I_i^{mea}\left(V^t, \vec{b}^t\right) \approx \ln I_i^{mod}\left(V_0, \vec{b}_0\right) + \frac{\partial \ln I_i^{mod}}{\partial V}\Big|_{V_0} \times (\hat{V} - V_0) + \sum_{j=1}^{F} \frac{\partial \ln I_i^{mod}}{\partial b_j}\Big|_{b_{0,j}} \times (\hat{b}_j - b_{0,j}) + SCD_{Ring} \cdot \sigma_{i,Ring} + SCD_{usamp} \cdot \sigma_{i,usamp} + P_i$$

I_i	Sun-normalized spectral radiance
P_i	Low-order polynomial
V^t	True vertical column
$\vec{b}^t$	True atmosphere (pressure,temperature,...)
V_0	Assumed model vertical column
$\vec{b}_0$	Assumed model atmosphere
$\hat{V}$	Vertical column fit parameter
$\hat{\vec{b}}$	Atmospherical fit parameters
σ_{Ring}	Ring-Spectrum
σ_{usamp}	Undersampling-Spectrum
i	Wavelength index

$\ln I_i^{mod}$ reference intensity

$\frac{\partial \ln I_i^{mod}}{\partial V}, \frac{\partial \ln I_i^{mod}}{\partial b_j}$ weighting functions

Parameter	Input
Total Ozone	WF
NO_2	~~WF or~~ cross-section / SC Fit
BrO	~~WF or~~ cross-section / SC Fit
Temperature	WF
~~Pressure~~	~~WF (?)~~
~~Albedo~~	~~WF (?)~~
Ring-Effect	SC Fit
Undersampling	SC Fit

Look-Up Table

- Pre-calculated reference intensities (SCIATRAN 1.2, multilple scattering RTM)
  - ➔O3 and temperature weighting function *(Rozanov et al. 1998)*
  - ➔Ring-spectrum (nadir only, *Vountas et al. 1998*)
    - Includes molecular (ozone) filling-in
    - Off-nadir approximated by fitting scale factor to nadir Ring

Atmospheric Parameter	Min	Max	Δ	N
Total Ozone (high latitudes)	125 DU	575 DU	50 DU	10
Total Ozone (mid latitudes)	125 DU	575 DU	50 DU	10
Total Ozone (low latitudes)	225 DU	475 DU	50 DU	6
Solar Zenith Angle	15°	92°	5° if SZA $\leq$ 70° 1° if SZA > 70°	34
Line-Of-Sight	-34.5°	34.5°	11.5°	7
Relative Azimuth Angle	(*)	(*)		3
Surface Albedo	0.02	0.98	~0.2	6
Ground Altitude	0 km	12 km	2 km	7

(*) Min/Max depend on SZA and LOS.

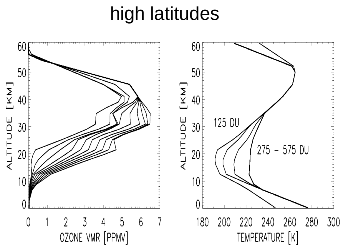
779,688 scenarios

A priori ozone and temperature climatology

Total Ozone and Profile Shape

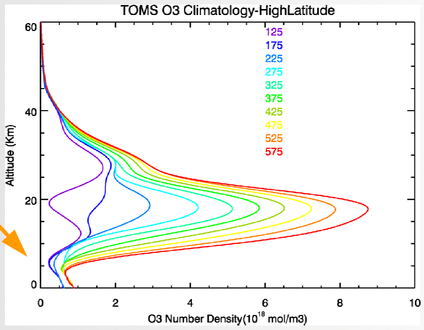
▷ TOMS V7 climatology

	Zone	Min - Max	N
High latitudes	60° - 90°	125 - 575 DU	10
Mid latitudes	30° - 60°	125 - 575 DU	10
Low latitudes	0° - 30°	225 - 475 DU	6



Wellemeyer et al. 1997

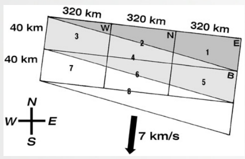
TOMS V7 profiles converted into 60 one wide km layers and number density



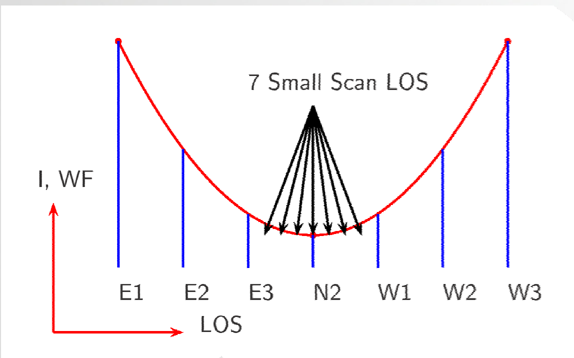
Line-of-sight (scan) simulation

▶3 LOS reference spectra averaged (weights: 1/6, 4/6, 1/6) for each ground pixel

- •E1, E2, E3 → East
- •E3, N1, W1 → Nadir
- •W1, W2, W3 → West

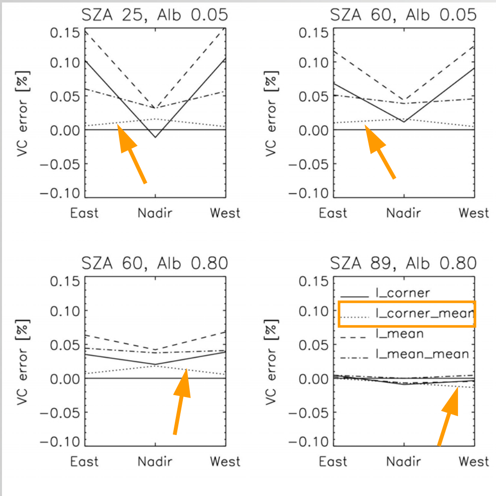


E1 : -34.5°
E2 : -23.0°
E3 : -11.5°
N2 : 0.0°
W1: 11.5°
W2: 23.0°
W3: 34.5°



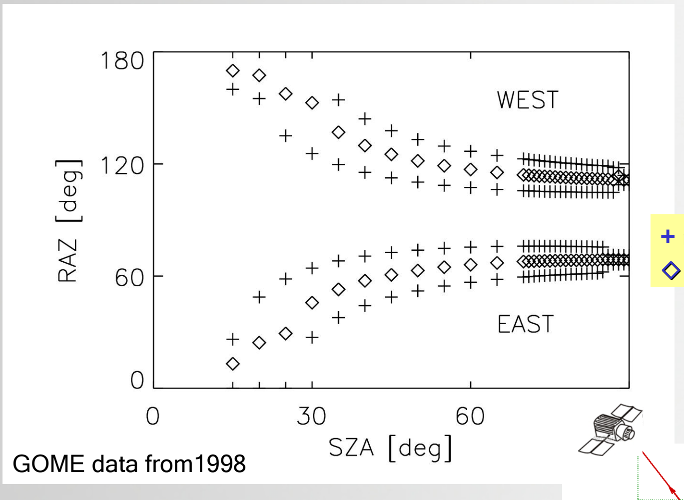
960 km

Line-of-sight (scan) simulation (2)

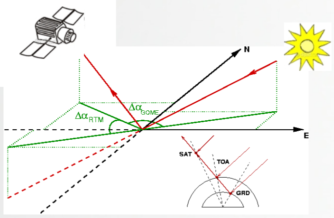


- ▶Averaging after fitting 3 LOS‘
  - ➔ I_corner (11.5°,23.0°,34.5° LOS)
  - ➔ I_mean (15.3°,23.0°,30.6° LOS)
- ▶Averaging 3 LOS‘ before fitting
  - ➔I_corner_mean (11.5°,23.0°,34.5°)
  - ➔I_mean_mean (15.3°,23.0,30.6°)

Relative azimuth (RAZ) as a function of SZA and LOS



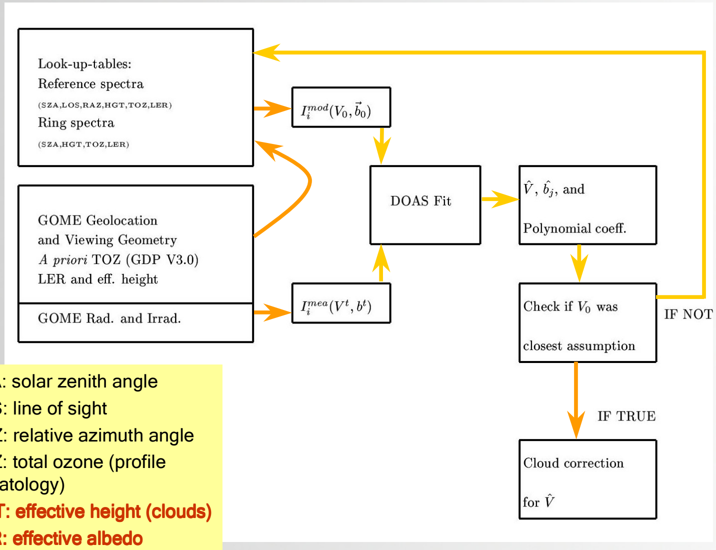
+ min / max RAZ
◇ mean RAZ



- ➩ three RAZ for a given SZA, LOS combination
- ➩ SZA dependence expressed as Chebyshev polynomial

779,688 scenarios ➞ 9828 reference files

WF DOAS Iterative Scheme



SZA: solar zenith angle
LOS: line of sight
RAZ: relative azimuth angle
TOZ: total ozone (profile climatology)
HGT: effective height (clouds)
LER: effective albedo
retrieved from GOME

Additional Settings and Fit Parameters

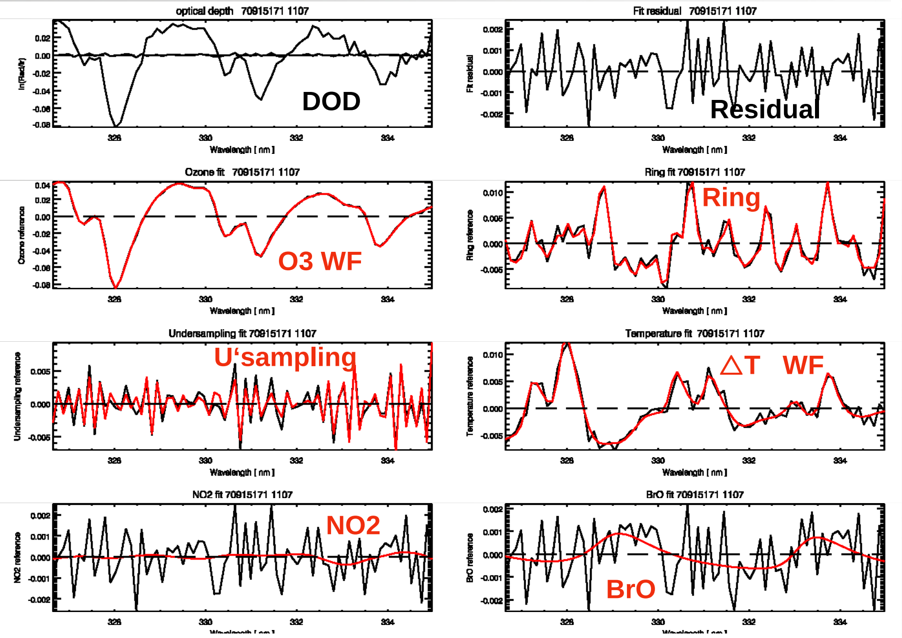
Settings

- Spectral window: **326.6-335 nm**
- **Fraunhofer fit** of solar spectrum (Kurucz' solar FTS data)
  ⇨ *Improved wavelength calibhration/ Doppler shift correction*
- **+0.017nm** shift of O3 cross-section (Burrows et al. 1999) in all reference spectra (van Roozendael, priv.comm.)
  ⇨ *No shift & squeeze except for earthshine (nadir) spectra*
- **Surface viewing geometry** (SZA, LOS) rather than TOA
  ⇨ *~1% effect at 90° SZA and 32° LOS*

WF DOAS Fit Parameter

- ozone (WF)
- temperature (WF)
- Ring (SCD)
- undersampling (SCD)
- NO2 (SCD)
- BrO (SCD)
- I_0 (SCD)
- Polynomial Coefficients

Spectral fitting: GOME 70915171 Pixel 1107 (tropics)



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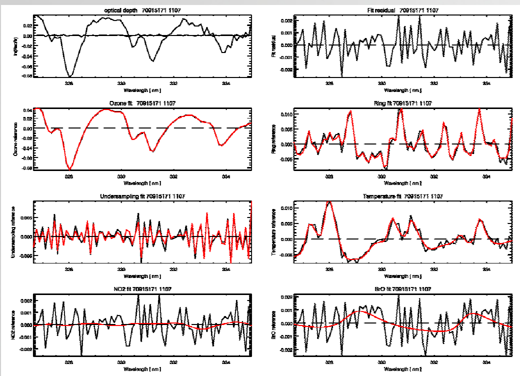

▶ Spectral fitting
- ➔ Fit residual about 0.001 (factor 2 improved over GDP V3)
- ➔ Fit residual remains unchanged when pure SC fit (two temperature x-section fits)
- ➔ Fit residuals cannot be used to test preferences for a-priori settings (climatology in O3 and Ring)

Summary: WF-DOAS algorithm

- Successful imlementation of look-up tables (LUT) for WF-DOAS algorithm using SCIATRAN V1.2 and TOMS V7 ozone profile climatology
  - ➔ Weighting functions of ozone and temperature
  - ➔ Reference intensity
  - ➔ New Ring data base
- Adaptation of LUT into DOAS algorithm (Fortran 90 code)
- Limiting shift & squeeze procedures to sun-normalized radiance
  - ➔ Fraunhofer fitting
  - ➔ Cross-section wavelength shift for O3
- Basic settings (fit paramaters) selected
- Very low fit residuals, reduced to 0.001 (factor two lower than GDP V3)

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  - ➔ **Clouds**
  - ➔ **Effective scene height**
- Ring effect (ozone filling-in)
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effective albedo retrieval

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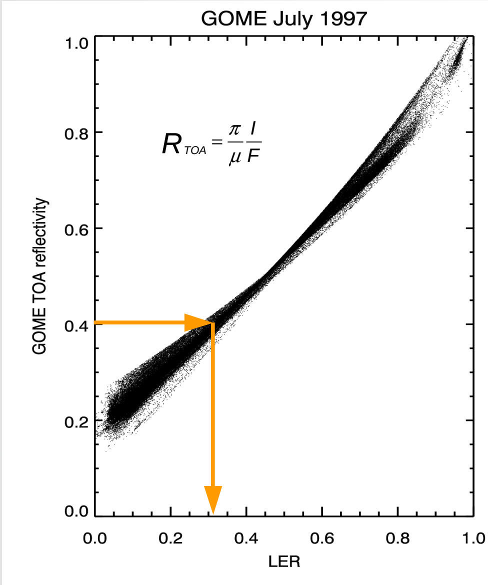
Look-up-table (SCIATRAN 1.2):

TOA reflectivity in aerosol free atmosphere @ 377.6 nm (Celarier & Herman 1997)
SZA,LOS,RAZ,GRD,ALB

GOME rad./irrad. SZA, LOS and RAZ

FRESCO : effective altitude

Lambertian Equivalent Reflectivity (LER)
= effective scene albedo



Cloud retrieval, effective height, and ghost vertical column

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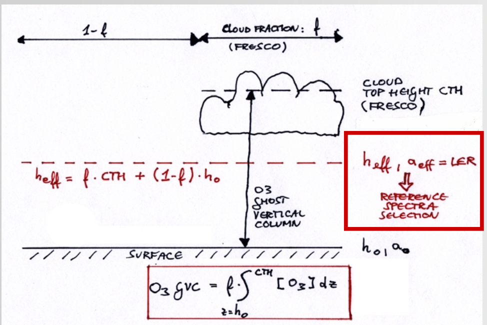
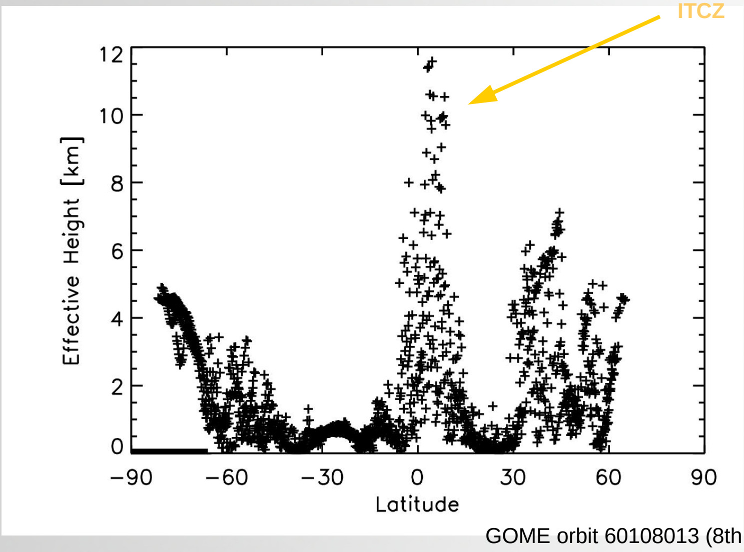


- ▶Ghost vertical column (hidden below clouds) derived from TOMS V8 climatology (zonal & monthly mean)
  - ➔ monthly zonal means better represents tropospheric ozone

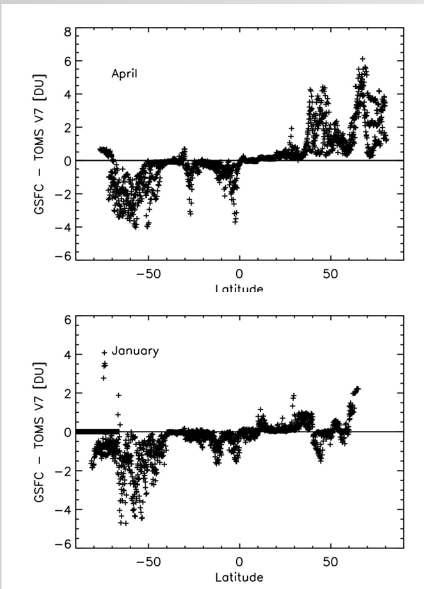
- ▶FRESCO (Koelemeijer & al 2001)
  - ➔cloud retrieval in O2 A-band
  - ➔Surface albedo a_o from GOME minimum LER database (Koelemeijer et al. 2003)
  - ➔Cloud reflectivity at 0.8
  - ➔Output
    - ❍ Cloud-top-height *cth*
    - ❍ Cloud fraction *f*
  - ➔Snow mode: only *cth* used

Effective Altitude vs. Latitude



GOME orbit 60108013 (8th Jan 1996)

GVC with TOMS V7 and TOMS V8



- Ghost vertical column differences between GDP V3 (TOMS V7 climatology) and WF-DOAS (TOMS V8 zonal monthly mean)
- More tropospheric ozone in NH (V8)
- Less tropospheric ozone in SH (V8)

Summary: Auxiliary Retrieval

- First time usage of combined cloud and albedo information directly retrieved from GOME
  - ➔ effective scene albedo from 377.6 nm (negligible molecular absorption and Ring contribution)
  - ➔ Cloud retrieval in oxygen A band (FRESCO)
  - ➔ Effective scene height derived from cloud-top-height and cloud fraction
- Use of zonal and monthly mean TOMS V8 climatology leads to different tropospheric ghost vertical columns in SH and NH

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  - ➔ Effective scene height
- **Ring effect (ozone filling-in)**
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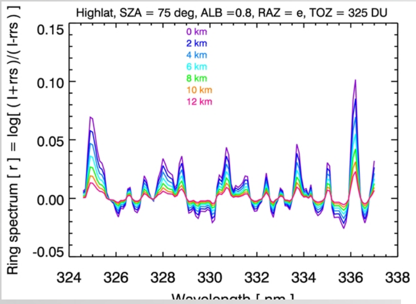
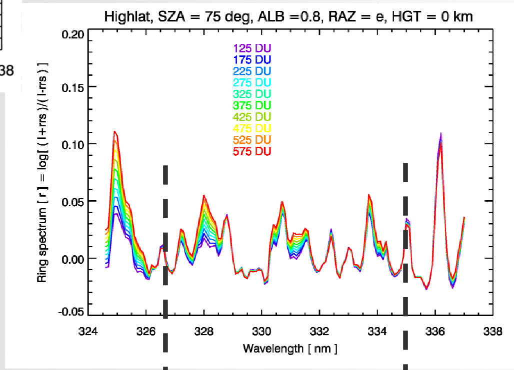
Ring spectra as a function of O3 VCD and altitude



effective height dependence

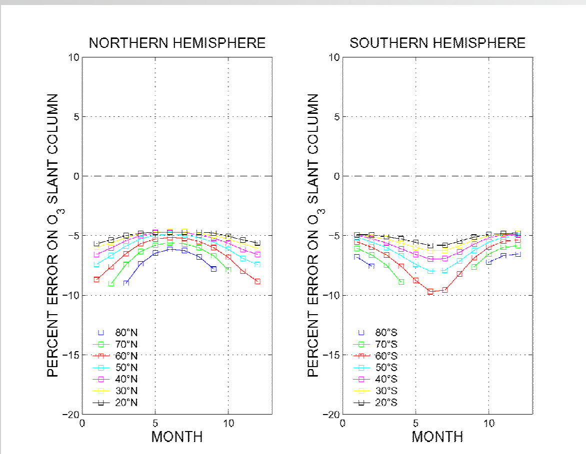
- Ring spectra: $\ln\left(\frac{I^{+Ring}}{I^{-Ring}}\right)$
- SCIATRAN V1.2 (Vountas et al. 1998)
  → full MS radiative transfer



total ozone dependence

Fitting window

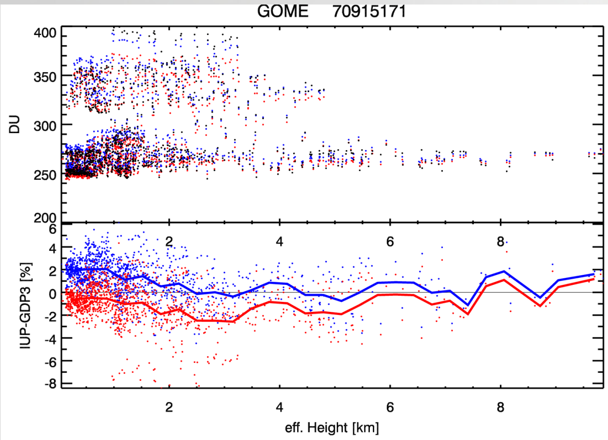
Error if molecular (ozone) filling-in is neglected



Roozendael et al. 2003

- Total column difference due to ozone filling-in (SCIATRAN V1.2) and Chance & Spurr Ring as in GDP V3
  → Fortuin & Kelder ozone profile climatology
    - monthly mean
    - 10° latitude band
- Bias on the order of -5 to -10%
- SZA dependence of error

Sensitivity to Raman-filling (1)



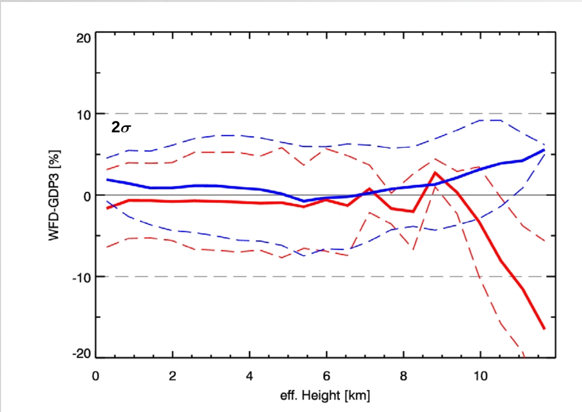
HIGH-LAT climatology

- Standard Ring scenario
  - ➔ Fixed atmospheric scenario
  - ➔ variation in SZA
- New Ring database parametrized by e.g.
  - ➔ Ozone VCD
  - ➔ Effective albedo
  - ➔ Effective height

⇨ differences on the order of +0 to 2% (V3) and +0 to+3% (standard Ring)

⇨ reduced molecular filling-in at high effective altitudes

Sensitivity to Raman-filling in (2)



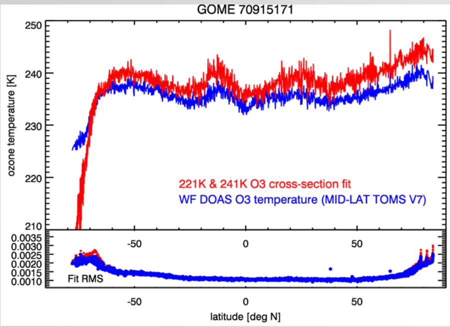
- Standard Ring scenario
- New Ring database parametrized

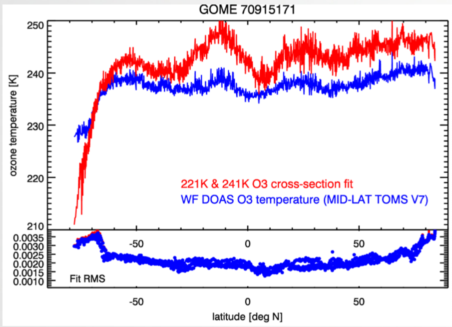
- MID-LAT climatology,
- 111 orbits
- Eight days from March, June, September, and December 1997

⇨ differences on the order of +0 to 2% (V3) and +0 to+3% (standard Ring)

⇨ reduced molecular filling-in at high effective altitudes

Retrieved ozone temperature and Ring





Standard Ring

Ring database

- ⇨ ozone temperature depends on Ring implementation (two x-section fits)
- ⇨ small temperature sensitivity with Ring in WF DOAS
- ⇨ fit residuals are identical for O3 SCD and WF DOAS fits
- ⇨ lower fit rms achieved when Ring calculated at GOME wavelength grid (left)

Summary: Ring effect and ozone filling-in

- ▶ Ozone filling-in has to be accounted for (up to 5% error if neglected)
- ▶ Combination of effective scene height (clouds) and ozone filling-in is important (see also de Beek et al. 2001, Joiner and Barthia 1995)
- ▶ Reduced molecular filling at high effective altitudes
- ▶ Ozone filling-in influences retrieved temperature shift (ozone temperature)

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  - ➔Effective scene height
- Ring effect (ozone filling-in)
- **Sensitivity study**
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Sensitivity to a-priori ozone (1)

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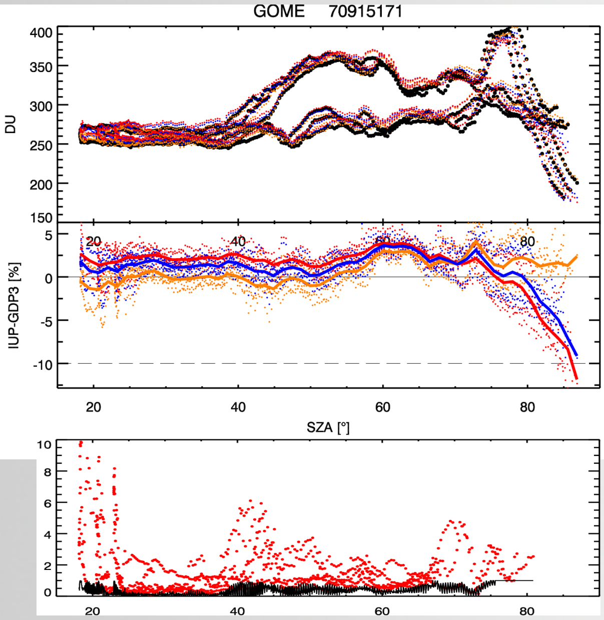


O3 climatology (TOMS V7):

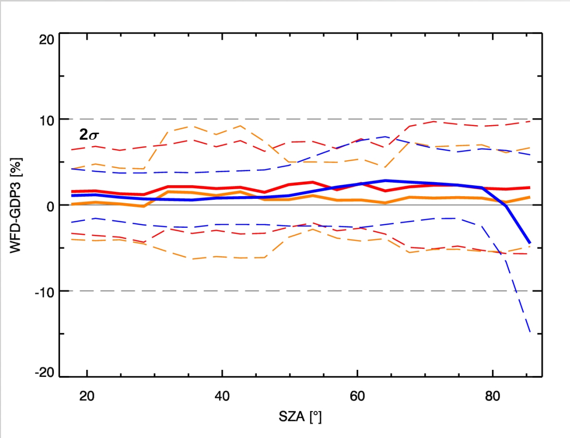
- Low latitude
- Mid-latitude
- High-Latitude

⇨ different sensititivies to clouds

⇨ overall ~1-2% higher than V3

⇨ differences to V3 depends on profile shape at high SZA (>75°)

Sensitivity to a-priori ozone (2)



O3 climatology (TOMS V7):

- Low latitude
- Mid-latitude
- High-Latitude

⇨ different sensititivies to clouds

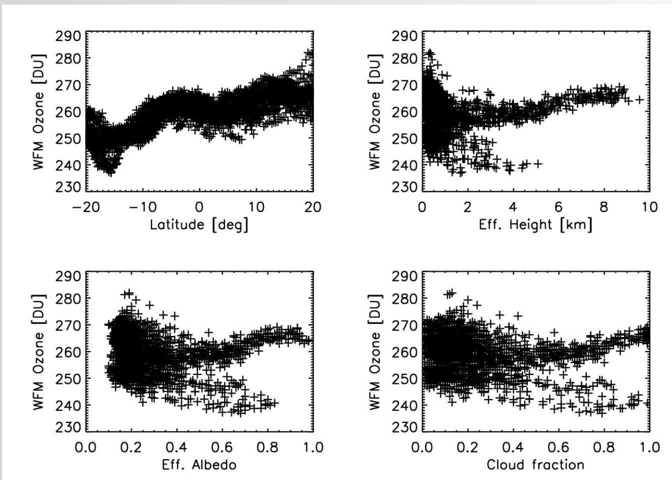
⇨ overall ~1-2% higher than V3

▷ 111 orbits

▷ Eight days from March, June, September, and December 1997

⇨ differences to V3 depends on profile shape at high SZA (>75°)

Selected Case Studies II
Tropical Clouds



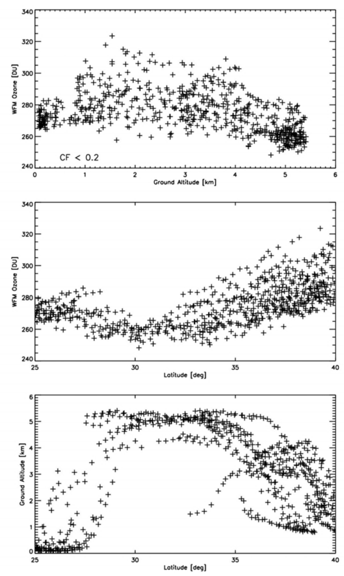
16-18 Sep 1997

Eastern Pacific : 20°S- 20°N, 120°W - 180°W

⇨ Correlation with cloud cover below 0.15

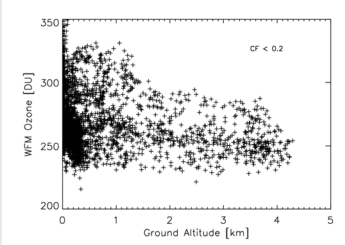
Selected Case Studies III
Mountains

Himalaya



June 1997
25°N - 40°S, 70°E - 100°E
cloud fraction < 0.2

Andes



September 1997
0° - 40°S, 60°W - 85°W
cloud fraction < 0.2

⇨ Slight reduction with ground altitude

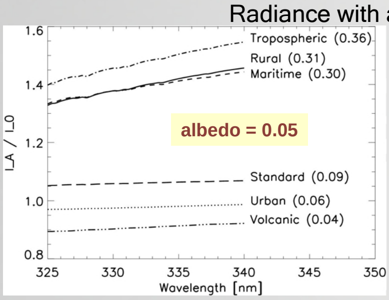
Selected Case Studies I
Enhanced Aerosol Loading

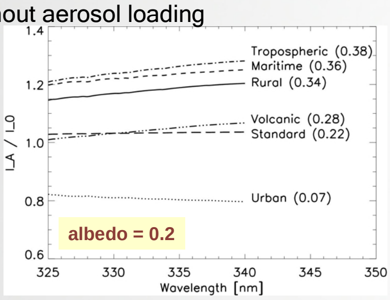
Aerosol Type	τ	ω_o @337.1 nm	LER [-]	O_3 [10^{16} molec/cm^2]	Error [%]	a_o [-]	O_3 [10^{16} molec/cm^2]	Error [%]
Standard $a_o = 0.05$	0.38	0.99	0.09	878.02	-0.17	0.05	881.50	0.22
Maritime	3.4	0.99	0.30	881.40	0.21	0.05	901.50	2.50
Tropospheric	5.0	0.96	0.36	878.96	-0.06	0.05	903.25	2.70
Rural	4.8	0.94	0.31	878.42	-0.13	0.05	899.19	2.24
Volcanic	0.6	0.81	0.04	870.14	-1.10	0.05	869.23	-1.17
Urban	4.6	0.66	0.06	871.95	-0.86	0.05	872.84	-0.76
Standard $a_o = 0.2$	0.38	0.99	0.22	880.09	0.06	0.2	881.89	0.27
Maritime	3.4	0.99	0.36	882.06	0.29	0.2	894.57	1.71
Tropospheric	5.0	0.96	0.38	879.56	0.00	0.2	893.31	1.57
Rural	4.8	0.94	0.34	878.68	-0.10	0.2	889.10	1.09
Volcanic	0.6	0.81	0.28	877.37	-0.25	0.2	884.11	0.52
Urban	4.6	0.66	0.07	871.32	-0.93	0.2	861.68	-2.03

⇨ non-absorbing aerosol error less than 0.3% (with LER)

⇨ absorbing aerosol error at 1% (with LER)

Radiance with and without aerosol loading





Summary: Sensitivity study

- **Climate zone in a-priori ozone** can lead to differences of up to 2%
- **profile shape effect** clearly detectable above 75°SZA
- difference to GDP V3 shows **sensitivity to clouds** in WF-DOAS
- No correlation between **tropical ozone and effective height**
- Reduction in total ozone observed above **high mountain ranges** (Andes, Himalaya
- Small errors due to **non-absorbing aerosols** if effective albedo is retrieved, larger errors of up to 1% to be expected in the presence of enhanced **absorbing aerosols**

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Global Error Budget

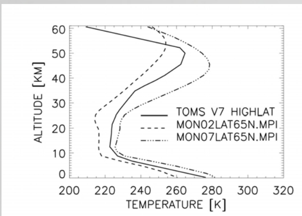
Error Source	Percent Error
A priori Errors	
profile shape: O_3 and T	1 % below 80°SZA 5 %beyond 80°SZA
profile shape (climate zone)	2 % below 80°SZA 5 %beyond 80°SZA
effective albedo	~ 1.5%
effective height	1%
LUT Interpolation error	
albedo	0.30%
altitude	0.25%
relative Azimuth Angle	0.05%
line-of-sight	0.02%
solar Zenith Angle	0.2% below 89°SZA
ozone	0.1% below 80°SZA 1.5% beyond 80°SZA
Other errors	
polarisation correction error	0.5% (1)
ground Al diffuser plate error	~0.3% (1)
signal-to-noise ratio	0.3% (1)
pseudo-spherical approximation	0.3% (1)
GVC error w.r.t. GVC	25%
GVC error w.r.t total ozone	0.15%
Error impact if not applied in WF-DOAS	
Fraunhofer fit (Kurucz)	~+2%
Bass-Paur vs. GOME FM98 ozone cross-section	2% (2)
Ring ozone filling–in	+2%
I_o effect	-0.2%

Overall precision
(excluding
error impact if not applied)

~ 3 % < 80° SZA
5% > 80°

(1) Kerridge et al. (2002)
(2) GDP V3 VALREPORT (2002)

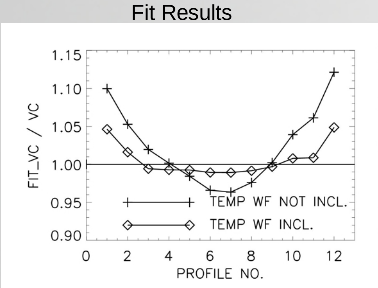
Error budget
a-priori ozone and temperature profile



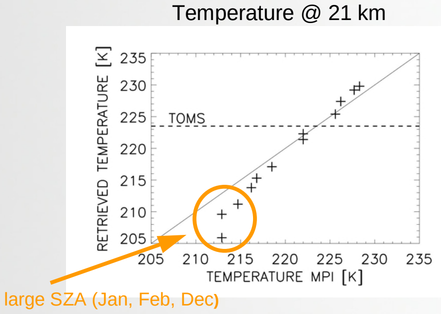
- ▷ Reference intensity: TOMS V7 high latitude
- ▷ twelve „measured“ spectra:
  MPI 2D Climatology 65°N, Jan – Dec
- ▷ SZA: 40° (June) -80° (Dec)

▶A-priori O3 and T profile error can propagate into 1% total column error (5% above 80°SZA)

Fit Results



Temperature @ 21 km

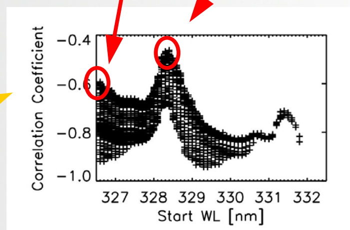


Fit Window

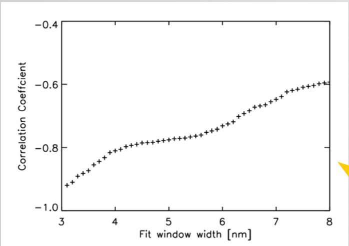
- Correlation between ozone and temperature weighting function
- No difference seen in retrieval results using 326.6-335.0 nm and 328.4-334.9 nm (Hradec-Kralove Brewer/Dobson time series)

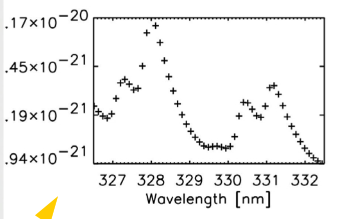
326.6-335.0 nm

328.4-334.9 nm



correlation coefficient as a function of window width and first wavelength





Correlation coefficient as a function of fit window width (start wl = 326.6 nm)

241 K ozone cross section [cm^{-2}]

Other error sources

Error sources from external sources

- Bass-Paur vs Burrows et al. 1999 O3 cross-section(*) 2%
- polarisation correction error 0.5%
- ground Al diffuser ~0.3%
- pseudo-spherical approximation 0.3%
- Pseudo-spherical approximation 0.3%

Other error sources investigated

- effective albedo ~1.5%
- effective height 1%/km
- LUT interpolation
  - → overall <0.3%
  - → ozone <0.1% below 80°SZA, <1.5% above 80°SZA
- Enhanced absorbing aerosols -1%
- Enhanced non-absorbing aerosols <0.3%
- I_o-effect -0.2%

Kerridge et al., GOME-2 error study, Eumetsat contract

(*) Roozendael et al. 2003, DOAS issues, ESA

Summary: Error budget

- **Detailed error budget** set up for WF DOAS
- Overall error budget: 3% for SZA below 80°
  5% for SZA above 80°
- *A-priori* errors (profile shape, climate zone, Ring) represents the largest error sources and are not necessarily random, but can be systematic (non-Gaussian distribution)

Topics

Part 1: Weighting Function DOAS

- Intoduction/Motivation
- Foreword: John Burrows
- WF-DOAS Algorithm
- Auxilliary Retrieval
  - → Effective albedo
  - → Clouds
  - → Effective scene height
- Ring effect (ozone filling-in)
- Sensitivity study
  - → A-priori ozone climatology
  - → Tropical clouds
  - → Mountains
  - → Aerosol
- Error Budget
- **Performance**

Computer Performance

- LUT table (750,000 scenarios)
  - → IBM Mantis (20 Gflops) ~2 weeks, 3 processors
- New Ring data base (37,000 scenarios)
  - → IBM Mantis ~1 month, 6 processors
- WF DOAS for one GOME orbit (only forward scans)
  - → SUN Ultra II
    - LUT from file ~25 min
    - LUT in memory **~5 min**

Conclusion

- Successful implementation of a new DOAS algorithm for total ozone using **weighting function** approach
- **Taylor expansion of DOAS equation** represents a straight forward and generalised approach valid for weak and strong absorbers alike
- By using LUT for RTM quantities, **fast processing speed** has been achieved
- New features as compared to GDP V3 has been introduced
  - → Use of **effective albedo and effective scene height** derived from GOME spectral information
  - → Dependence of **Ring effect** on ozone total column and profile shape **(ozone filling-in)** is accounted for
  - → Improved **wavelength calibration** (Fraunhofer fit, x-section shift)
- Improved spectral **fit residual RMS** by factor of two (against GDP V3)
- Overall **precision** is about **3%** (5% at high SZA)