Atmospheric Physics
UNIVERSITY OF TORONTO

The 2007 Noble Lecture Series

Atmospheric Chemistry and the Remote Sensing of the Global atmosphere March 26-30th 2007.

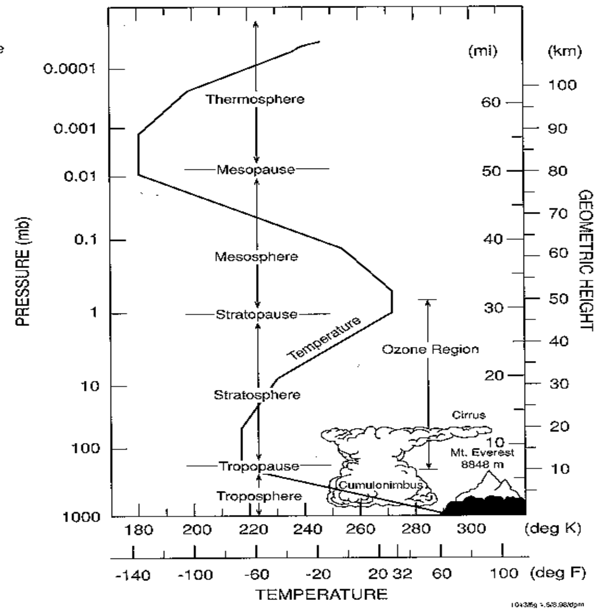
Lecture 2: Retrieval for Nadir and Limb Sounders in the UV visible and near IR DOAS and FURM

John P. Burrows
Department of the Physics and Chemistry of the Atmosphere
Institute of Environmental Physics and Remote Sensing
University of Bremen, Bremen, Germany

Introduction and Content: L2

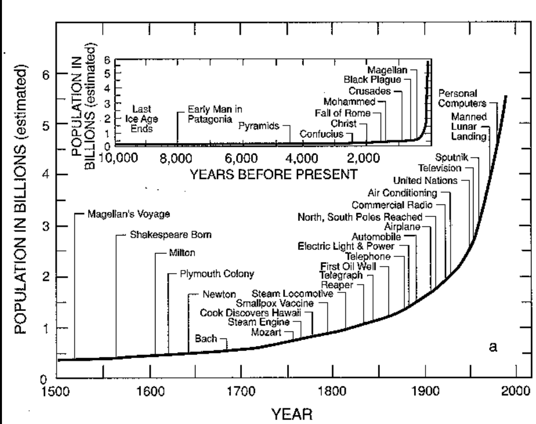
- Atmospheric Issues,
- Observations from Space using back Scattered Solar Radiation
- Retreiveal of Data Products

Figure 1.5. Vertical profile of the temperature between the surface and 100 km altitude as as defined in the U.S. Standard Atmosphere (1976) and related atmosphere layers. Note that the tropopause level is represented for midlatitude conditions. Cumulonimbus clouds in the tropics extend to the tropical tropopause located near 18 km altitude.



Population and Emissions to the atmosphere

Atmospheric Chemistry and the Earth System



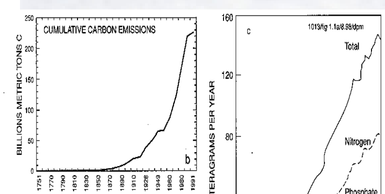


Figure 1.1. Evolution of (a) the world population, (b) the cumulative emissions of carbon in the atmosphere since 1750 (courtesy of G. Marland, 1994), and (c) world fertilizer use between 1940 and 1990 (from OUR CHANGING PLANET 2/E by Mackenzie/Mackenzie, ©1998, adapted by permission of Prentice-Hall, Inc., Upper Saddle River, NJ).

Mesospheric Issues:

- Is the Mesospheric composition a potential early warning signal for Climate Change???
- Noctiluscent or Polar Mesospheric clouds???
- Quantify global NO_x source for the stratosphere??
- Impact of meteorites (also of stratospheric sig)??
- Do we understand the O_2 and O_3?? Photolysis rates, $O_2(^1\Delta)$, $O_2\ (^3\Sigma)$, NO etc.
- Impact of SPE – changing magnetic fields etc. (also stratospheric sig)

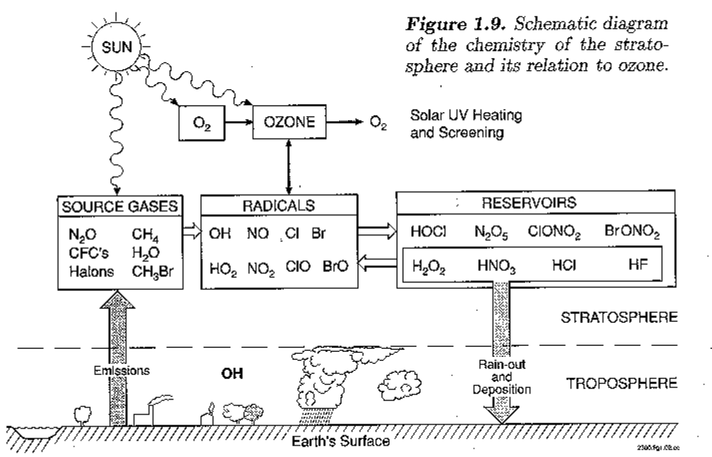
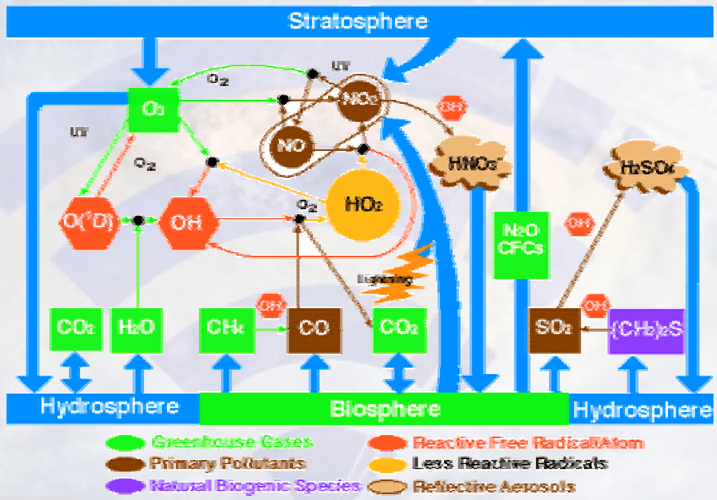


Figure 1.9. Schematic diagram of the chemistry of the stratosphere and its relation to ozone.

Universität Bremen ife
Noble Lectures - University of Toronto, 26-30th March 2007, J. P. Burrows - Lecture No. 2.

Tropospheric Chemistry



SOME (PRE-) HISTORY

- 1920s Dobson et al develop a Spectrophotometer and technique for atmospheric O3 column
- 1957 International Geophysical Year – Dobson network -Singer and Wentworth propose BUV technique
- 1960s Soviet make first attempts to measure O3 from space
- 1974 – 1979 BUV launched aboard NASA Nimbus 4
- 1975 –1990 Development of DOAS (Differential Optical Absorption Spectroscopy)
- 1979 – 1991 SBUV and TOMS launched on NASA Nimbus 7
- 1991- 1994 TOMS on Russian Meteor
- 1996 - TOMS on ADEOS and EPTOMS
- 1979-2006 SAM-II, SAGE, I, II and III occultation

Universität Bremen ife

Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

The unabridged History of SCIAMACHY - GOME – GeoSCIA-GeoTROPE

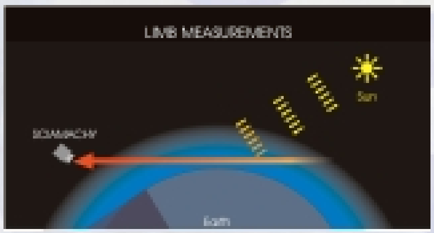
03-1985	MAP (Measurement of Atmospheric Pollution) proposal idea to ESA for EURECA *not selected*
05-1985	Stratospheric Ozone hole observed by Farman et al (Nature).
1985 – 1988	Submission of the *SCIAMACHY proposal,* supported by Germany to ESA for the Polar Platform, now ENVISAT.
1988	Proposal of SCIA-mini for ERS-2
1989	Descope of *SCIA-mini to GOME (Global Ozone Monitoring Experiment)*
1989 – 2002	*Selection, Design and Development of SCIAMACHY as German/Dutch/Belgian contribution to ENVISAT*
20.04.1995	Launch of ERS-2 with GOME

The unabridged History of SCIAMACHY - GOME – GeoSCIA-GeoTROPE

1997-1998	Development of GeoSCIA C0ncept
12.1998	Proposal of GeoSCIA to ESA – recommended for further study
1997-2000	Selection of GOME-2 for the EUMETSAT operational series Metop.
2000	GeoSCIA++ - Geostationary Idea for ESA Earth Explorer
2000-2001	Development of GeoFIS
01.2002	Proposal of *GeoTROPE(GeoSCIA+GeoFIS) Geostationary TROPospheric Explorer* to ESA for EEOM-2 recommended for further study -
28.02.2002	Launch of ENVISAT with SCIAMACHY on board.
12.2003	Proposal GeoSCIA-Lite – small sat for national EO programme Germany – not selected
15.08.2005	Proposal GeoTROPE-R for the ESA Earth Explorer - not selected for Phase A
17.10.2006	Launch of Metop-A with GOME-2 and IASI on board.

SCIAMACHY and GOME Measurement Geometry

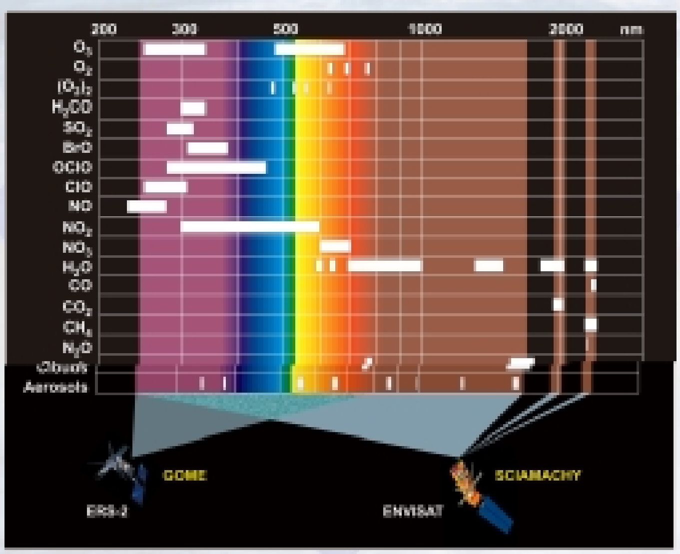
- Typical spatial resolution in nadir:
  GOME-1 - 40x320 km^2 1995-?
  SCIAMACHY - 30x 60 km^2 2002
  GOME-2 - 40x80 km^2 2005/6
- Vertical resolution in limb/occultation: 1.5-3 km
- Global coverage for limb and nadir



Universität Bremen ife

Noble Lectures - University of Toronto, 26-30th March 2007, J. P. Burrows - Lecture No. 2.

GOME SCIAMACHY Targets and Spectral Coverage



Universität Bremen ife

Noble Lectures - University of Toronto, 26-30th March 2007, J. P. Burrows - Lecture No. 2.

Introduction and Content: L2

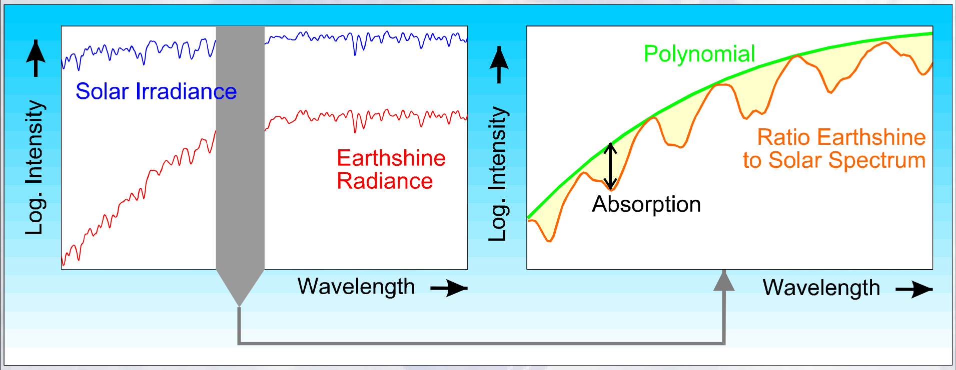
- •FURM, Optimal Estimation and Inversion Theory
- •DOAS Differential Optical Absorption Spectroscopy
- •DOAS + TEM or Reference Sector Method
- • WFM-DOAS retrieval algorithm

NADIR Retrieval Principles

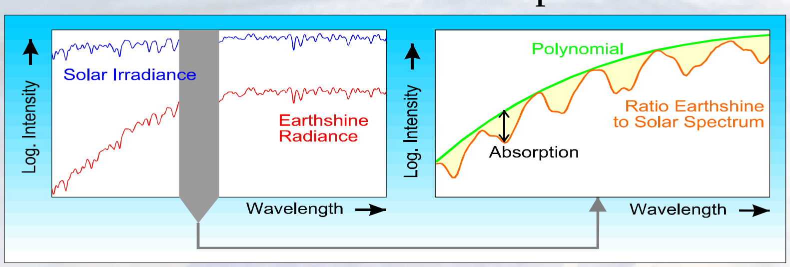
- DOAS - Differential Optical Absorption Spectroscopy
- FURM – FUll Retreival Method

Universität Bremen ife
Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

DOAS



DOAS made simple!



Derive the Slant Column Amount of species i:

$$\min [\Sigma_{\lambda}\{(\ln(Io/I))_{\lambda}\} - \Sigma_{\lambda}\{\Sigma_i (\Delta\sigma_{i\,\lambda} (c_i\, l_{\lambda})+P_{\lambda}\}]$$

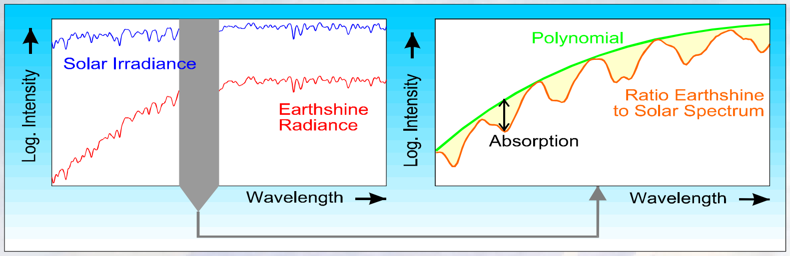
$$SC_i = \Sigma_{\lambda}(c_i\, l_{\lambda})$$

Assume l_{λ} constant over small spectral window and thereby derive Vertical Column Amount

VC = SC/AMF

AMF is the Air Mass factor

DOAS made simple (2)!



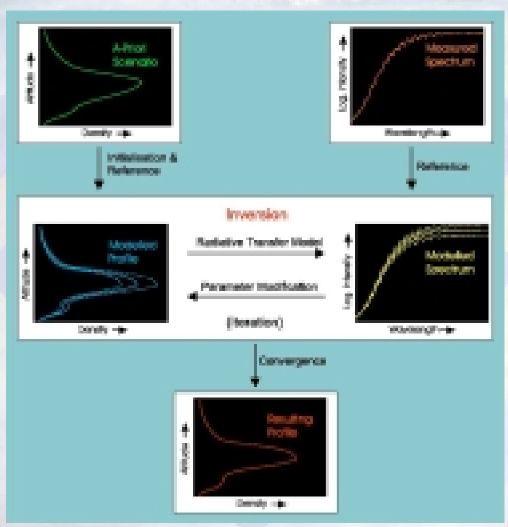
VC = SC/AMF

The AMF must be derived using a Radiative Transfer Model – RTM.

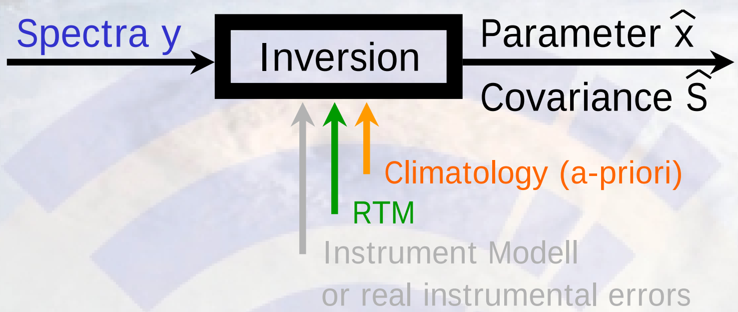
The RTM describes the path of light through the Atmosphere.

In its simplest form i.e. Ignoring scattering, the AMF is determined by the geometry

FURM

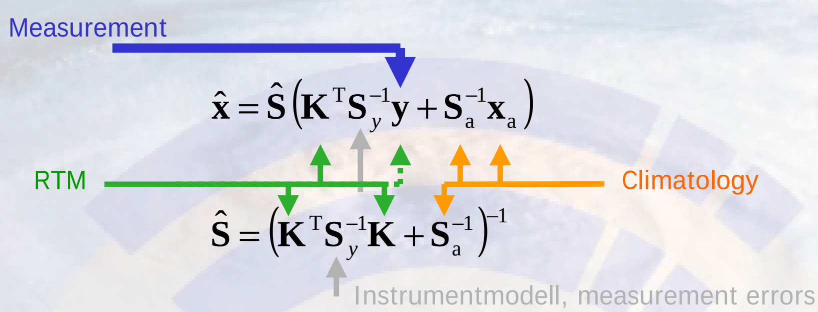


Inversion using Optimal Estimation



- Optimal Estimation (Rodgers 1976)
- Simultaneous fit of all parameters

Optimal Estimation



$$\hat{\mathbf{x}} = \hat{\mathbf{S}}\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{y} + \mathbf{S}_a^{-1}\mathbf{x}_a\right)$$

$$\hat{\mathbf{S}} = \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} + \mathbf{S}_a^{-1}\right)^{-1}$$

$\hat{\mathbf{x}}$: vector of atmospheric parameters, retrieval covariance $\hat{\mathbf{S}}$

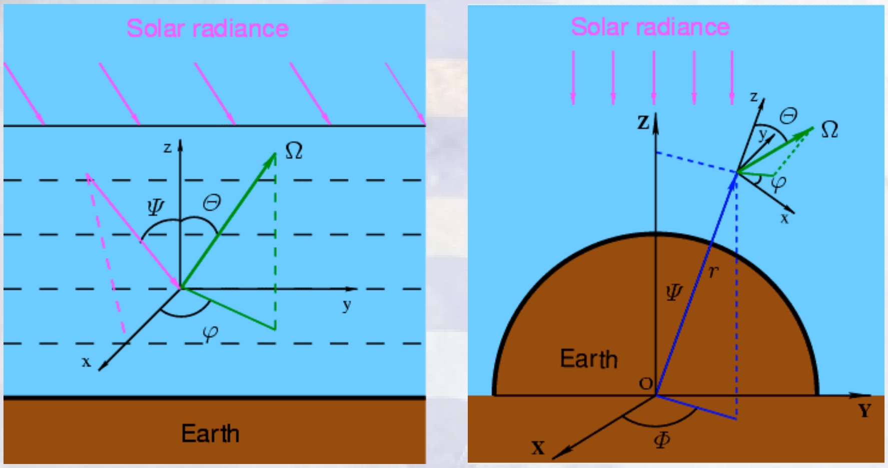
$\mathbf{y}$: measurement vector, measurement covariance $\mathbf{S}_y$

$\mathbf{x}_a$: climatological state vektor, a-priori covariance marix $\mathbf{S}_a$

$\mathbf{K}$: weighting function, from RTM

Coordinate systems

Plane-parallel atmosphere | Spherical atmosphere



GOMETRAN/SCIATRAN RTM

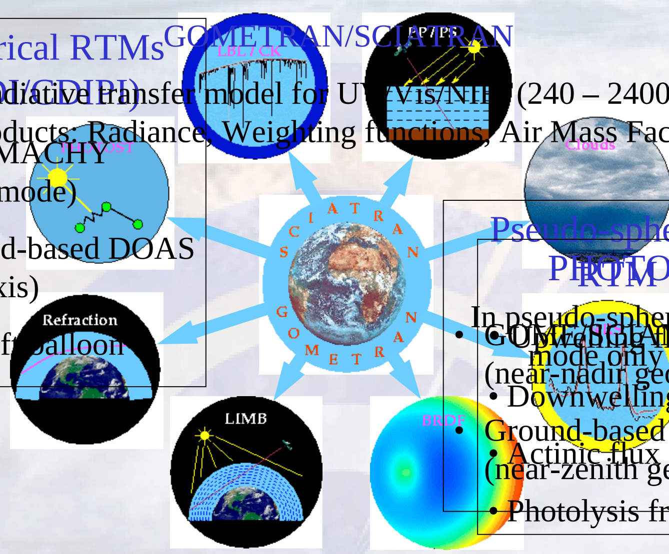
GOMETRAN/SCIATRAN

A radiative transfer model for UV/Vis/NIR (240 – 2400 nm)

Products: Radiance, Weighting functions, Air Mass Factors

Spherical RTMs (CDI/CDIPI)

- SCIAMACHY (limb mode)
- Ground-based DOAS (off-axis)
- Aircraft, balloon



Pseudo-spherical RTM

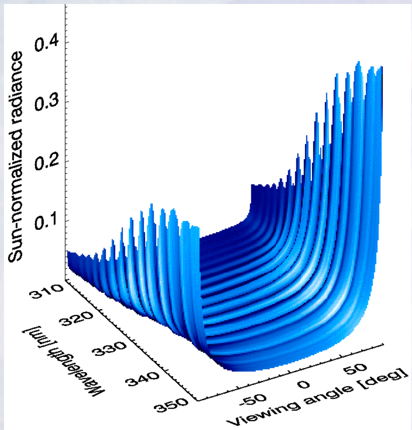
- In pseudo-spherical mode only
- GOME, SCIAMACHY (near-nadir geometry)
- Ground-based DOAS (near-zenith geometry)

PROTOST

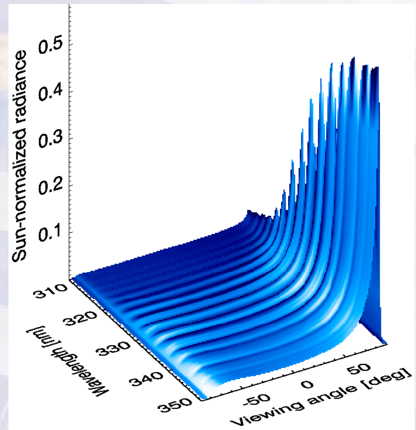
- Upwelling flux
- Downwelling flux
- Actinic flux
- Photolysis frequency

Outgoing radiation at SZA = 89 deg

Pseudo-spherical model



Spherical model



Ozone Profile Retrieval with GOME

The FURM Technique Utilises

i) the penetration as a function of wavelength in the UV,

I i) Some additional information in the T-dependence of the Huggins bands

However the retrieval is strongly dependent on the

Radiometric calibration!!!

Universität Bremen ife
Noble Lectures - University of Toronto, 26-30th March 2007, J. P. Burrows - Lecture No. 2.

Ozone Profile Retrieval from GOME

- GOME: Global Ozone Monitoring Experiment
- retrieval algorithm: FURM (FUll Retrieval Method)
- moderate linear dependencies between Ozone x and Radiance y :

$\Rightarrow y(x) \approx y(x_0) + \frac{\partial y}{\partial x}(x - x_0))$

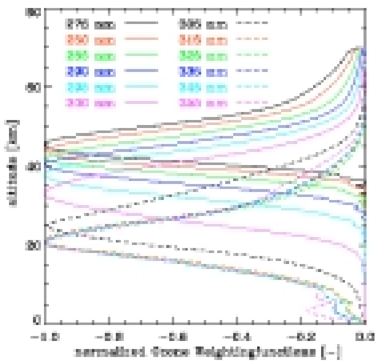
$$\Delta y = K \cdot \Delta x$$

y : Radiance

x : Ozone Profile

$$K_j^i = \frac{\partial y_i}{\partial x_j}$$

weighting function



" True" and Retrieved Profile : The Averaging Kernel Matrix

$$x_{ret} = x_a + \tilde{A}(x_{true} - x_a)$$

x_{true} : True atmospheric Profile

x_{ret} : Retrieved Profile

x_a : a priori Profile

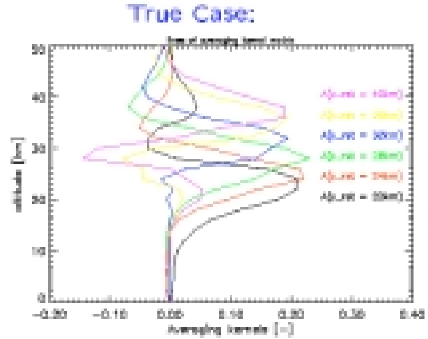
$\tilde{A}$: Averaging Kernel Matrix

Ideal Case:

$$\tilde{A} = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$

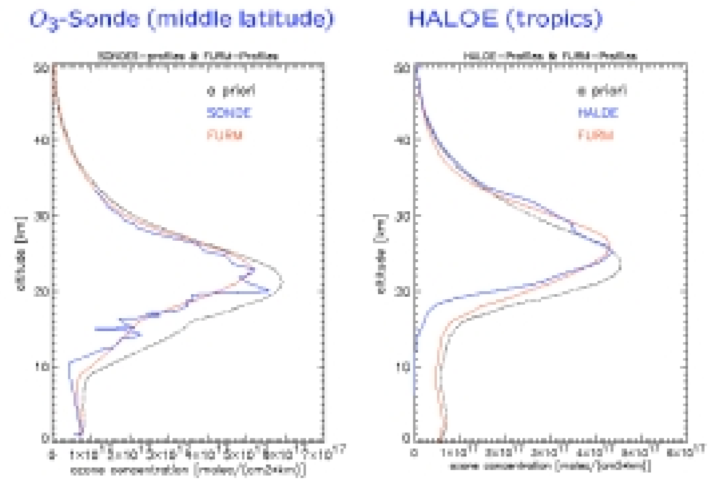
$\Rightarrow x_{ret} = x_{true}$

True Case:



Results

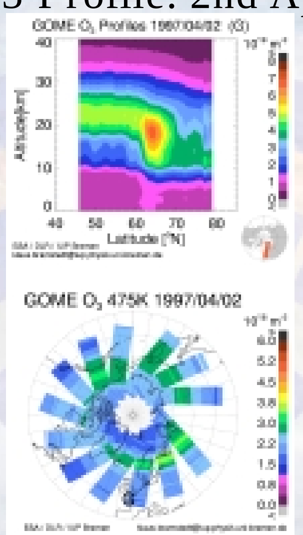
Comparison with independent data



Universität Bremen ife

Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

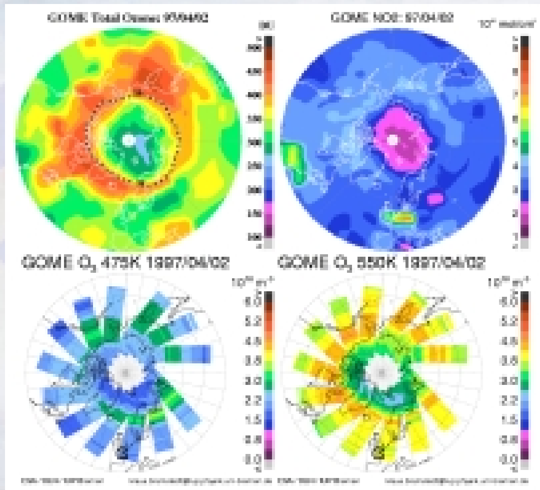
GOME O3 Profile: 2nd April 1997



Universität Bremen ife

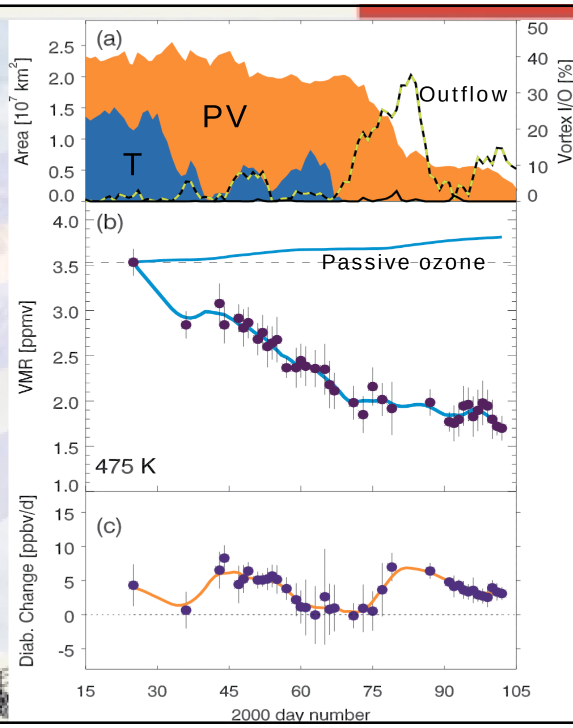
Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

O_3, NO_2 and O_3 at 475K and 550K Levels: 2nd April 1997

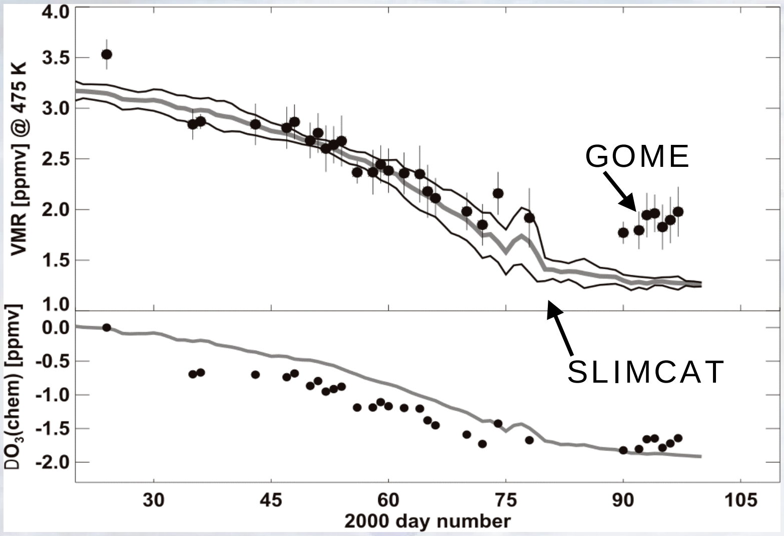


FURM Ozone

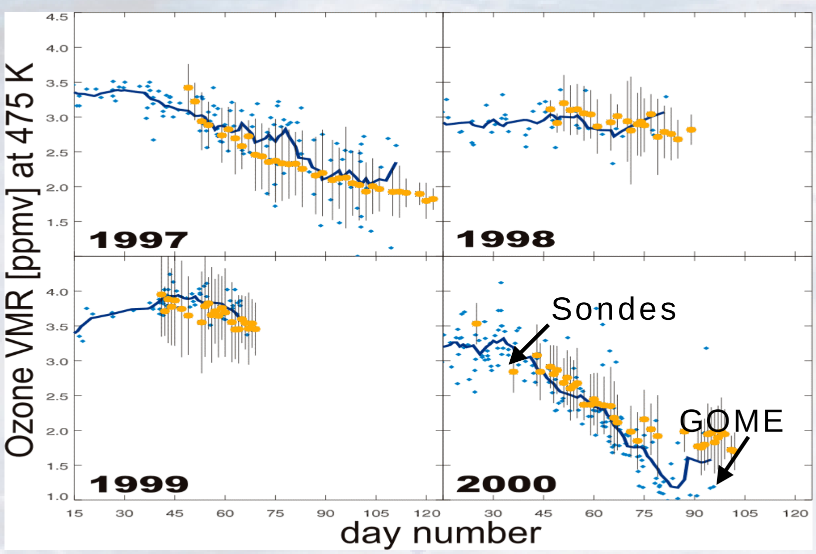
- Vortex- and PSC-Area
- FURM Ozone VMR and passive Ozone
- Diabatic Ozone-change



FURM Ozone vs. SLIMCAT

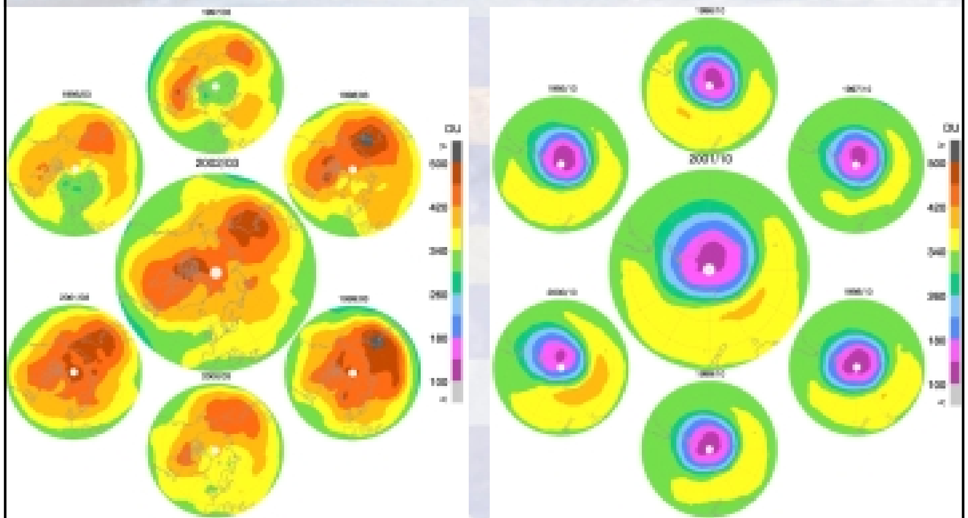


GOME-FURM Ozone vs. Ozonesondes



Universität Bremen ife
Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

GOME: Polar Ozone [DU] NH March and SH October 1995-2002



Universität Bremen ife

Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

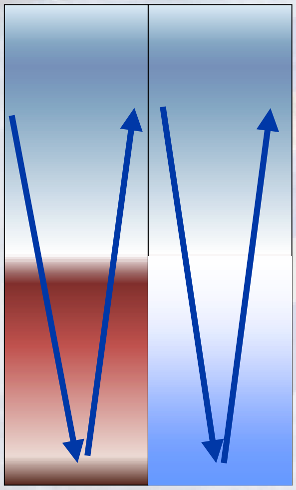
Tropospheric Trace Gas Information

- Origin of Information
  - Total Column - Stratospheric Column from other sources (limb sounders on LEO, data assimilation)
  - Reference Sector Method (depends on coverage)
  - Cloud Slicing (spatial and temporal)
  - wavelength dependence of mean scattering height (example BUV)
  - SZA dependence of mean scattering height (McKenzie et al.)
  - Combined IR (thermal emission) and UV-Vis (solar backscatter) retrieval

Universität Bremen ife

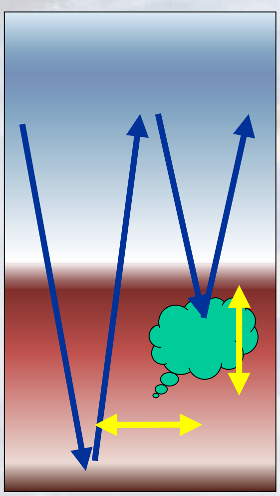
Noble Lectures - University of Toronto,
26-30th March 2007,
J. P. Burrows - Lecture No. 2.

Reference Sector Method



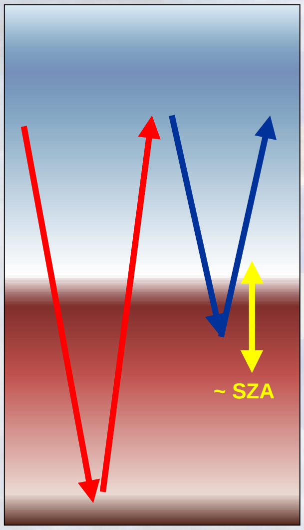
- tropospheric “clean” reference ground pixels (no sources, clean air region etc.)
- Stratospheric contribution assumed to be negligible or homogeneous over relevant ground pixel area
- NO_2, HCHO,CHO.CHO, SO_2, BrO ...

Cloud Slicing



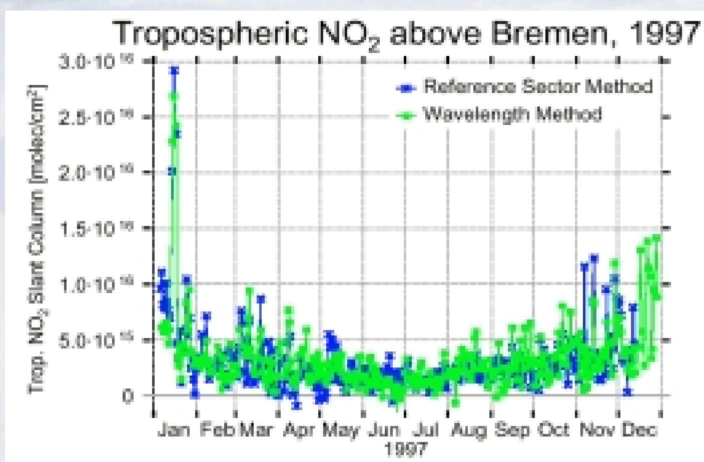
- **Spatial and/or temporal cloud slicing** techniques applicable
- Assumption: tropospheric concentration reasonable constant within relevant temporal and/or over spatial scales
- Heritage: O_3 TOMS Cloud Slicing
- Applicable: O_3,NO_2, HCHO, SO_2 etc.
- High precision tropospheric trace gas data requires co-located cloud top pressure data (for example from O_2 A-band and/or Ring effect analysis)
- **Cloud slicing with deep convective cloud systems in the tropics will allow profiling**

Mean scattering height



- Wavelength dependence of mean scattering height
- **solar zenith angle dependence of mean scattering height** (McKenzie et al., Fish et al.)
- Atmospheric Composition w.r.t. strong absorbers and scatters known
- High precision tropospheric trace gas data requires co-located measurement of mean scattering height (for example via O_2 A-band)
- O_3, NO_2, BrO, Aerosol

Tropospheric NO2 above Bremen

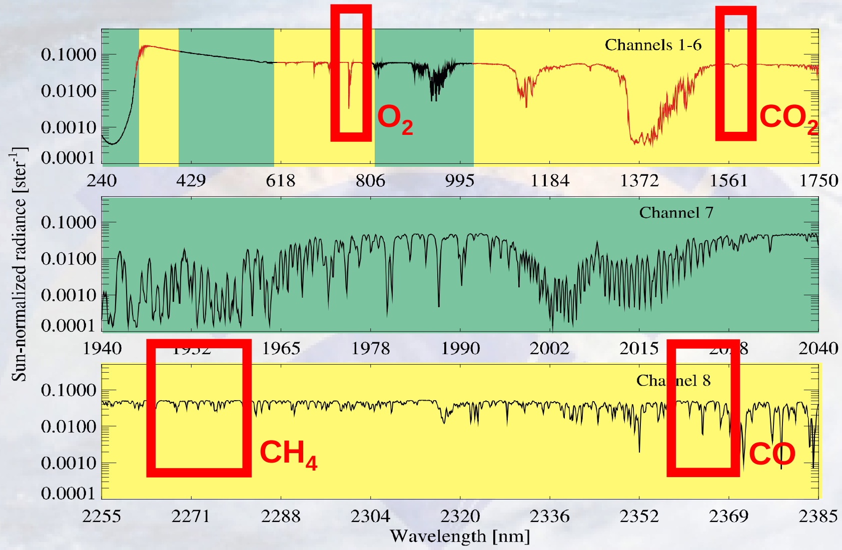


» Consistent tropospheric columns from two independent approaches!

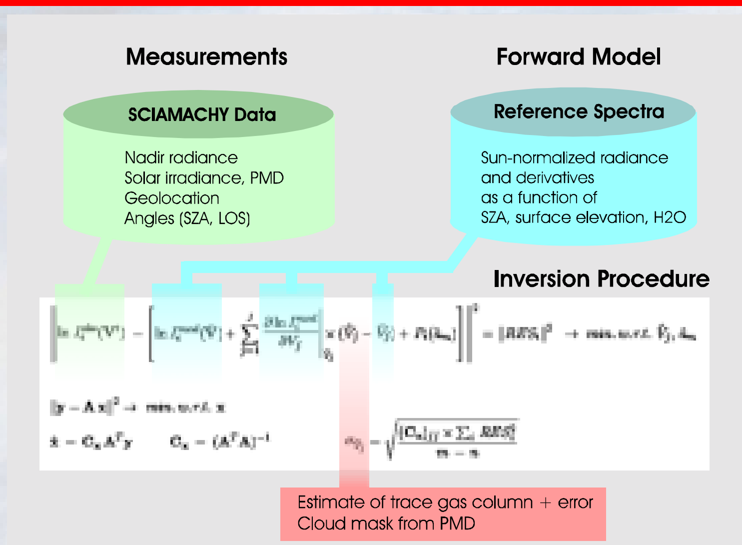
© A. Richter IUP/IFE Bremen

Universität Bremen ife
Noble Lectures - University of Toronto, 26-30th March 2007, J. P. Burrows - Lecture No. 2.

SCIAMACHY Nadir spectrum CO, CO_2 and CH_4



WFM-DOAS algorithm



WFM-DOAS look-up-table

Currently implemented look-up-table:

Constant:

• US Standard atmosphere (USS), no clouds, maritime aerosol, nadir viewing (no scan)

Variable:

• SZA: 0º-90º in steps of 5º

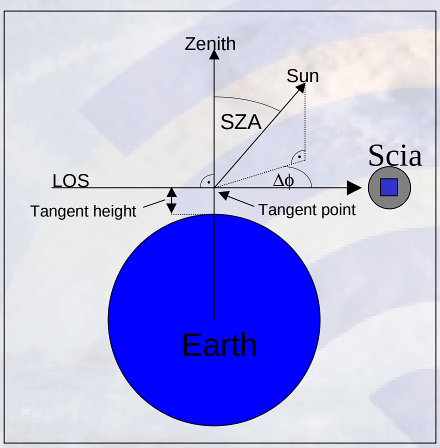
• Surface elevation (pressure): 0, 1, 2, 3 km

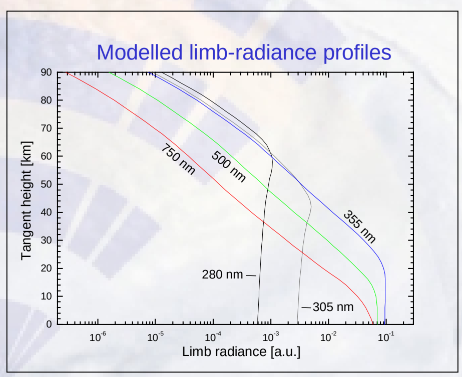
• Albedo,

• H_2O column: 0.5, 1.0, 1.5, 2.0, 4.0 x USS H_2O column

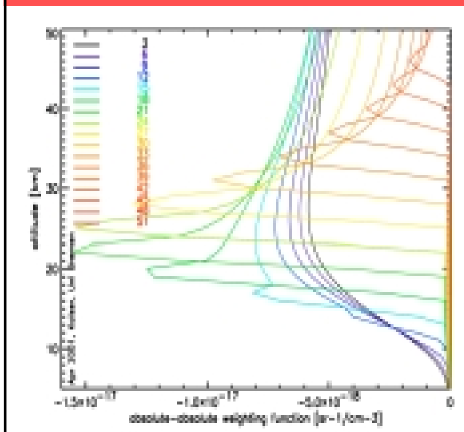
The limb-scattering geometry

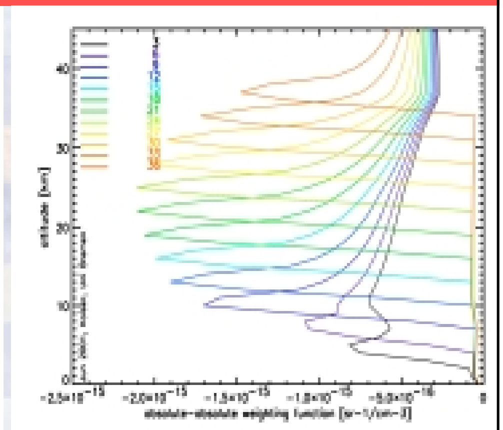
• Limb radiance corresponds to the solar radiation that is Rayleigh and Mie-scattered along the LOS and transmitted in to the FOV of the observer





O_3 Weighting Function for Limb



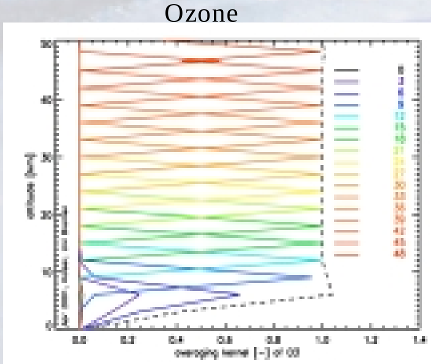


- 360 nm 790 nm
- Light path is wavelenght dependence => multi spectral advantage

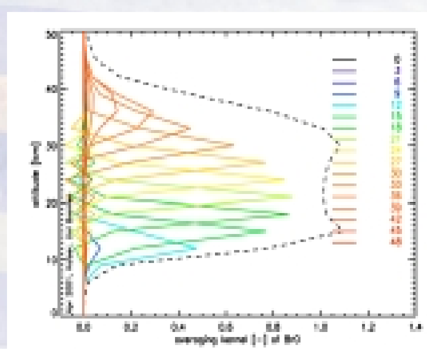
Averaging Kernels Limb

- 300 –370 nm

Ozone



- BrO



- Useful height range: 5—50 km
- Above 12 km all information comes from the measurement
- No smoothing

- Useful height range: 15—30 km
- Information determined by the measurement
- some smoothing

Summary and Conclusions

1 Requirements for measurements from Space

2 Passive Remote Sensing using back scattered solar radiation

3 Radiative Transfer Issues

4 Retriveal techniques for Limb and Nadir