GOME-1 and O3 Retrieval

Methodology: an overview

J.P. Burrows

University Bremen FB1, Institut für Umweltphysik (iup)

GOME Total Ozone Column Retrieval Development,
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Mark.Weber@uni-bremen.de
http://www.iup.physik.uni-bremen.de

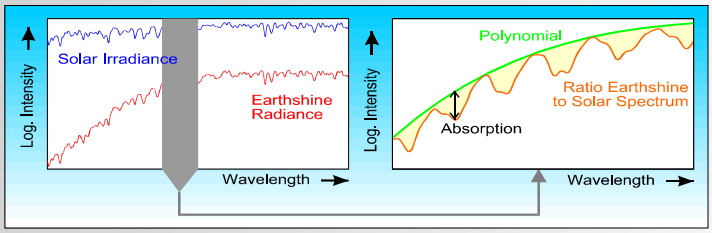
Topics

- Differential Optical Absorption Spectroscopy

SCIAMACHY, SCIA-mini and GOME-1: some relevant facts

1970-1982	Long path Differential Optical Absorption Spectroscopy (DOAS) developed by D. Perner and U. Platt. SAOZ Balloon instruments (Pommereau) Noxon then later Mount and Solomon ground based Zemith sky and SME.
03 -1985	MAP (Measurement of Atmospheric Pollution) proposal idea to ESA for EURECA first attempt to apply DOAS from Space - Burrows and Perner *no significant agency response - ignored,*
05-1985	Stratospheric Ozone hole observed by Farman et al (Nature).
1985 - 07-1988	Development and submission of the *SCIAMACHY (Scanning Imaging Absorption Spectrometer for atmospheric CHartographY) proposal,* supported by Germany in response to ESA call for instruments for the Polar Platform - now called ENVISAT. Simultaneous Limb and Nadir observations to separate mesosphere, stratosphere and troposphere
12- 1988	Proposal of SCIA-mini in response to ESA call for an atmospheric constituents monitor on ERS-2 Simultaneous - Limb and Nadir - UV visible only!!!
1989	SCIA-mini selected by ESA but descoped of *SCIA-mini to GOME (Global Ozone Monitoring Experiment)*
1990-1994	GOME designed - basis SCIAMACHY nadir - constructed, characterised, and calibrated.
20-04-1995	Launch of ERS-2 with GOME

DOAS made simple!



Derive the Slant Column Amount of species i:

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

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

Assuming

a) l_λ ***constant over small spectral window***

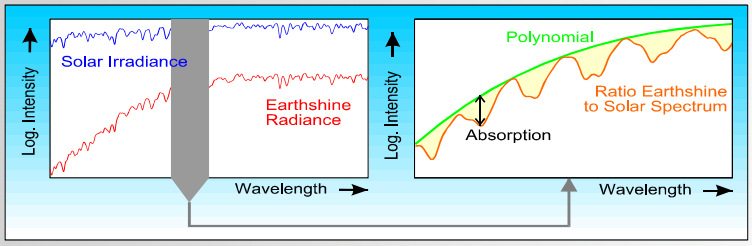
b) ***Weak absorption at all*** λ

Thereafter derive Vertical Column Amount

VC = SC/AMF

AMF is the Air Mass factor

DOAS made simple (2)!



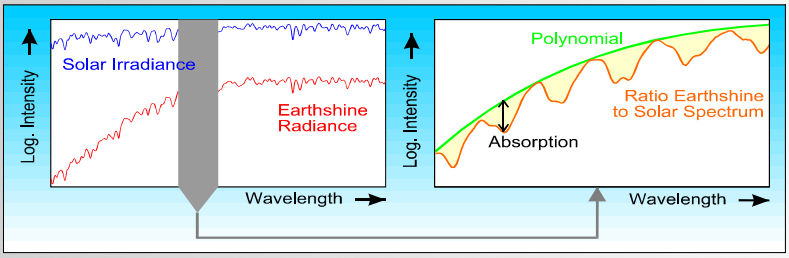
VC = SC/AMF

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

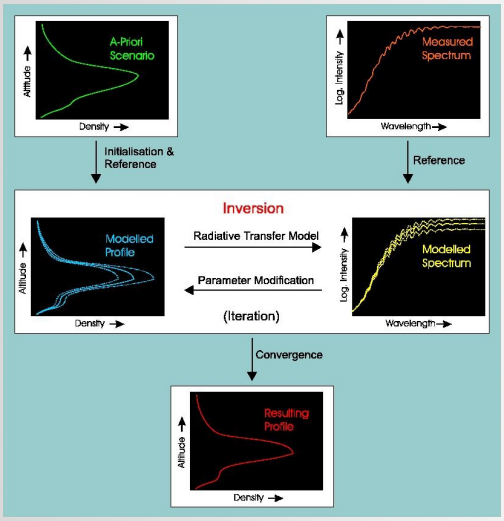
DOAS made simple (3)- Limitations!



Simplest AMF is the geometric factor – This works well for wavelengths where the scattering in the atmosphere is negligible!

In the UV penetration is strongly wavelength dependent as a result of
- Molecular scattering (Rayliegh)
- strong Ozone absorption ($\lambda \geq 320$ nm) basis of BUV and FURM O3 profile retrieval
- particle scattering aerosol and clouds
As a consequence the surface spectral reflectance becomes of great significance

FURM



Optimal Estimation

Measurement

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

RTM

Climatology

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

Instrument modell, measurement errors

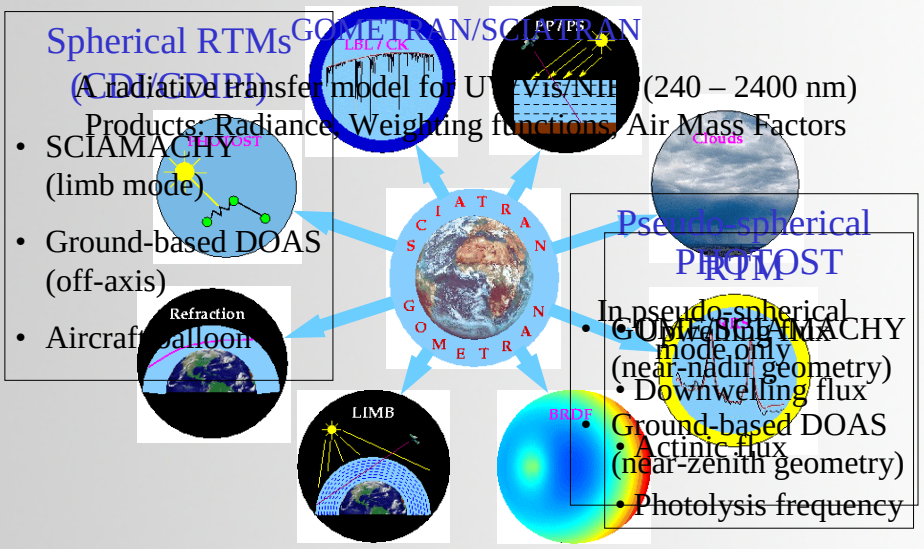
$\hat{\mathbf{x}}$: vector of atmospheric parameters, retrieval covariance $\hat{\mathbf{S}}$

$\mathbf{y}$: 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

GOMETRAN/SCIATRAN RTM



Spherical RTMs (CDI/GDIPI)

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

GOMETRAN/SCIATRAN

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

Products: Radiance, Weighting functions, Air Mass Factors

Pseudo-spherical PP/PR/TOST RTM

In pseudo-spherical mode only

- GOME/SCIAMACHY (near-nadir geometry)
- Downwelling flux
- Ground-based DOAS (near-zenith geometry)
- Actinic flux
- Photolysis frequency

GOME-1 Retrieval Studies: some relevant historical Information

1990	Scientific Radiative Transfer Programme GOMETRAN, developed by Rozanov and Burrows for GOME and SCIAMACHY applications. Concept of Linearisation and thereby direct calculation of Weighting functions to optimise and speed analysis.
1990	After a short phase A Study - Selection of GOME for ERS-2 but limited ESA ground segment granted.
1991	DLR offers to support the development of an operational prototype level 0 to 1 and level 1 -2 processor for GOME.
1992-1994	Scientific Prototype DOAS level 1-2 processor for GOME developed at UB with support from University of Heidelberg and MPI. - Transfer to GDP ESA Trace Gas Study No 1 (scientific Consortium UB, UH and RAL + consultants) investigates total Ozone and Ozone profiling from GOME. GOMETRAN provided to RAL, DLR, UH etc.
1994	Several Important Conclusions of Trace Gas 1 e.g. Simple DOAS depends on the assumption that absorption in a spectral window is weak i.e. AMF is constant over a spectral window. This breaks down for O3 at larger SZA. Consequence - modified DOAS recommended for SZA above 70° Several O3 windows investigated including 325-335 nm Recommendations for optimal settings Cross Sections, Ring etc. ESA selects 325-335 nm window as first spectral window for operational processor.
1994-1995	ESA Trace Gas Study No. 2 Further investigation of the total O3 and O3 profile error sources. Recommendation for the use of modified DOAS at high SZA confirmed.

GOME-1 Retrieval Studies:
some relevant historical Information

1995-1996	ESA Ring Study (IUP/IFE-UB led scientific consortium UB, UH and consultant -) Conclusions (Report: Burrows et al 1997 and later published in part in Vountas et al 1998) - Ring is indeed RRS and gas phase Vibrational Raman scattering is small - Experimental Ring as proposed by Solomon et al introduces some systematic error - Ring can be calculated but requires accurate RTM including all physics - Both in-filling of Fraunhofer lines and molecular features of significance. - Theoretical calculation of Ring recommended for implementation in GDP.
1995-1996	GOME Validation shows strong SZA bias - increasing strongly beyond SZA 70° Rozanov, Buchwitz et al at UB-IUP/IFE show that „simple DOAS" may be extended to about SZA 80° by appropriate selection of the most representative wavelength for the calculation of AMF in the spectral window 325-335 nm. Adopted by ESA after GSAG recommendation and implemented in GDP as quick fix for the breakdown of simple DOAS the GDP. Doppler Shift of the Solar Irradiance and small thermal drift around the orbit, reported by by Burrows, Eisinger, Richter et al at IUP/IFE to GSAG ESA and GDP.
1996	Intensive phase of the Validation of GDP completed – Many systematic errors found and identified in the GDP and list of recommendations provided to ESA. This list includes recommends the use of GOME cross sections, improved Ring and Modified DOAS for large SZA,