Radiative Transfer in the Atmosphere in the UV, Visible and Near-IR

SCIAMACHY Instrument and SCIATRAN: a Family of Computer Programme

Lecture 2

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ENVISAT Launch: 1st March 2002, 2:07 CET

In Orbit

SCIAMACHY

Scanning Imaging Absorption Spectrometer for Atmospheric Chartography

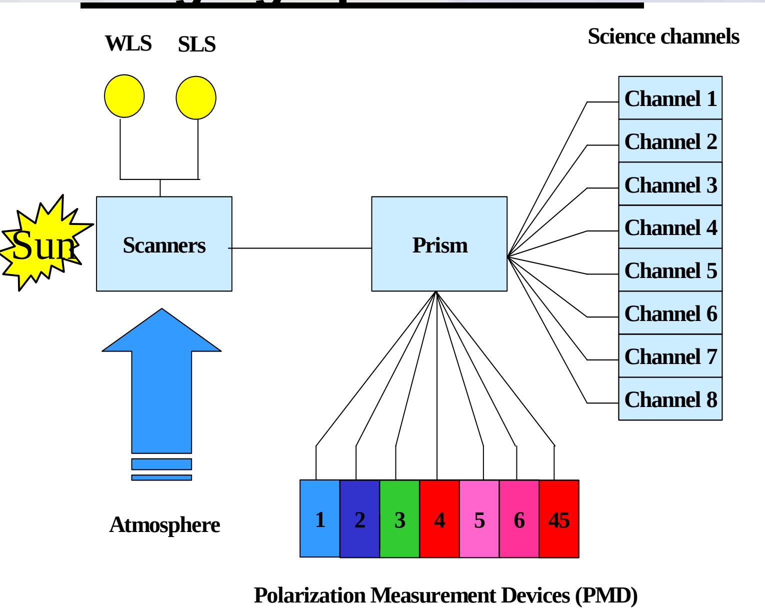
Viewing Geometry

Nadir

Limb

Occultation

Imaging Spectrometer



Combination of Prism and 8 high resolution channels (each having its own grating)

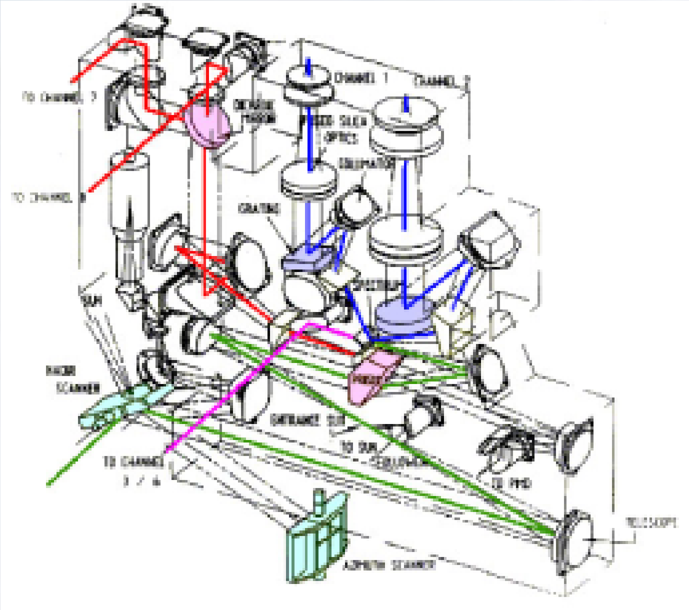
Spectral range from 214 to 2380 nm

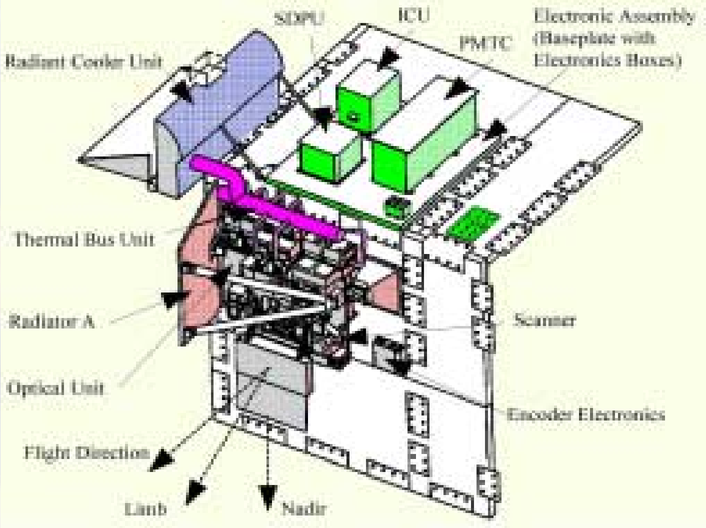
Spectral resolution from 0.2 to 1.5 nm

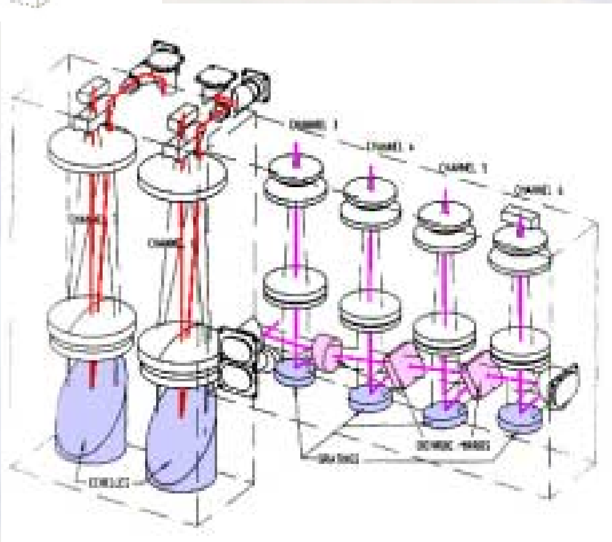
7 broadband polarization measurement Devices PMDs

On-board calibration H/W

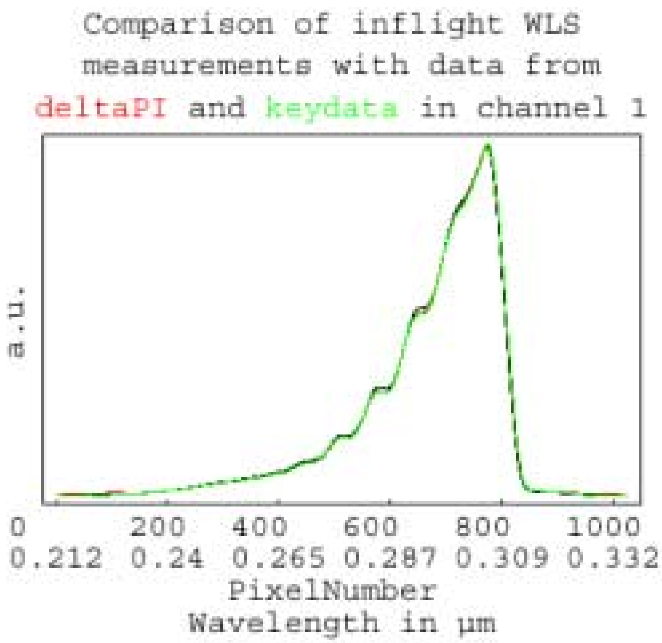
SCIAMACHY Instrument

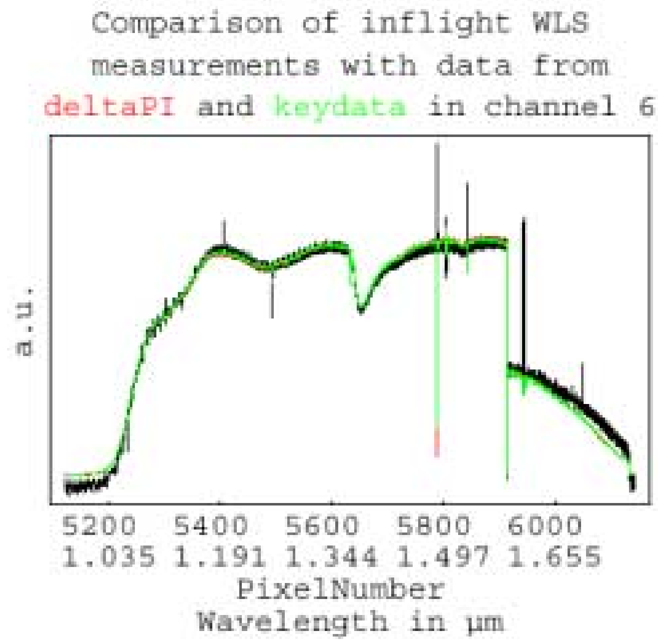


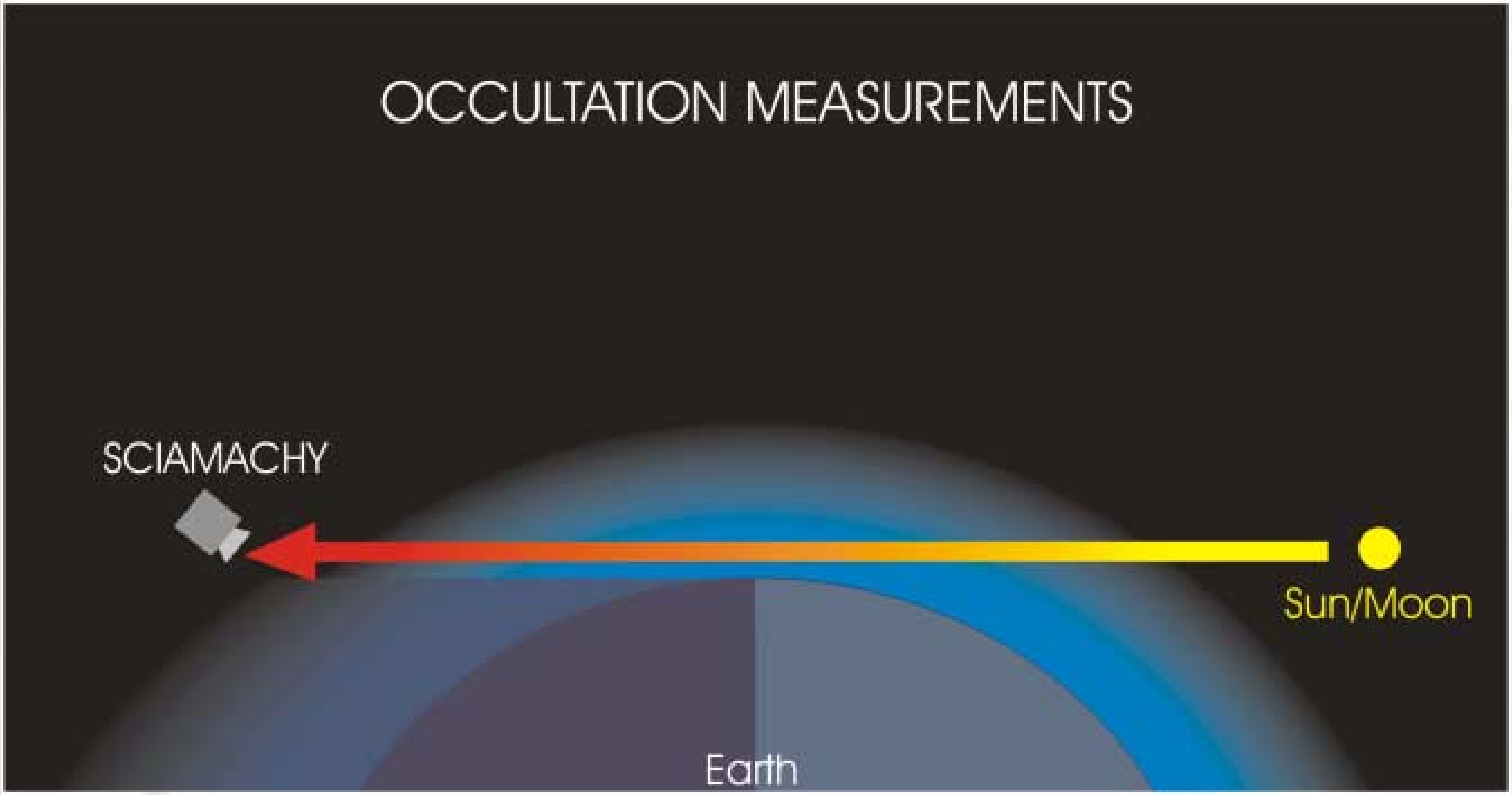




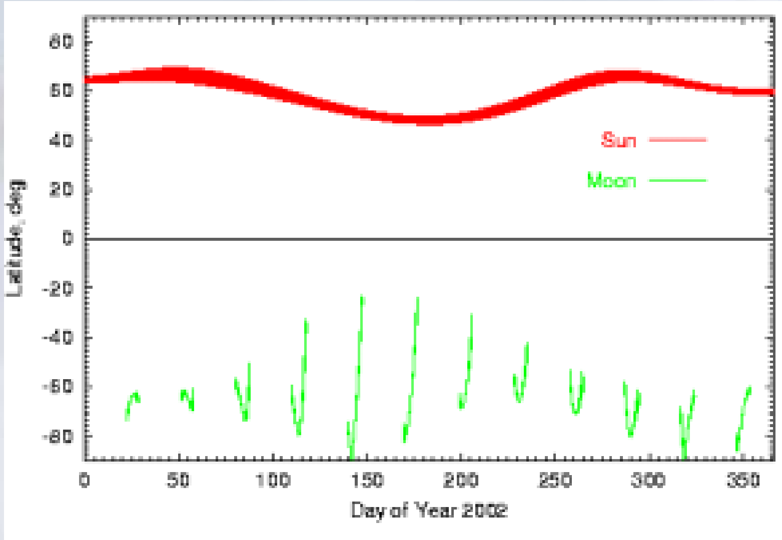
SCIAMACHY First In-Flight WLS Spectra from Orbit 252

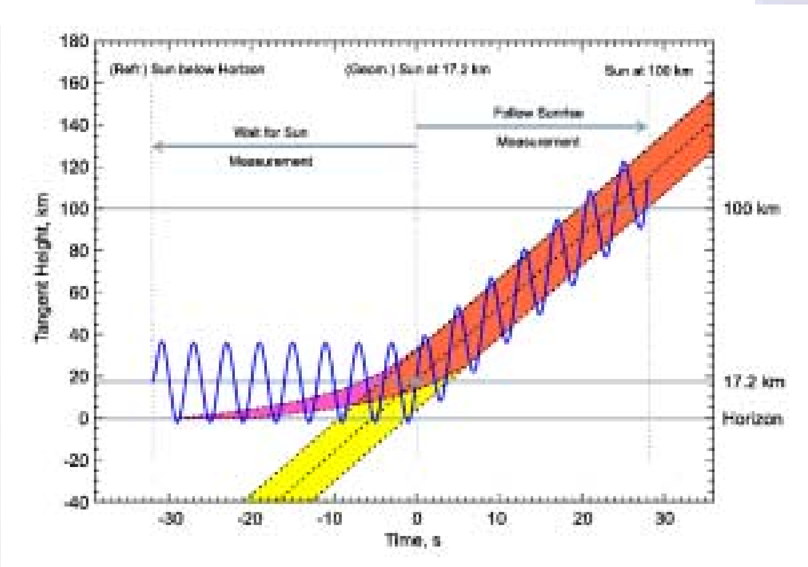





OCCULTATION MEASUREMENTS
SCIAMACHY
Sun/Moon
Earth

Occultation Measurements





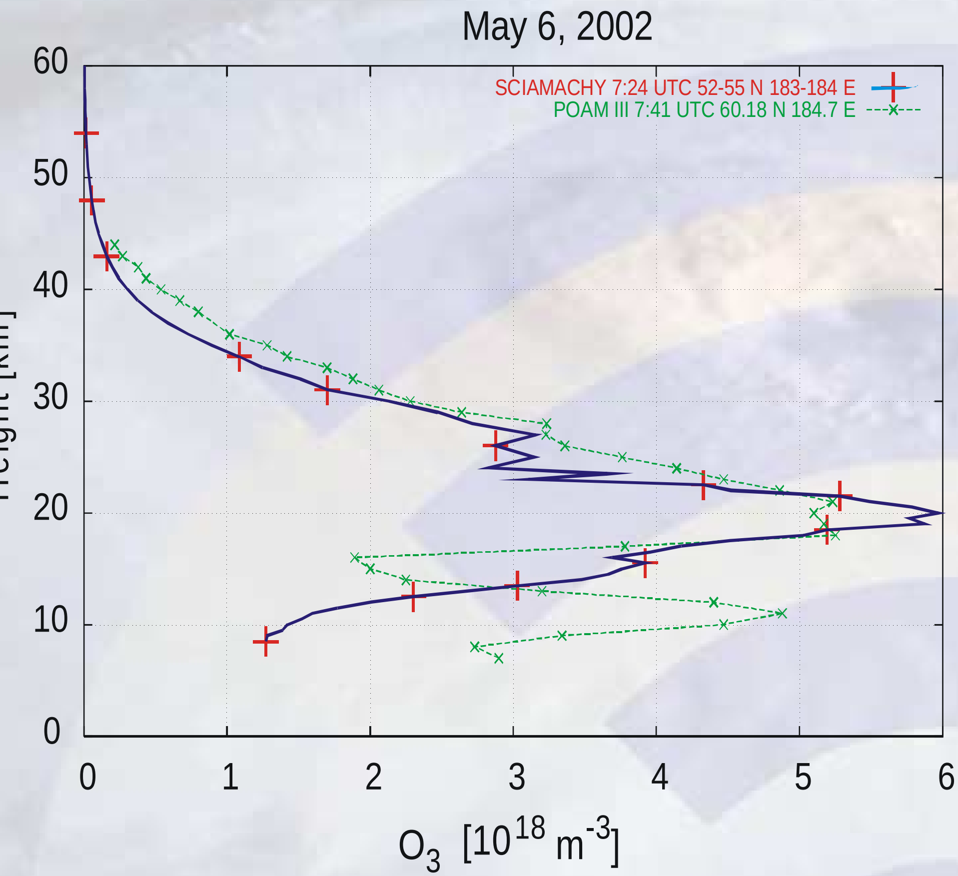
Solar occultation:

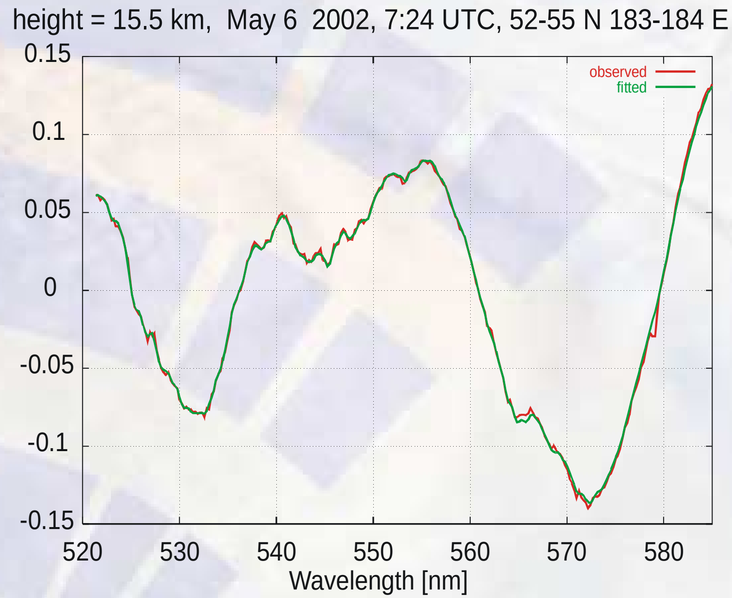
- **Measurements during sunrise (scans over sun)**
- **Once per orbit**
- **Vertical res.: 2.6 km**
- **Horizontal azimuth: 30 km**
- **Horizontal in-flight: 400 km**
- **NH, 65°S-90°S**

Lunar occultation:

- **Measurements during moonrise**
- **Moon only visible for about one week per month (highly variable)**
- **SH, 30°S- 90°S**

O_3 Profile from Solar Occultation compared to POAM III

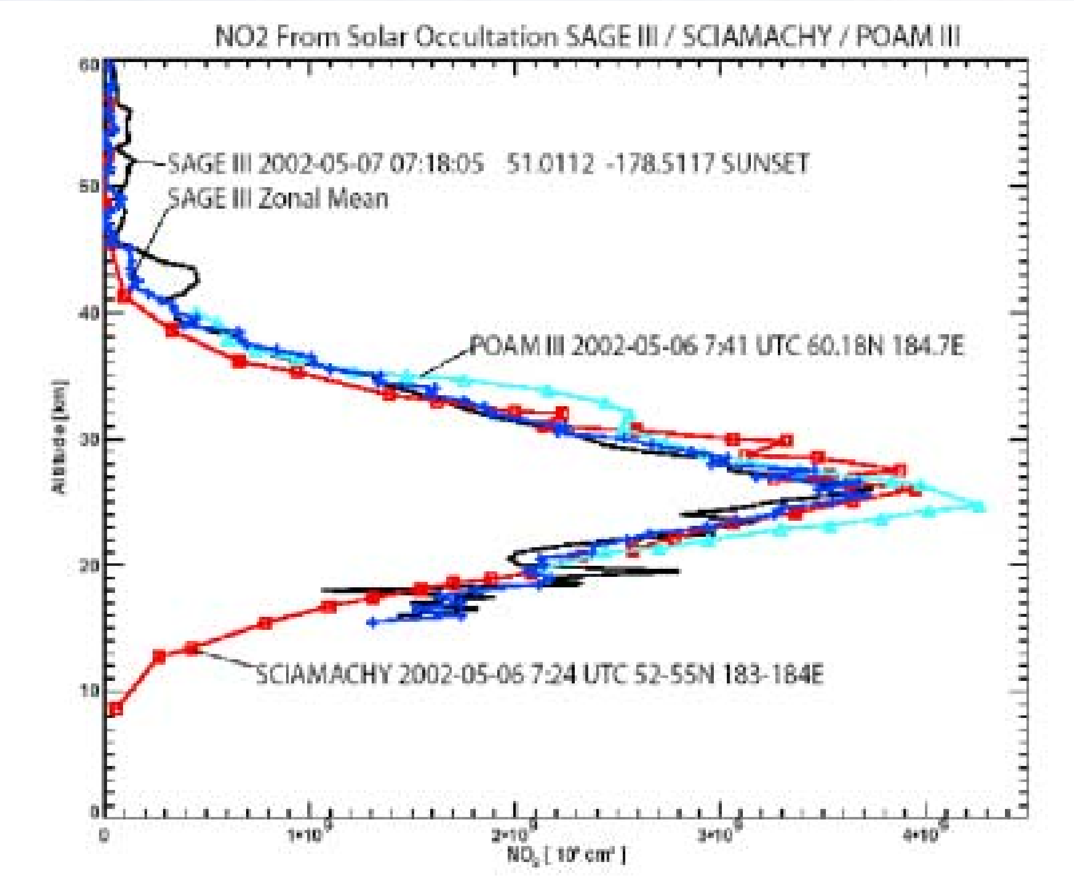




J. Meyer & A. Schlesier 07/2002

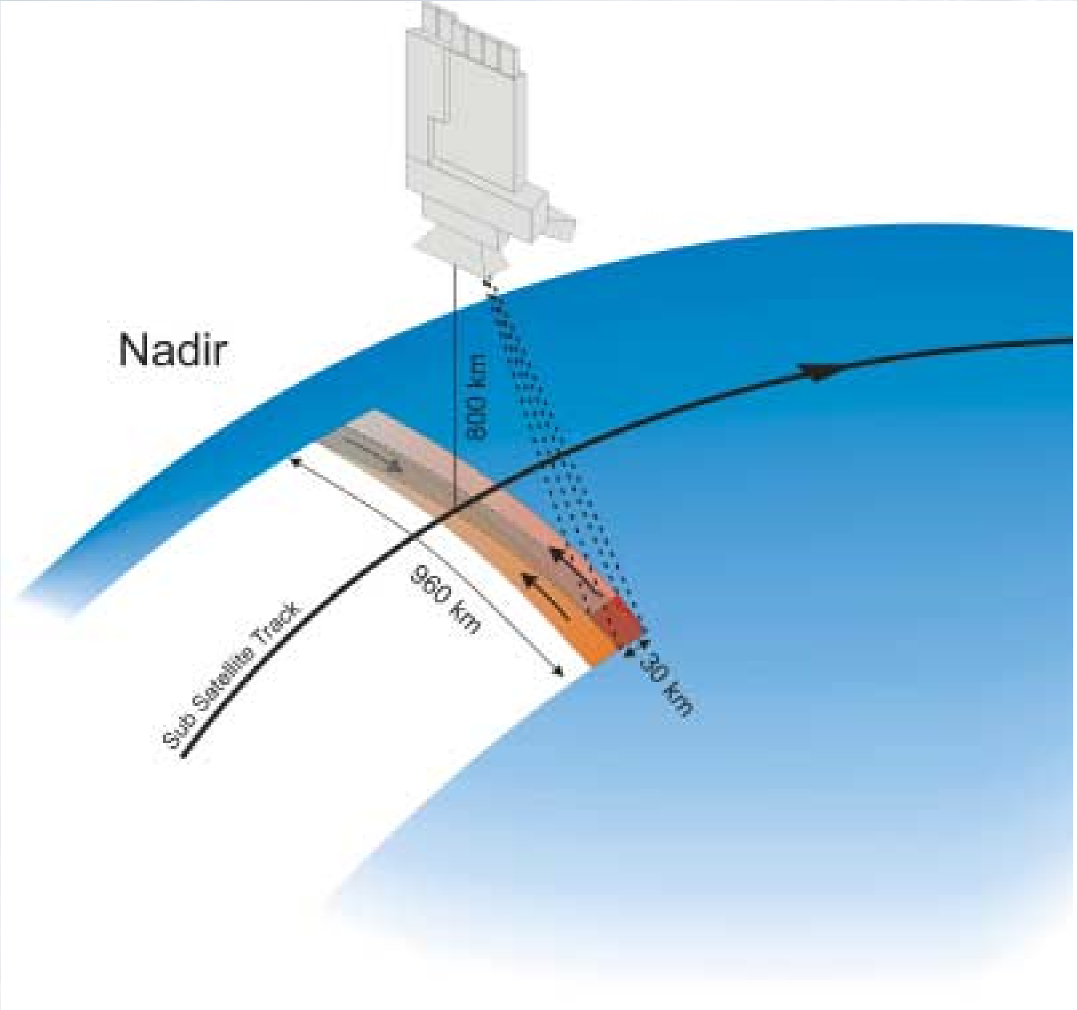
Preliminary results!

NO_2: SAGE III / SCIAMACHY / POAM III



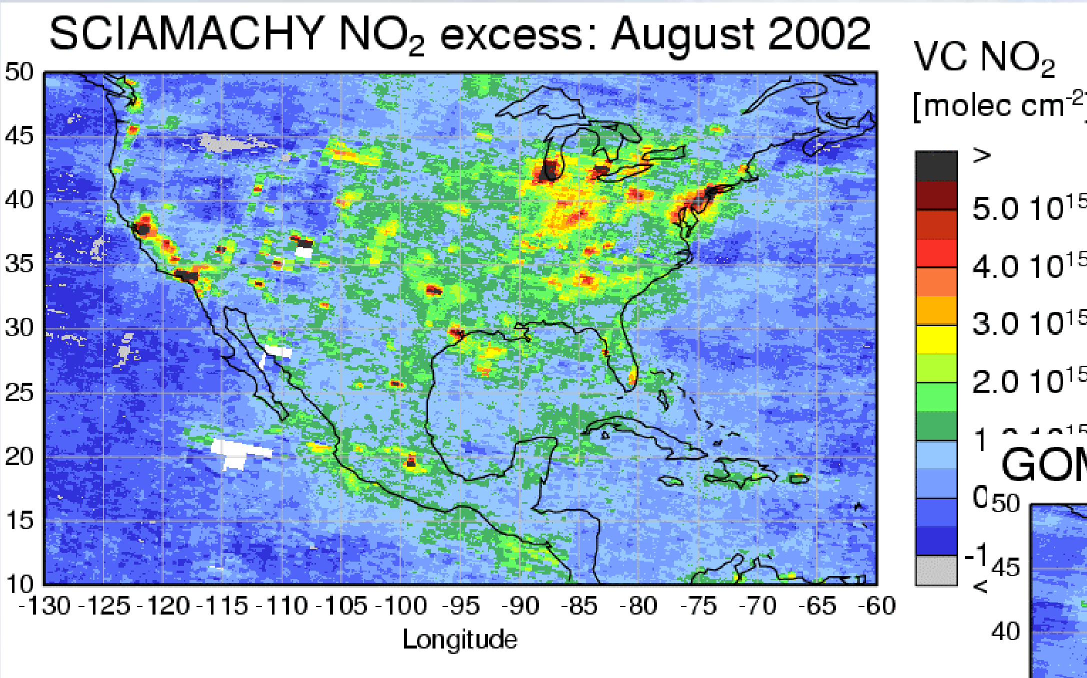
Preliminary Data

Nadir Geometry



- horizontal resolution in across track:
  - 30 - 240 km
  - (60 km typ.)
  - 960 km swath
- horizontal resolution in along track:
  - 30 km
- Observation optimised to match limb with nadir measurements
- Duration of Limb sequence: 60 sec.
- Global coverage: 6 days at the equator

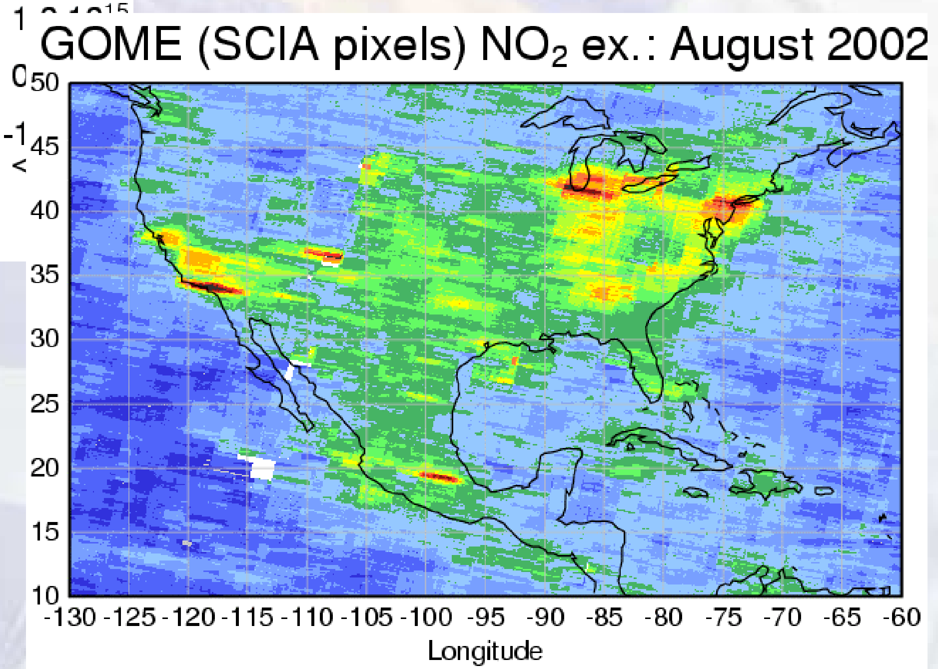
Effects of spatial resolution US



Maximum values

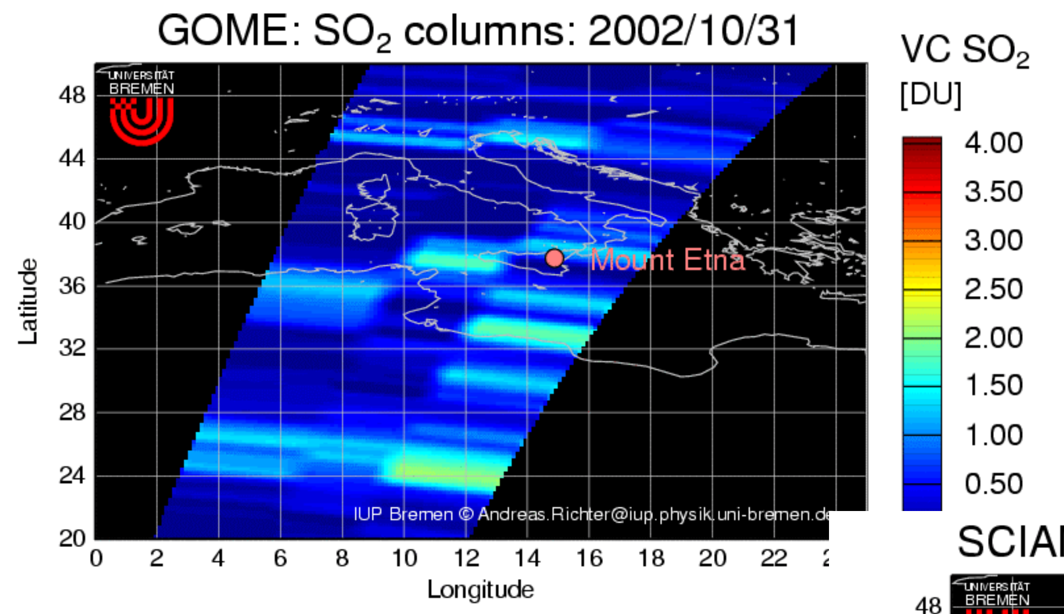
GOME 7E15 molec/cm2

SCIA 17E15 molec/cm2

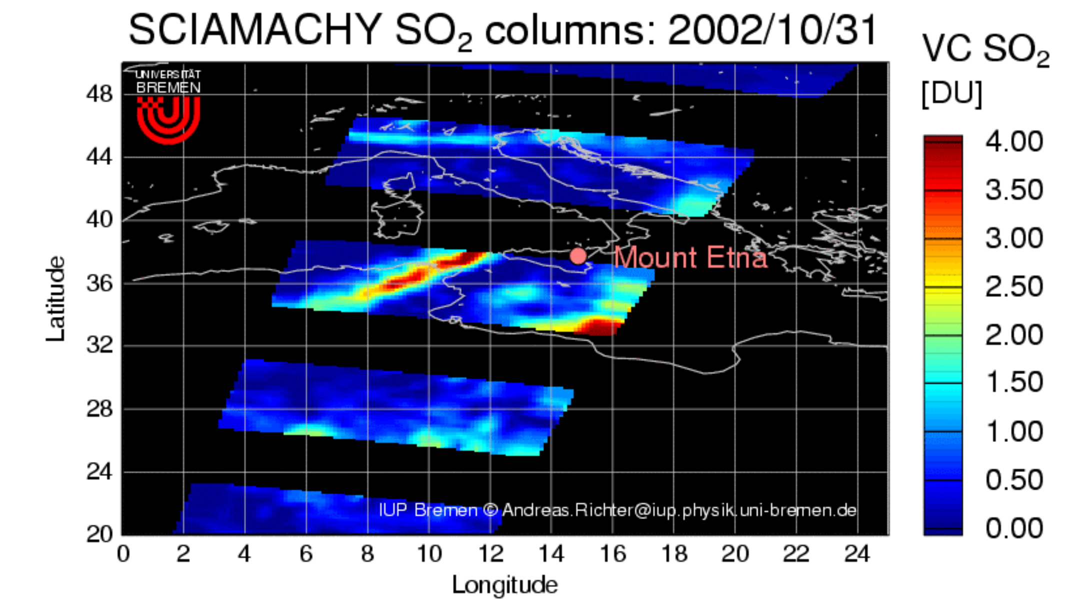


- **GOME: only pixels with corresponding SCIA measurements**
- **SCIA: all available raw data for August 2002**

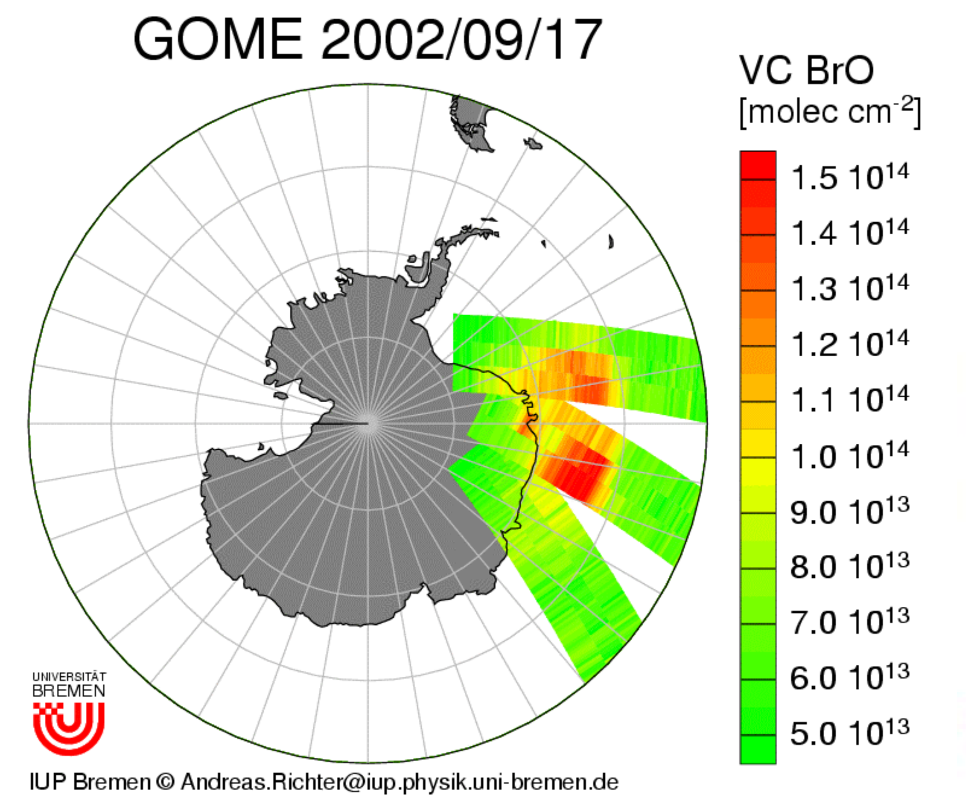
SO_2 from Mount Etna October. 2002

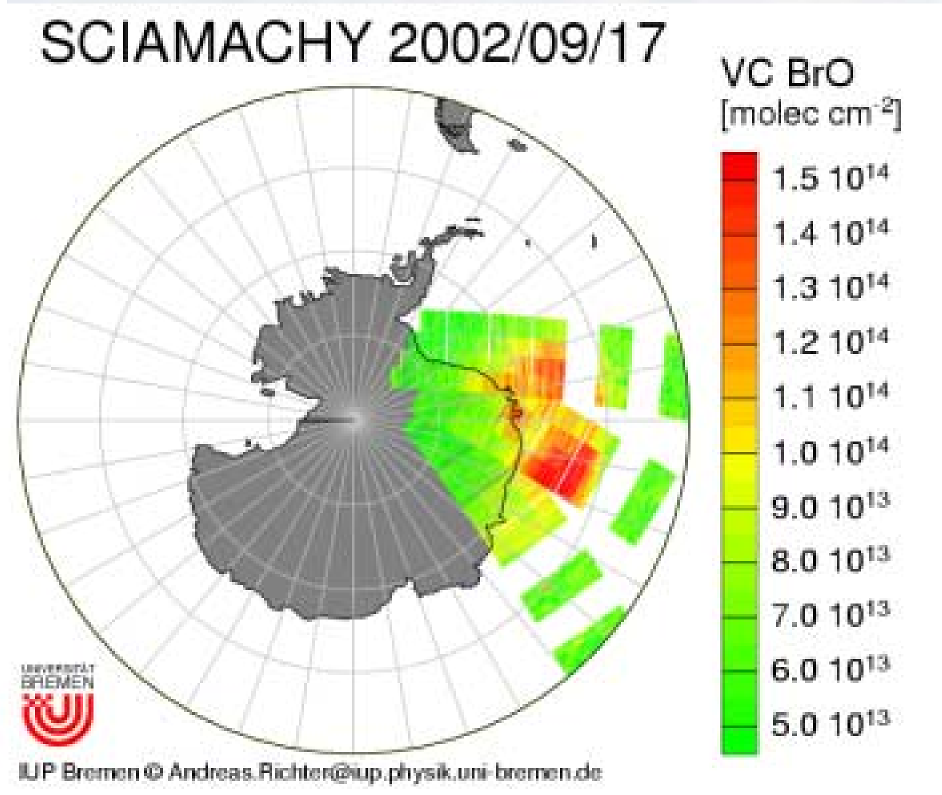


- **good general agreement of values**
- **much better spatial resolution possible over regions with high values**

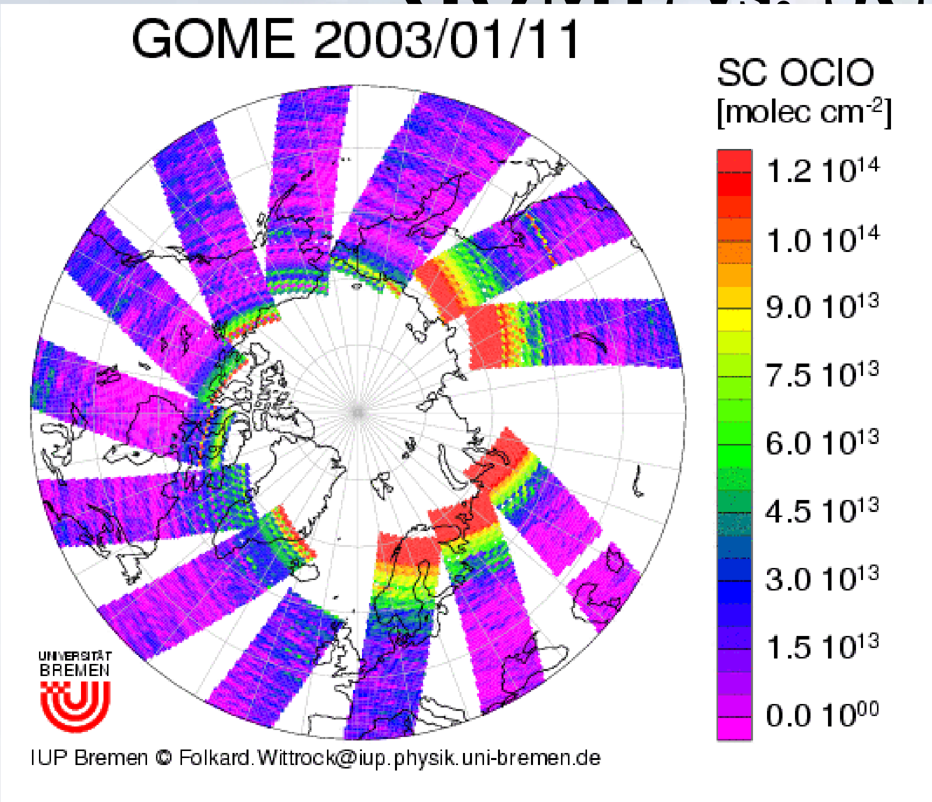


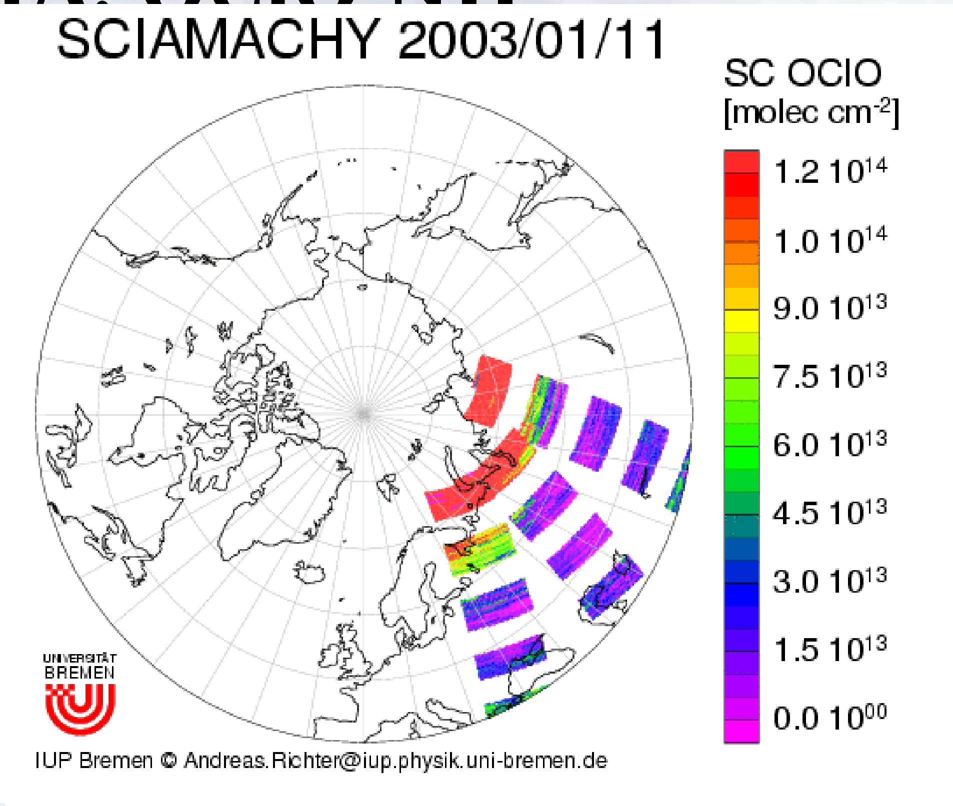
GOME-SCIA: SH BrO





GOME vs. SCIA: OClO NH





- **High chlorine activation within NH polar vortex 2002/2003**
- **SCIA measures approx. 30 min. earlier than GOME**

Why do we need accurate RTM?

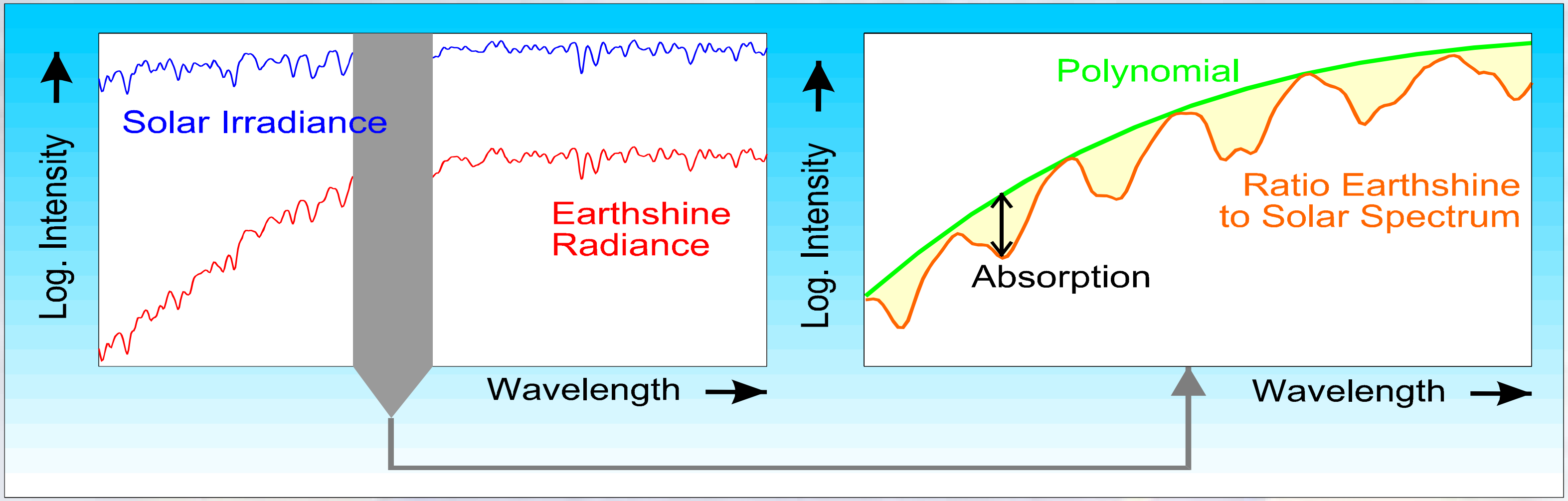
The Radiance observed at TOA comprises, the extra terrestrial irradiance modified by absorption and scattering along the path of light within the atmosphere.

Key Issues: Wavelength dependent of

i) Surface Spectral Reflectance

ii) Multiple scattering.

DOAS made simple!



Derive the Slant Column Amount of species i:

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

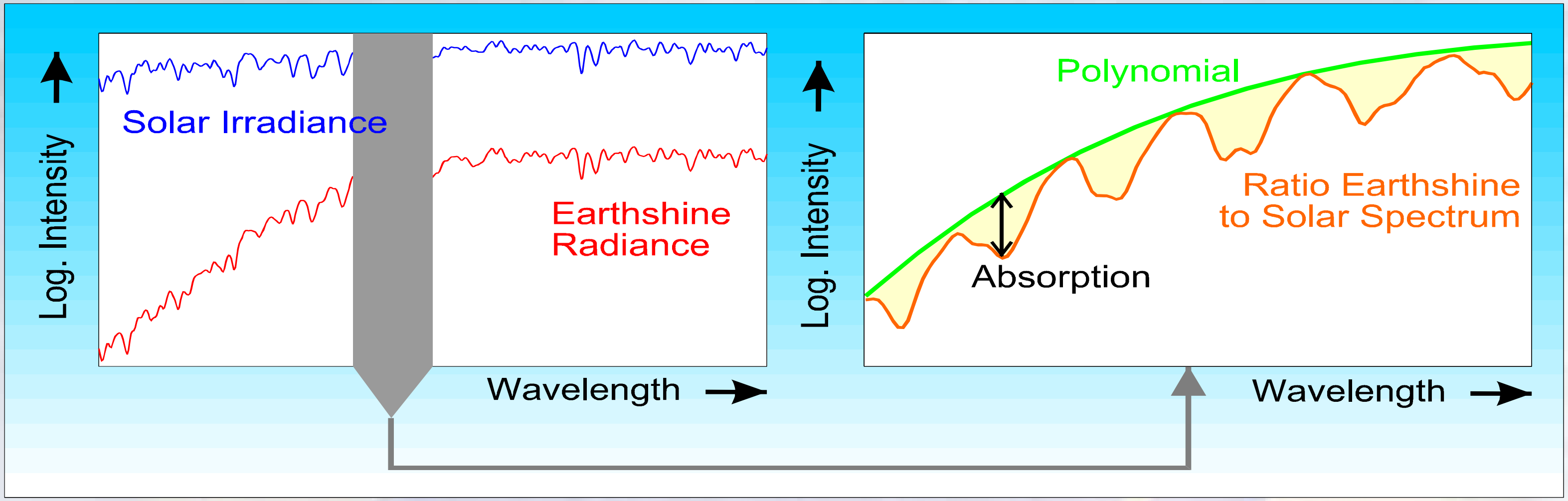
$$SC_i = \Sigma_{\lambda}(c_i\, l_{\lambda})$$

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)!



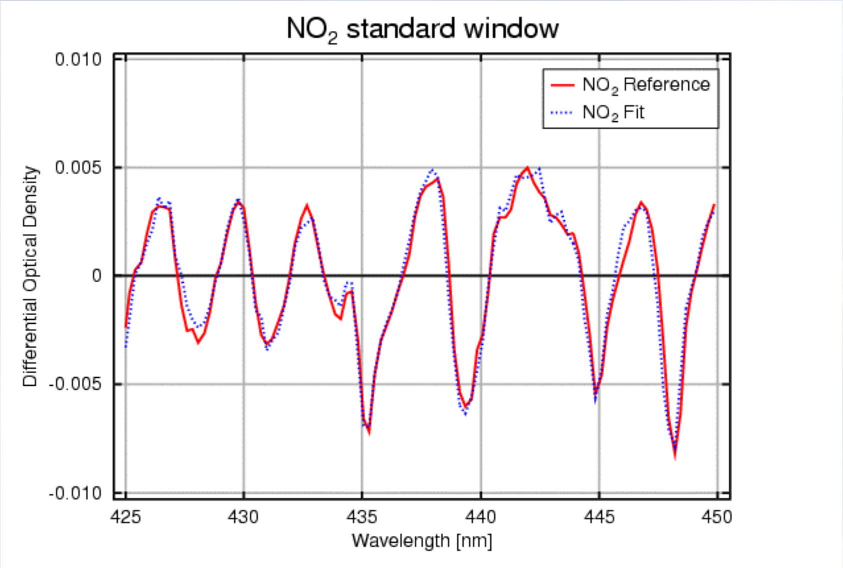
VC = SC/AMF

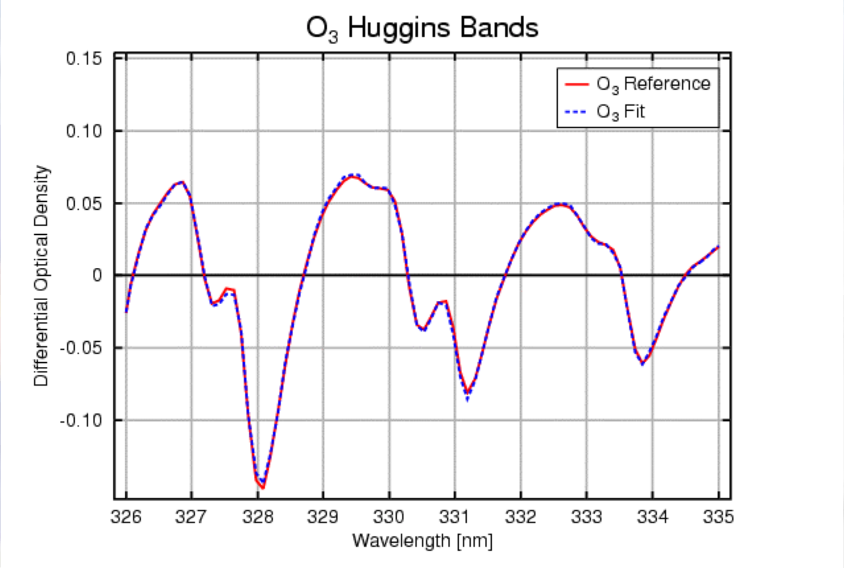
The AMF must be derived using a Radiative Transfer Model – RTM.

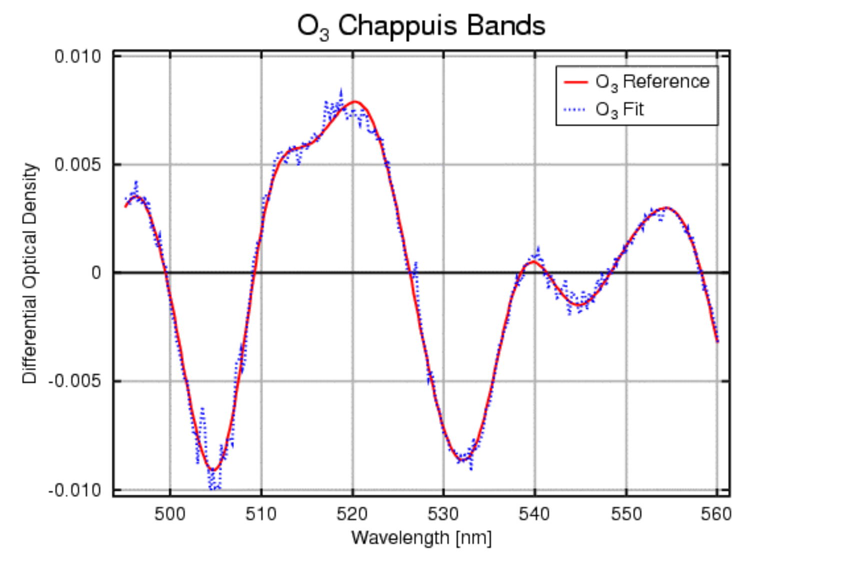
The RTM describes the path of light through the Atmosphere.

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

First SCIAMACHY Nadir Spectral Fits



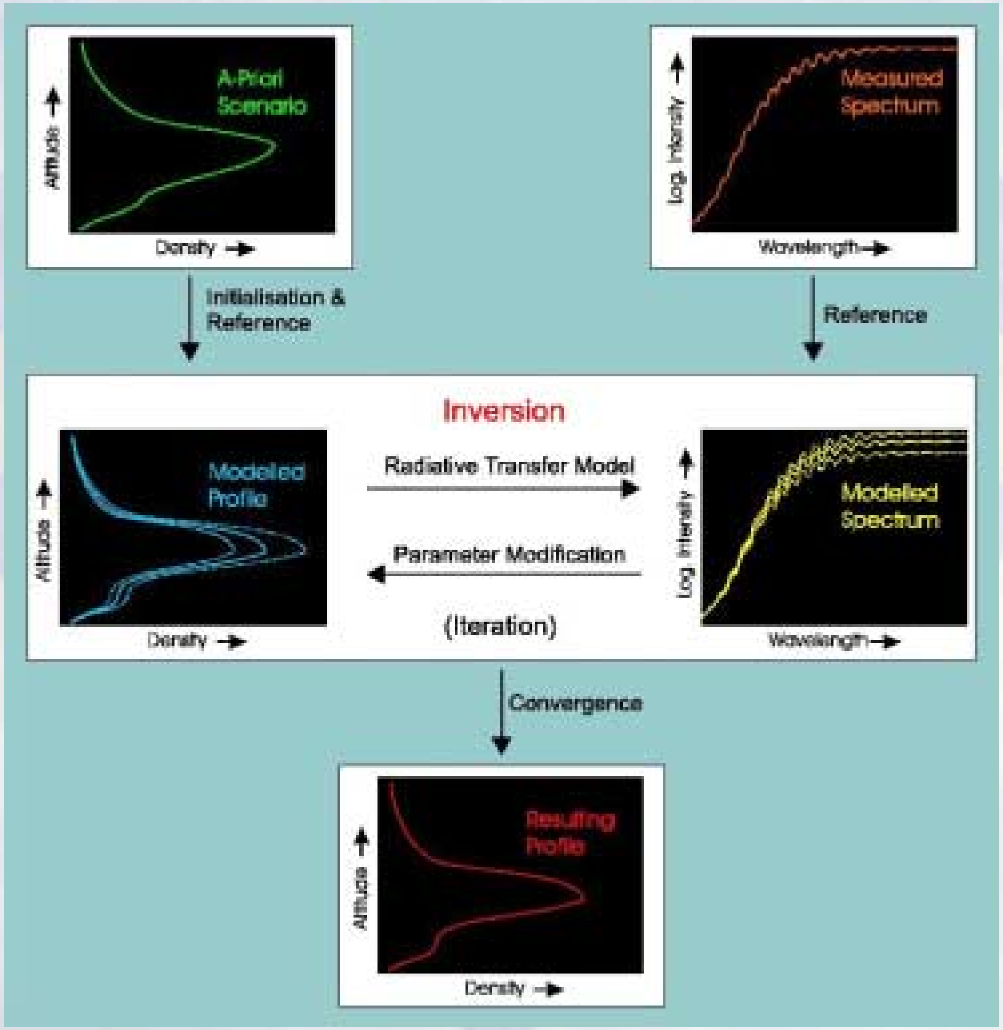




date: 20/06/2002
location: 67.6°N, 20°E
SZA: 80.5°
uncalibrated raw data (lv0)
DOAS analysis using GOME settings

Richter et al., 07 / 2002

FURM



A-Priori Scenario
Altitude
Density
Measured Spectrum
Log. Intensity
Wavelength
Initialisation & Reference
Reference
Inversion
Modelled Profile
Altitude
Density
Radiative Transfer Model
Parameter Modification
(Iteration)
Modelled Spectrum
Log. Intensity
Wavelength
Convergence
Resulting Profile
Altitude
Density

Optimal Estimation

Measurement

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

RTM

Climatology

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

Instrument modell, measurement errors

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

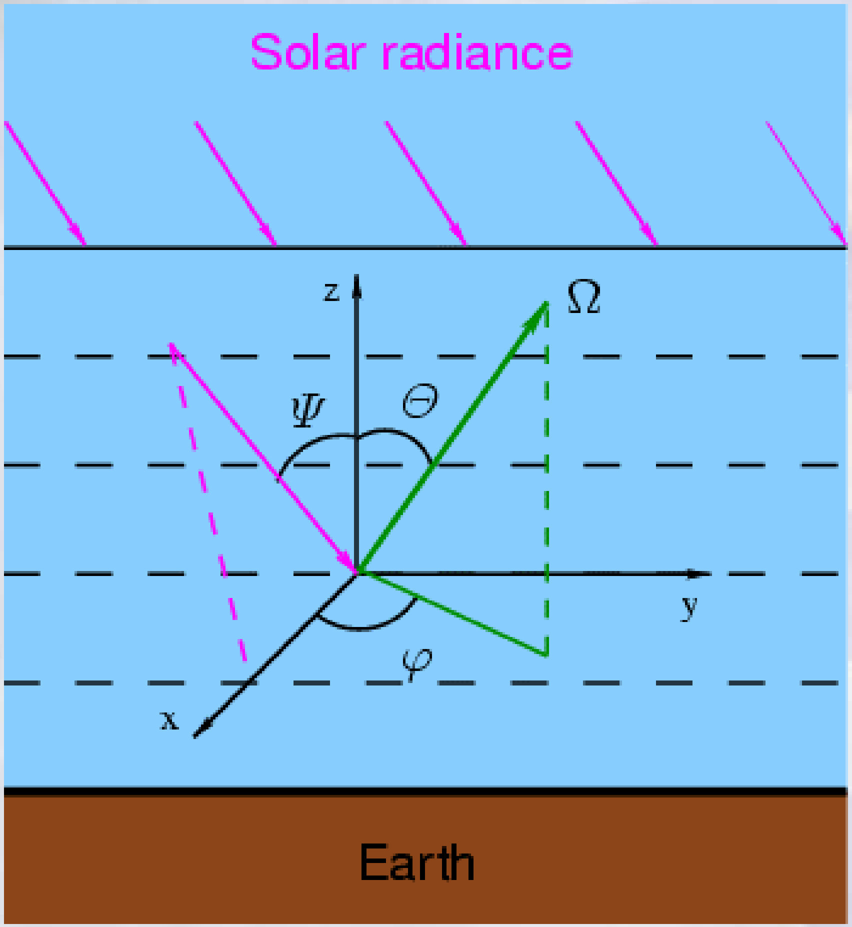
$\mathbf{y}$: measurement vector, measurement covariance $\mathbf{S}_y$

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

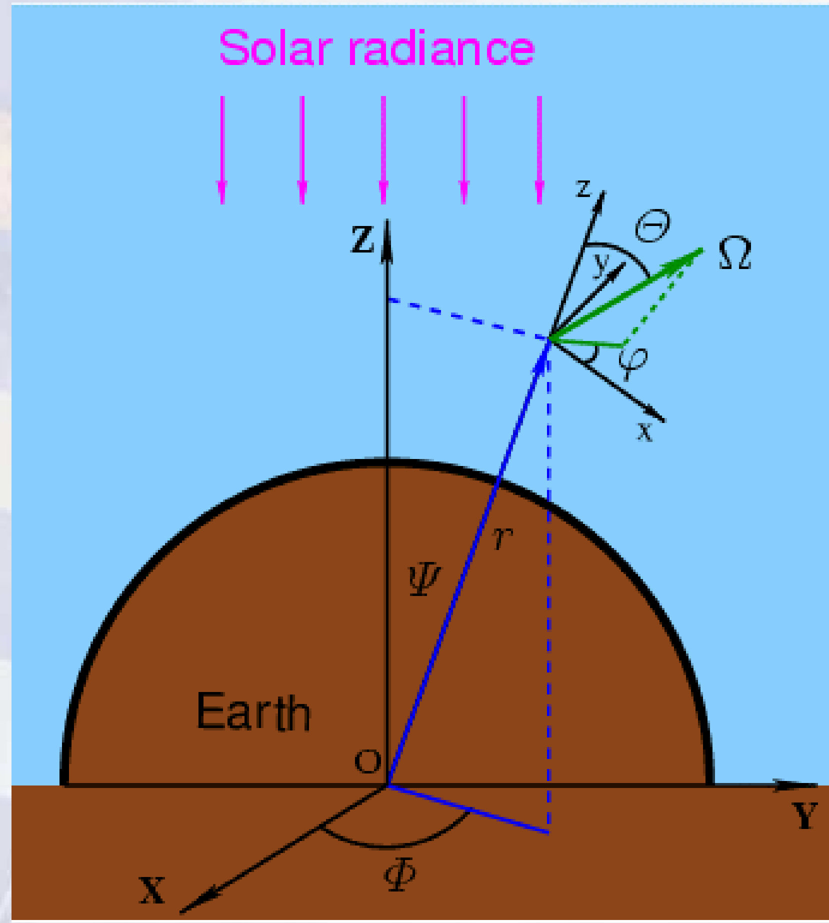
$\mathbf{K}$: weighting function, from RTM

Coordinate systems

Plane-parallel atmosphere

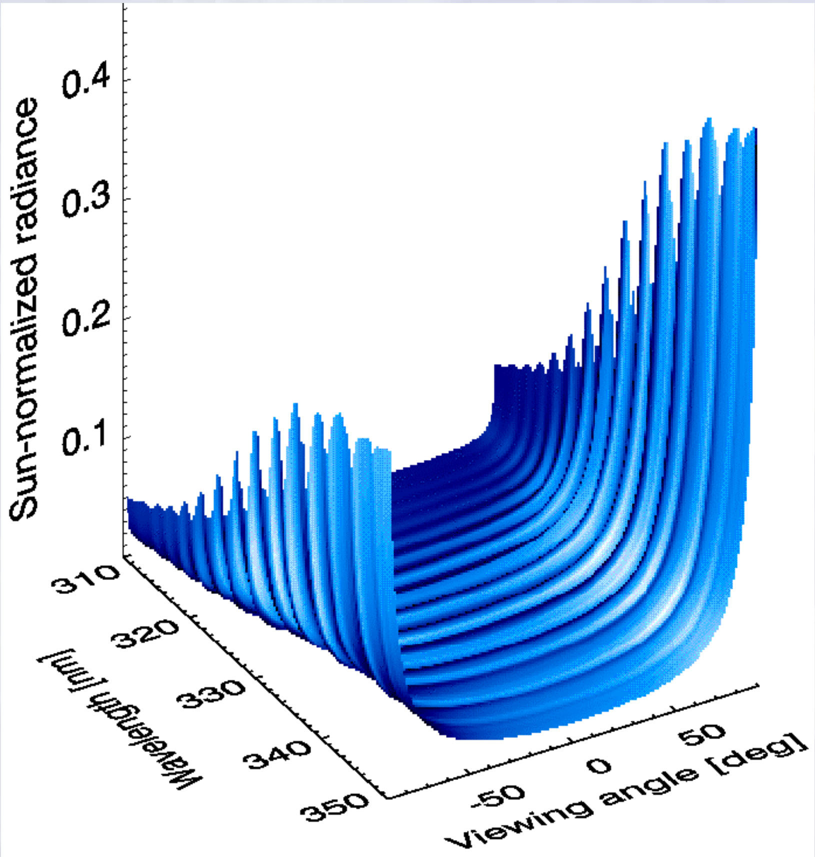


Spherical atmosphere

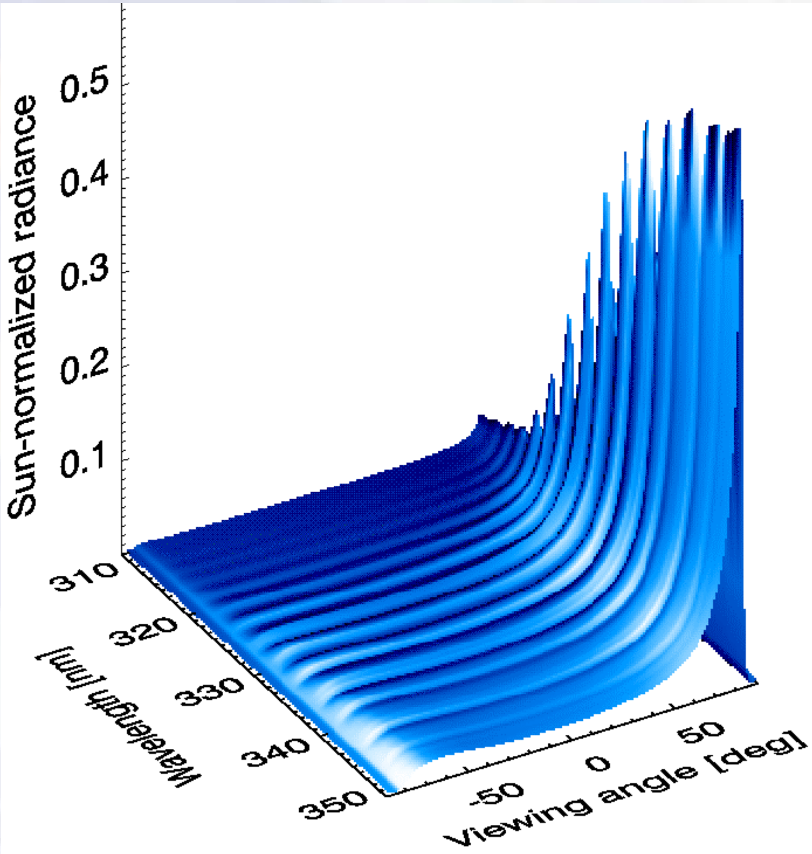


Outgoing radiation at SZA = 89 deg

Pseudo-spherical model



Spherical model



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

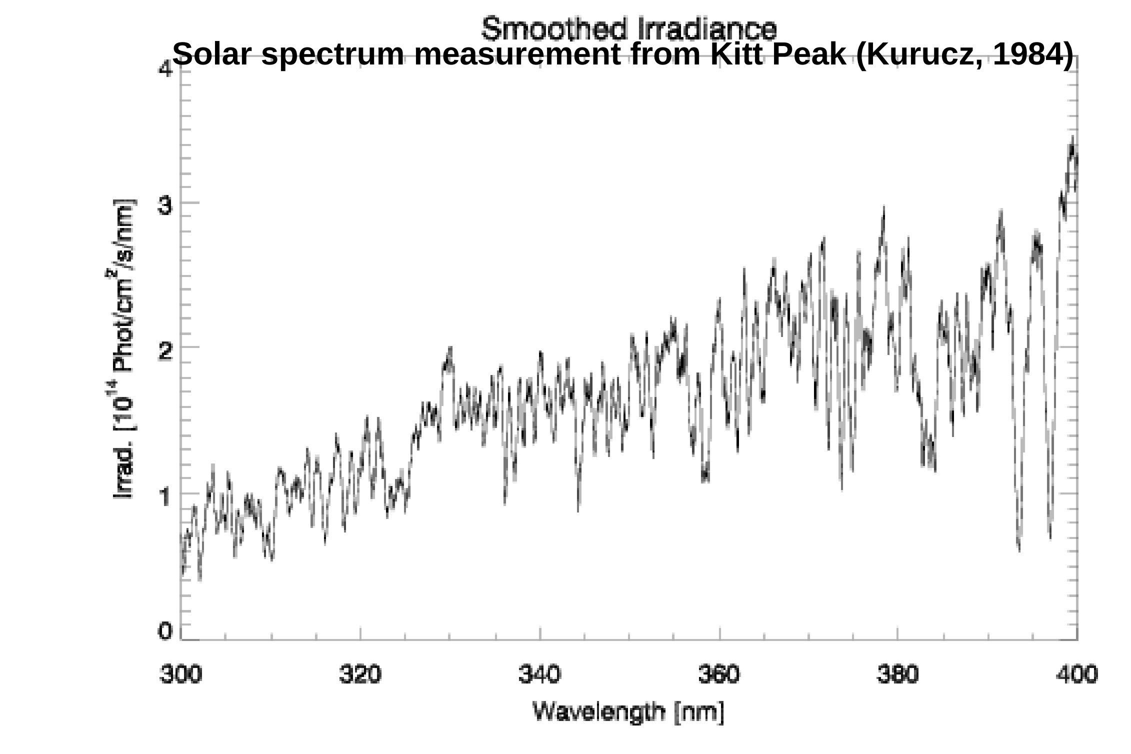
- GOME / SCIAMACHY (near-nadir geometry)
- Ground-based DOAS (near-zenith geometry)

PHOTOST

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

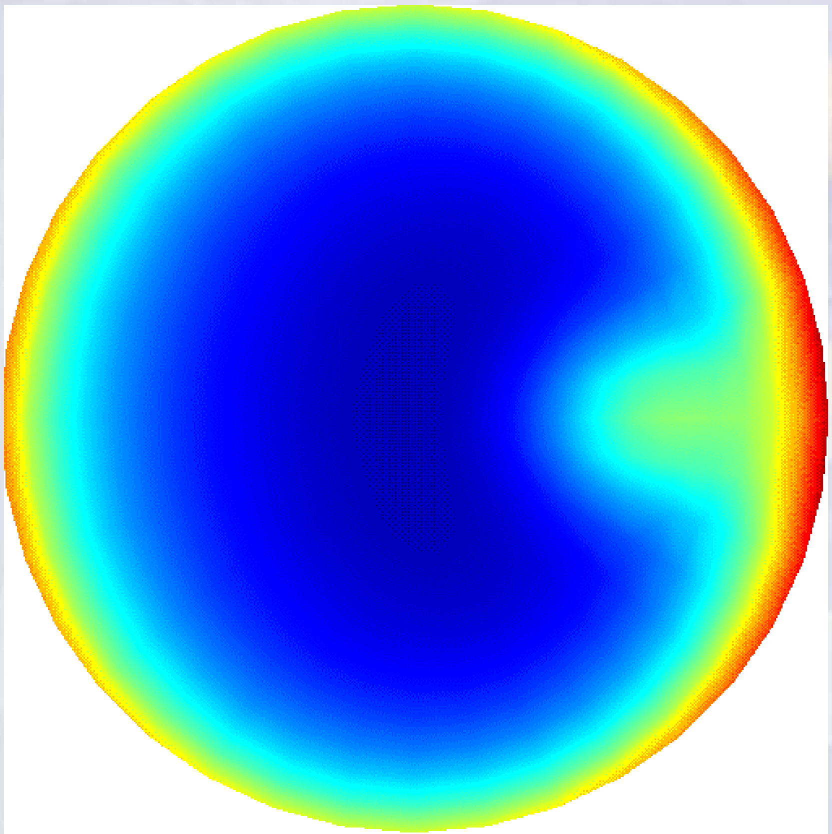
Solar Spectrum

- **The Solar spectrum consists out of a Planck emission Spectrum (T~ 5800 K) and superimposed line-structure.**
- **The line structure appears in absorption and emission – Fraunhofer Lines**
- **A section of the solar spectrum with strong Fraunhofer variability can be found in the**

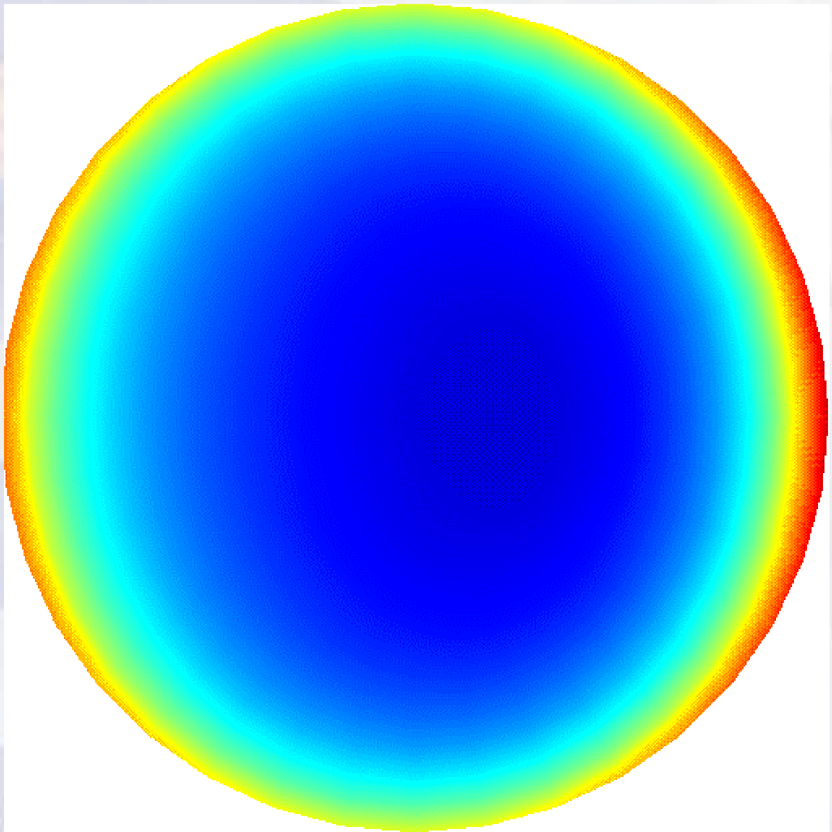


Sun-normalized radiance at TOA (SZA = 40 deg)

Ocean



Lambertian surface



Radiative transfer equation: Conservation of Energy/First Law of Thermodynamcs

$$\mathcal{E} = I\, d\sigma\, d\nu\, d\omega\, dt \implies d\mathcal{E} = dI\, d\sigma\, d\nu\, d\omega\, dt$$

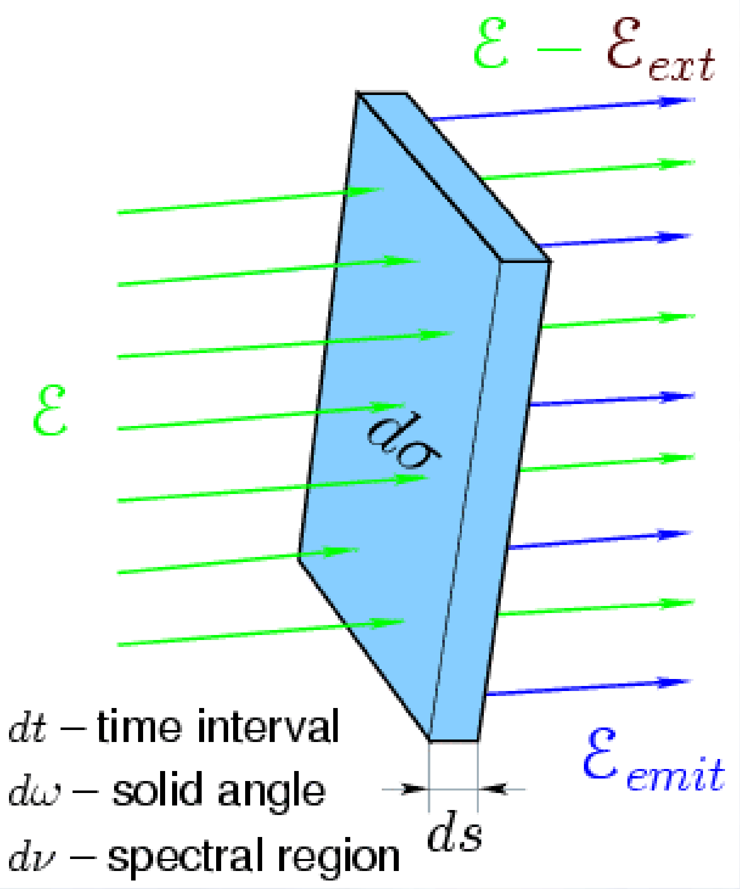
$$\mathcal{E}_{ext} = \alpha\, ds\, \mathcal{E} \implies \mathcal{E}_{ext} = \alpha\, ds\, I\, d\sigma\, d\nu\, d\omega\, dt$$

$$\mathcal{E}_{emit} = \alpha\, J\, ds\, d\sigma\, d\nu\, d\omega\, dt$$

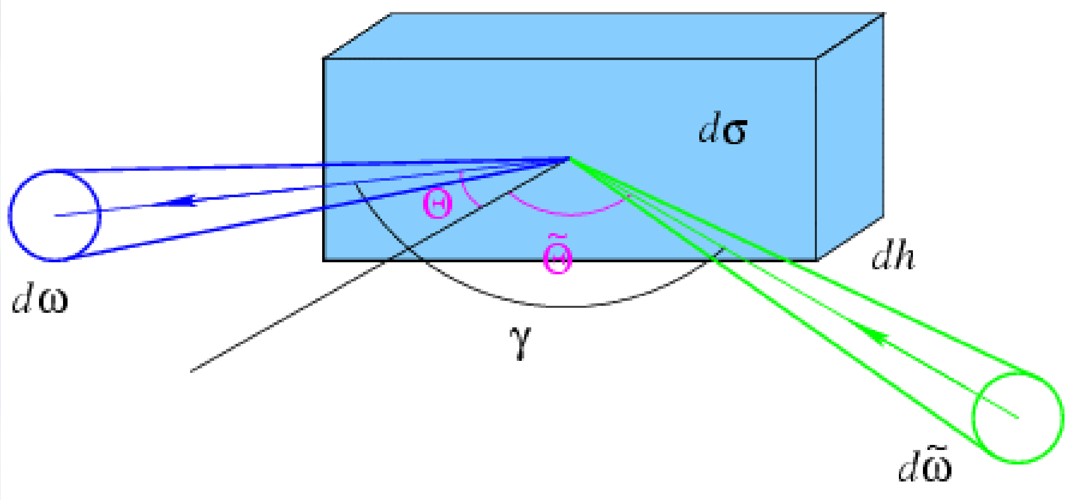
$$d\mathcal{E} = -\mathcal{E}_{ext} + \mathcal{E}_{emit}$$

$$\Downarrow$$

$$\frac{dI}{ds} = -\alpha(I - J)$$



Radiative transfer equation (source function)



$$\mathcal{E} = I\, d\tilde{\omega}\, d\sigma \cos\tilde{\Theta}$$ →

(Incoming energy)

$$\mathcal{E}_{ext} = \alpha\, ds\, \mathcal{E} = \alpha\, dh\, d\sigma\, I\, d\tilde{\omega} \quad \left(ds = \frac{dh}{\cos\tilde{\Theta}} \right)$$ →

(Total energy loss)

→ $$\mathcal{E}_{scat} = \varpi\, p(\gamma)\, \mathcal{E}_{ext}$$ →

(Scattered part of energy)

$$\varpi\, \alpha\, dh\, d\sigma \frac{d\omega}{4\pi} \int p(\gamma)\, I\, d\tilde{\omega} = \frac{\mathcal{E}_{emitt}}{d\nu\, dt}$$

(Energy gain due to scattering from all possible incoming angles)

→ $$J = \frac{\varpi}{4\pi} \int p(\gamma)\, I\, d\tilde{\omega}$$

/ Elastic scattering source function /

Elastic & Inelastic (molecular) Scattering Coefficients

Molecular Scattering coefficients

- Rayleigh scattered energy (by scattering in air) is the sum of
  - Cabannes line (unshifted) and
  - Rotational (Raman) lines (shifted).
  - Vibrational Raman in the atmosphere is weak and therefore neglected
- In standard radiative transfer models this shift is not accounted for and the scattering coefficient remains unseparated:

$$\beta_{ray}(z;\lambda) = N(z)\sigma_{ray}(\lambda) = N(z)\frac{32\pi^3(n-1)^2}{3\lambda^4 N_s^2}\frac{6+3\rho}{6-7\rho}.$$

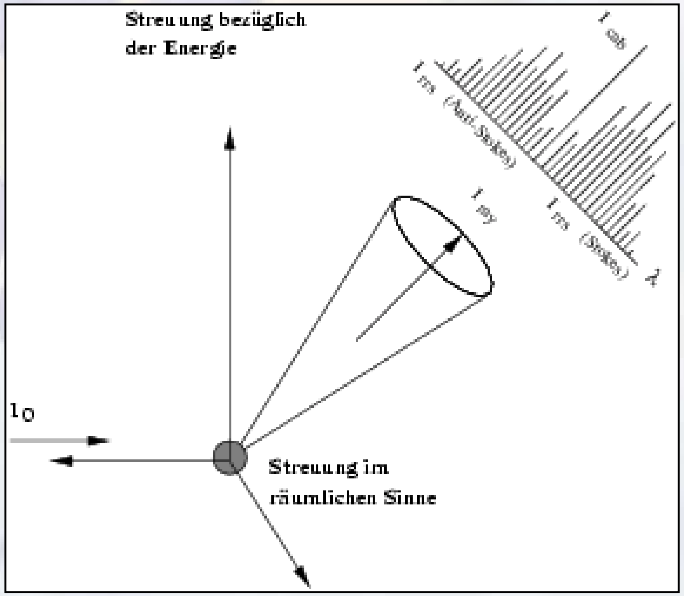
Rayleigh splits into

- Rotational Raman lines:

$$r(z;\lambda,\lambda') = N(z)\ \sigma_{rrs}(\lambda,\lambda') = N(z)\ w(J;T)\frac{256\pi^5 b_J\gamma^2}{27(\lambda+\Delta\lambda_{J\to J'})^4},$$

- and Cabannes line:

$$\beta_{cab}(\lambda) = N(z)\frac{128\pi^5}{3\lambda^4}\frac{(n-1)^2}{4\pi^2 N_0^2}.$$



Inelastic Scattering in Atmosphere and Ocean

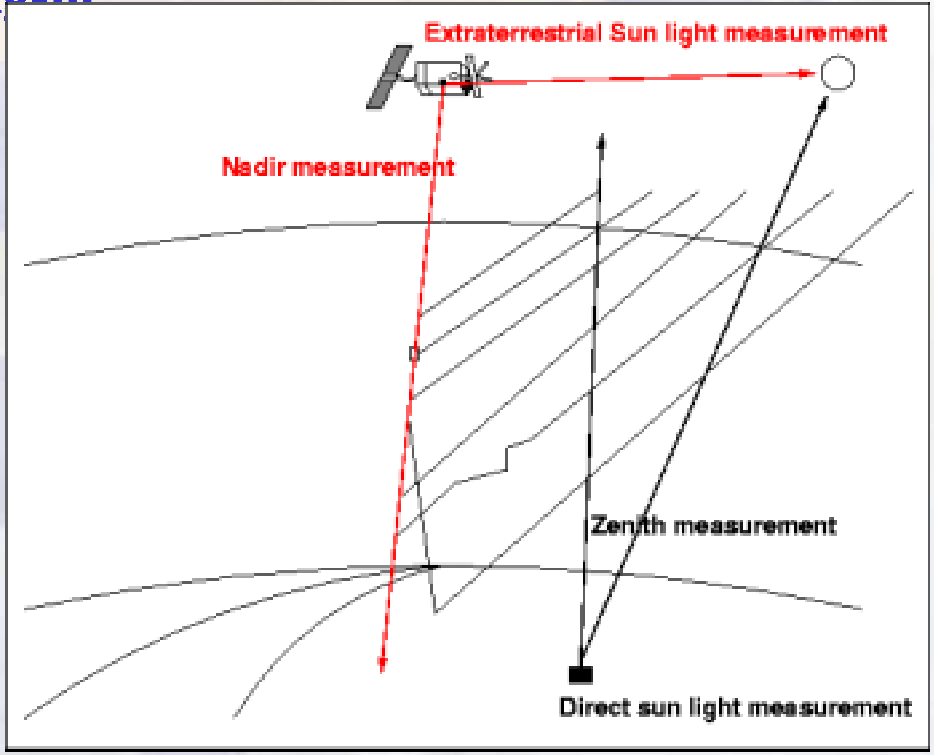
Impact on Trace Gas Retrievals

Universität Bremen ife

What is the Ring Effect?

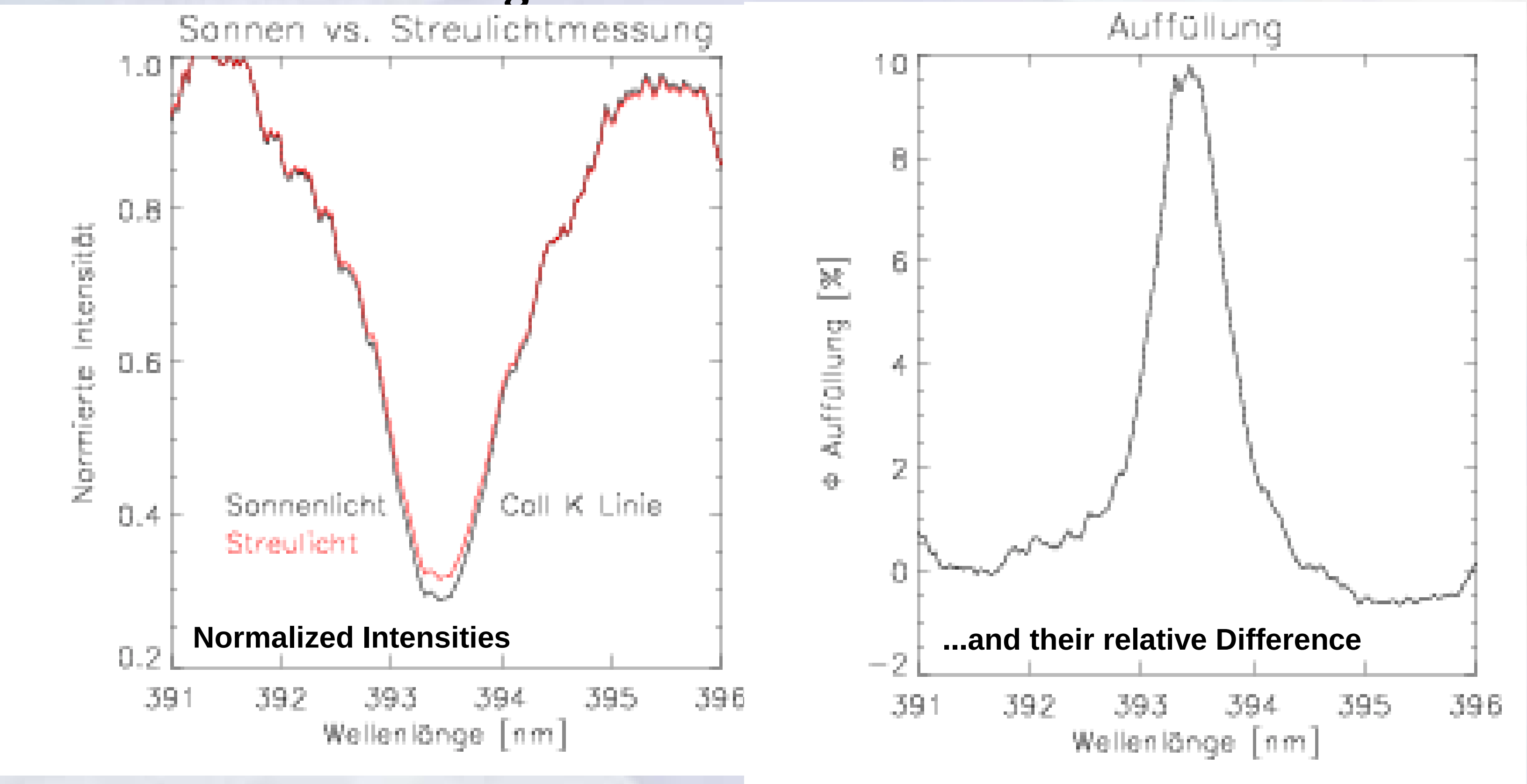
- **Solar Fraunhofer lines are different in shape comparing scattered light and direct sun light (Grainger & Ring, 1962).**
- **Usually the ratios of scattered and sun light spectra reveal an in-filling of Fraunhofer lines – Resulting spectral structure is called Ring spectrum or filling-in**

Measurement geometries



Filling-In

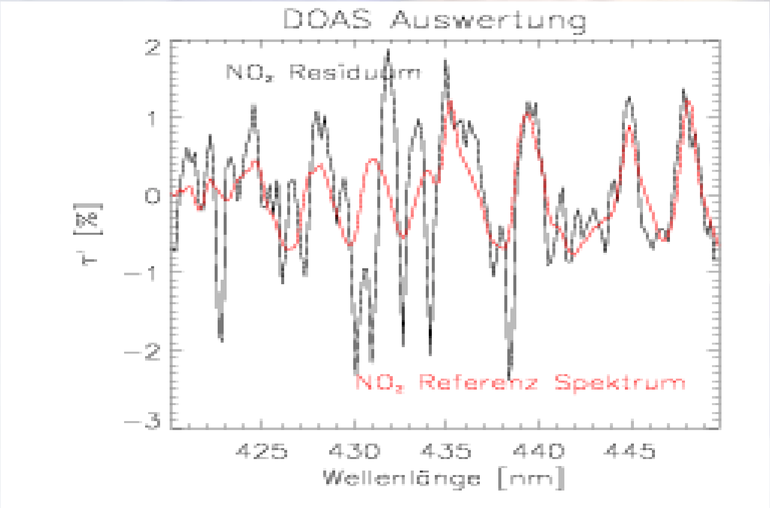
- **The deformation, or filling-in, of a Fraunhofer line is illustrated for one of the strongest Fraunhofer lines- the Ca II-K line:**



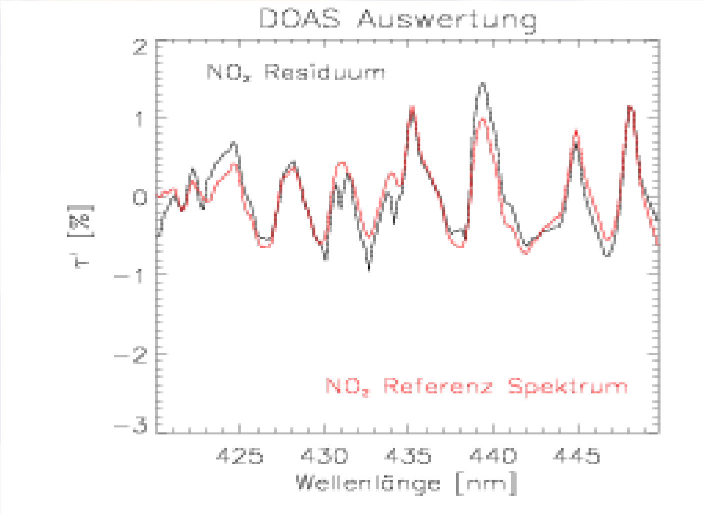
- In-filling is a relative quantity!

Why is the Ring effect important?

- **To improve our understanding of fundamental processes in planetary (not only terrestrial) atmospheres.**
- **To remove the impact of the effect on trace gas retrievals (especially in UV-Vis):**



NO_2 Retrieval without accounting for the effect



...and taking it into account

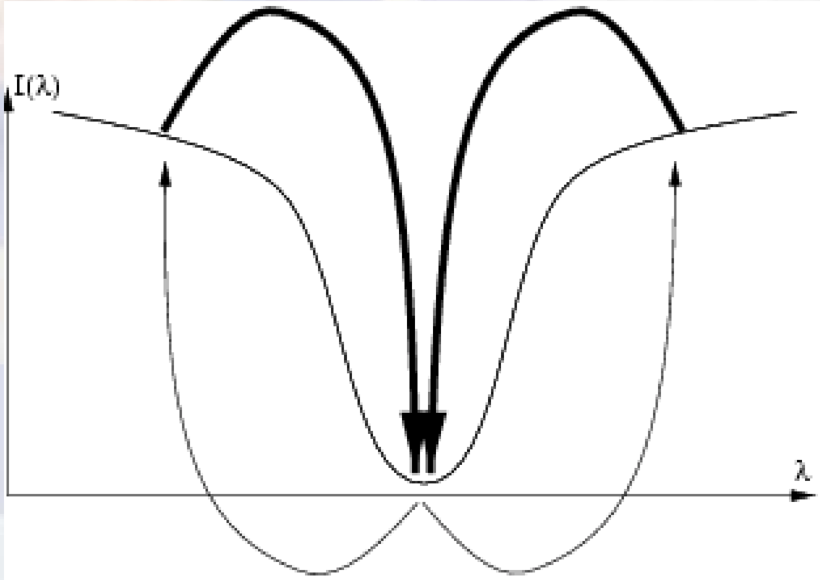
- Errors in slant column UV-Vis-retrievals from DOAS will be significant for weak absorbers and moderate for strong absorbers like Ozone.

Characteristics of Ring

- **More than fourty years of research in this area mainly show similar characteristics.**
- **Experiences are mainly based on experiments.**

Increase of	Filling in
Solar zenith angle	+
Ground Albedo	+
Wavelength	-
Clouds	+/-
Spectral Resolution	-

- Strong depolarization of line cores.

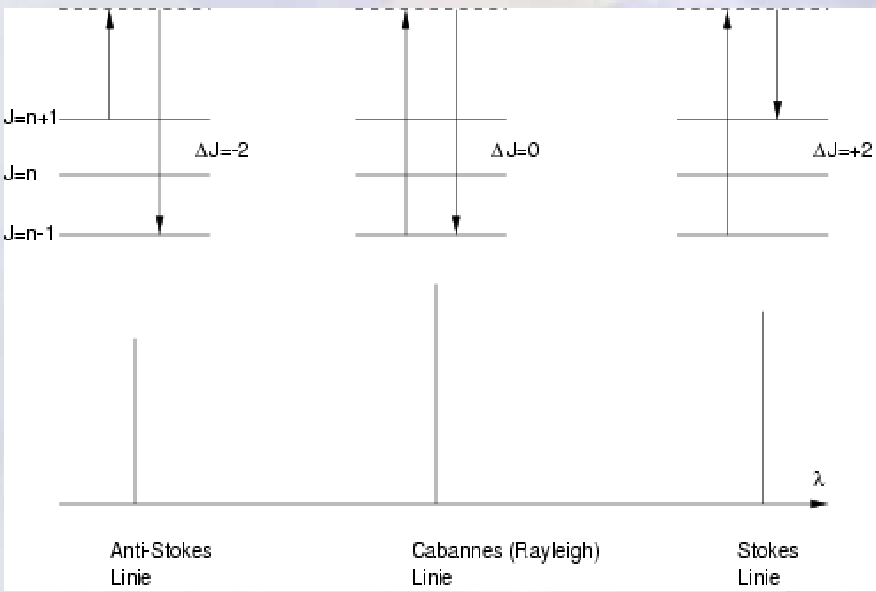


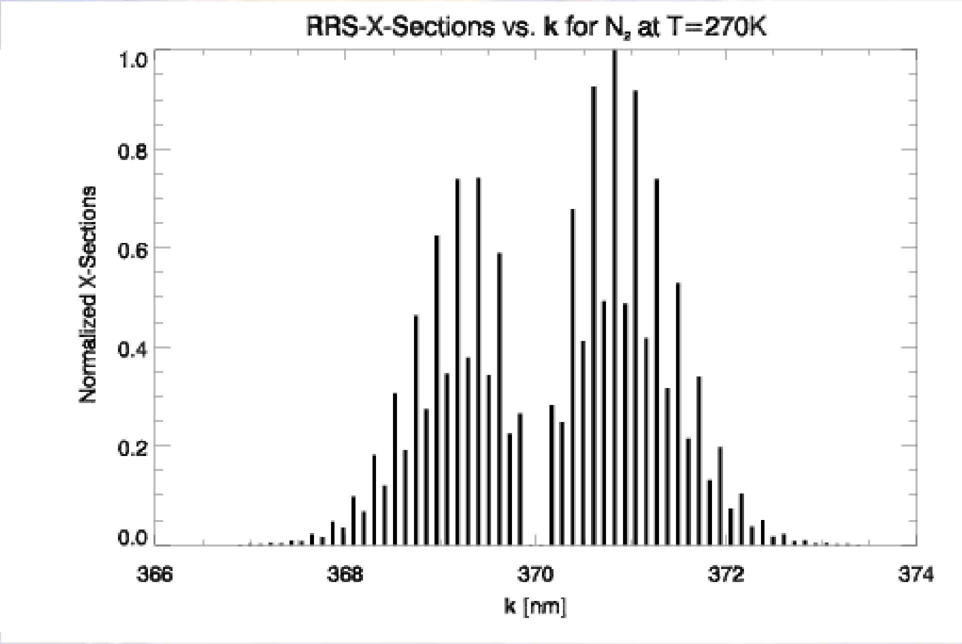
Photon redistribution

- **Rotational Raman Scattering** (RRS) at air molecules (O_2 & N_2) is the process that contributes predominantly to the filling in.

Reminder: Raman scattering

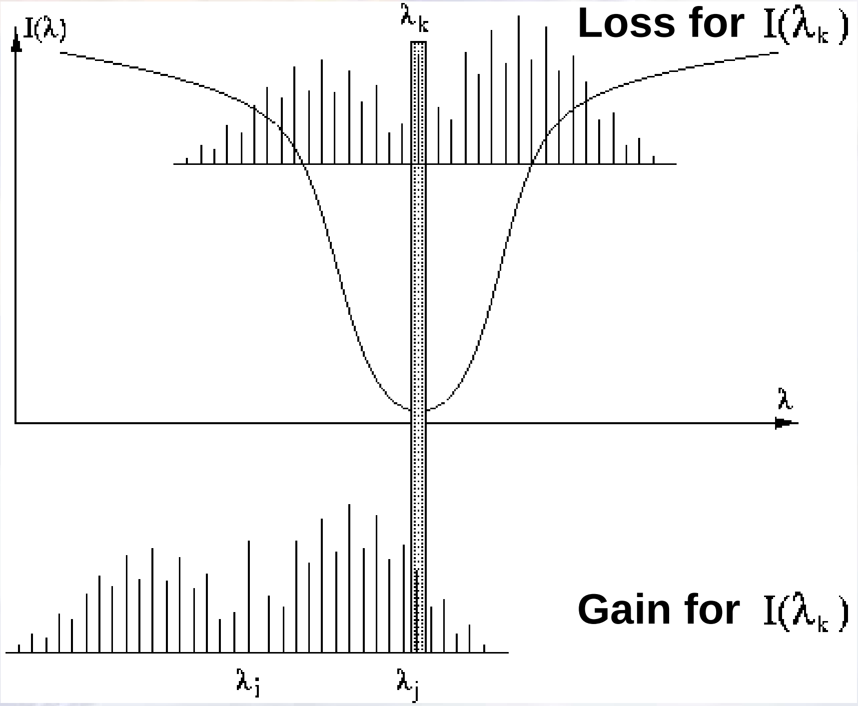
- **Stokes-Transitions**: Molecule takes part of scattered photon energy.
- **Anti-Stokes-Transitions**: Molecule adds part of its energy to scattered photon.





Filling-in by RRS

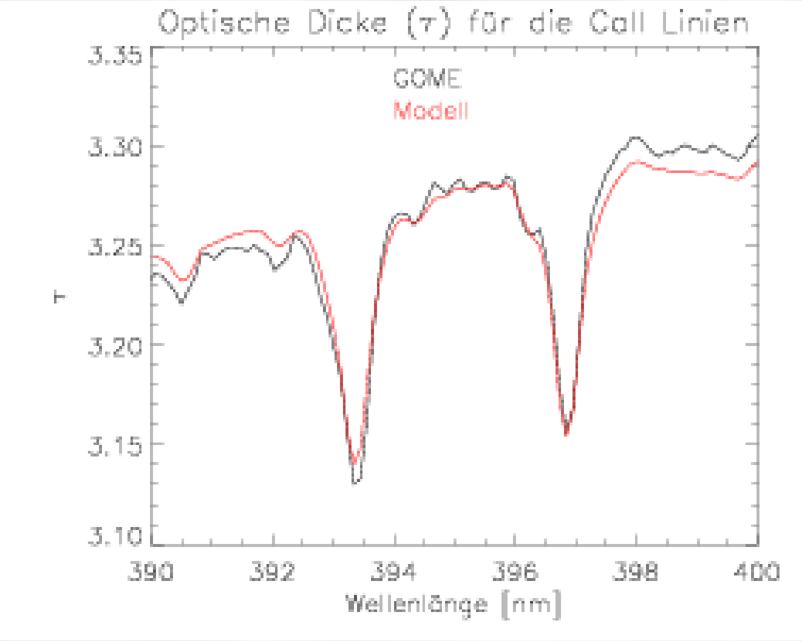
- **RRS redistribution is based on**
  - **Loss of photons at wavelength of interest by expanding the amount of light to Stokes & Anti-Stokes transitions.**
  - **Gain of photons by RRS lines (Stokes and Anti-Stokes) corresponding with the wavelength of interest.**



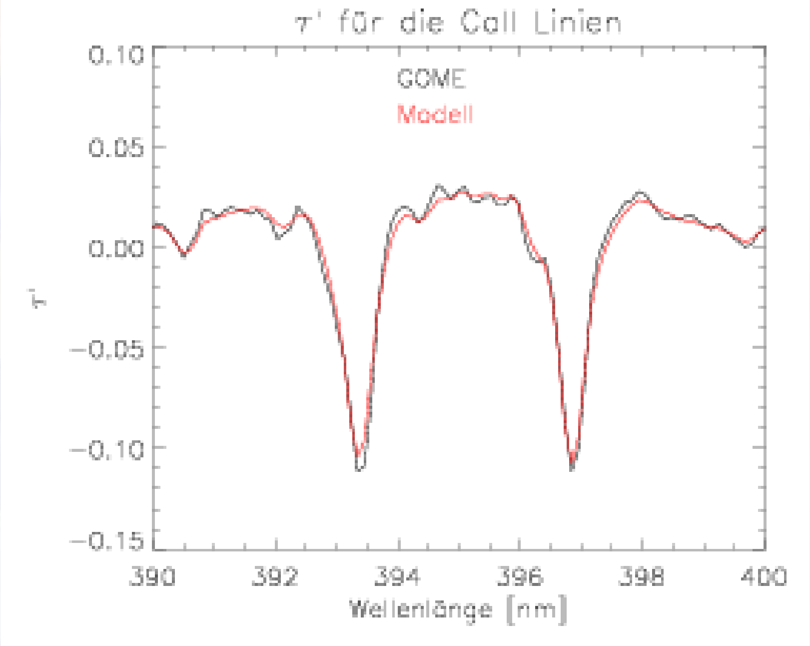
- This approach takes into account single „wavelength scattering“ but multiple spatial scattering w.r.t. (Vountas et. al., 1997)

Validation of the Model

- RRS redistribution within radiative transfer has been incorporated in Sciatran1.2
- Validation of the model with data of GOME.
- Investigation of Fraunhofer lines between 390-400 nm



Direct comparison of opt. Depth

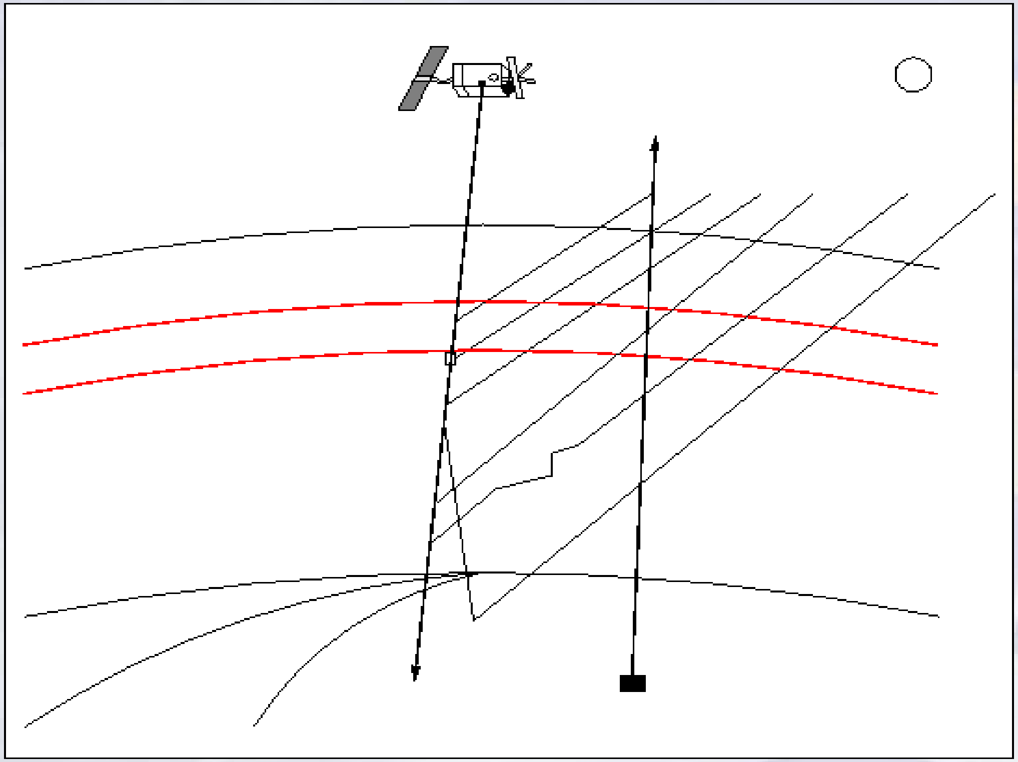


... and after removing a polynomial

- Very good agreement in a wavelength range that is dominated by Ring!

Extension of Ring: Molecular Ring

- In principle there is no difference between Fraunhofer lines and gas absorption lines.

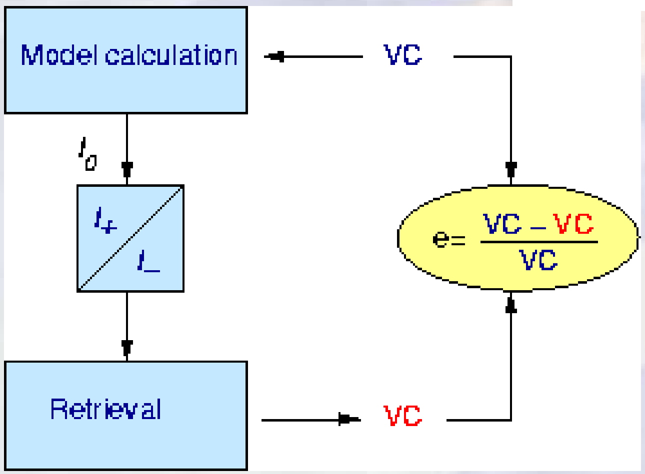


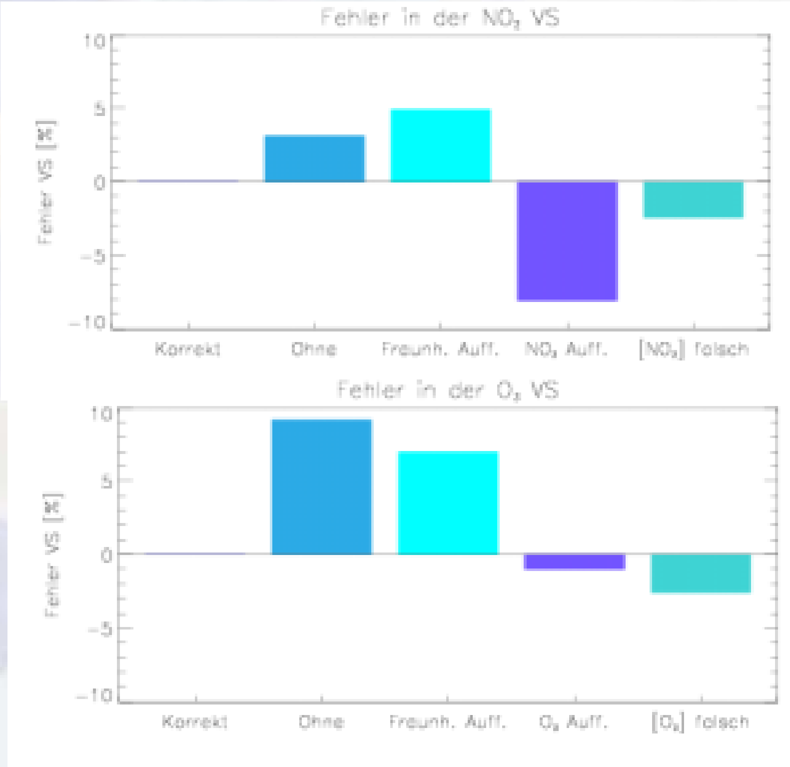
- Pure Fraunhofer Filling-in is independent of state of the atmosphere
- Filling-In of absorption lines will certainly depend on it!
- This leads to a significant problem accounting for this issue in TG-retrievals

- A separation or parameterization of „molecular Ring“ failed because of correlation. This an iterative approach is required.

DOAS Retrievals

- A clear quantitative statement about the impact of Ring on DOAS retrievals can be done only using model data
- Tests with O_3 and NO_2
- Accounting for Ring: $r_r(\lambda) = ln \frac{I^{+RRS}(\lambda)}{I^{-RRS}(\lambda)}$

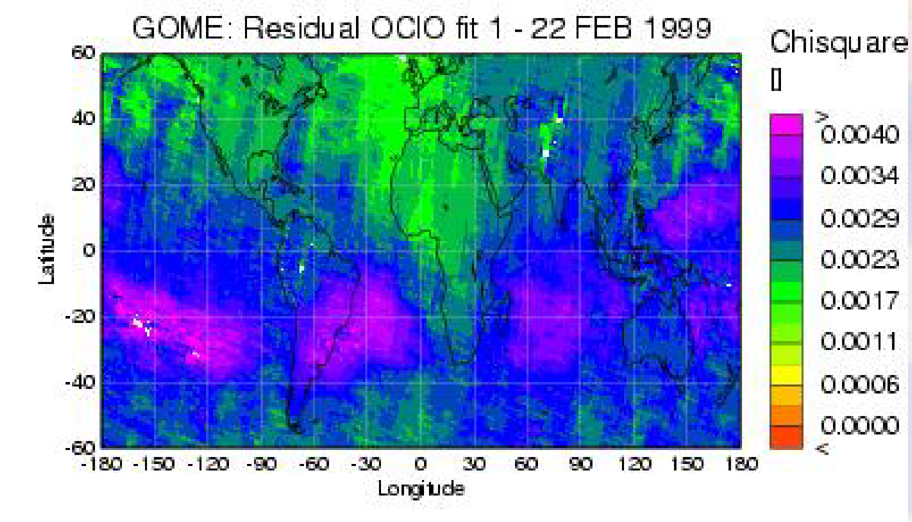




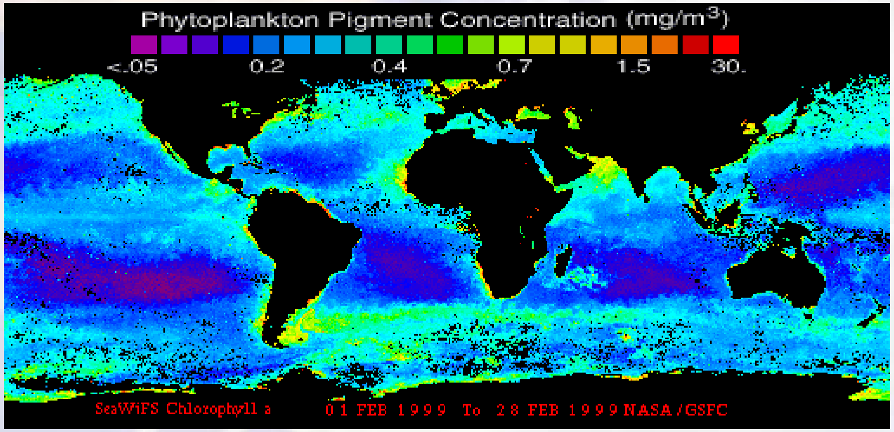
- Error in VC for both gases lies between 0-10%
- Wrong Ring spectrum can be worse than using none.
- For Ozone Fraunhofer Filling-in is more important. Absorption line Filling-in is more important for NO_2

Water Ring: Historical Background

- Global retrieval of minor trace gases using DOAS in the UV/Vis.: GOME-Data
- Spectral structures could not be attributed and remained as a residual.
- X^2 is an indicator for the fit quality



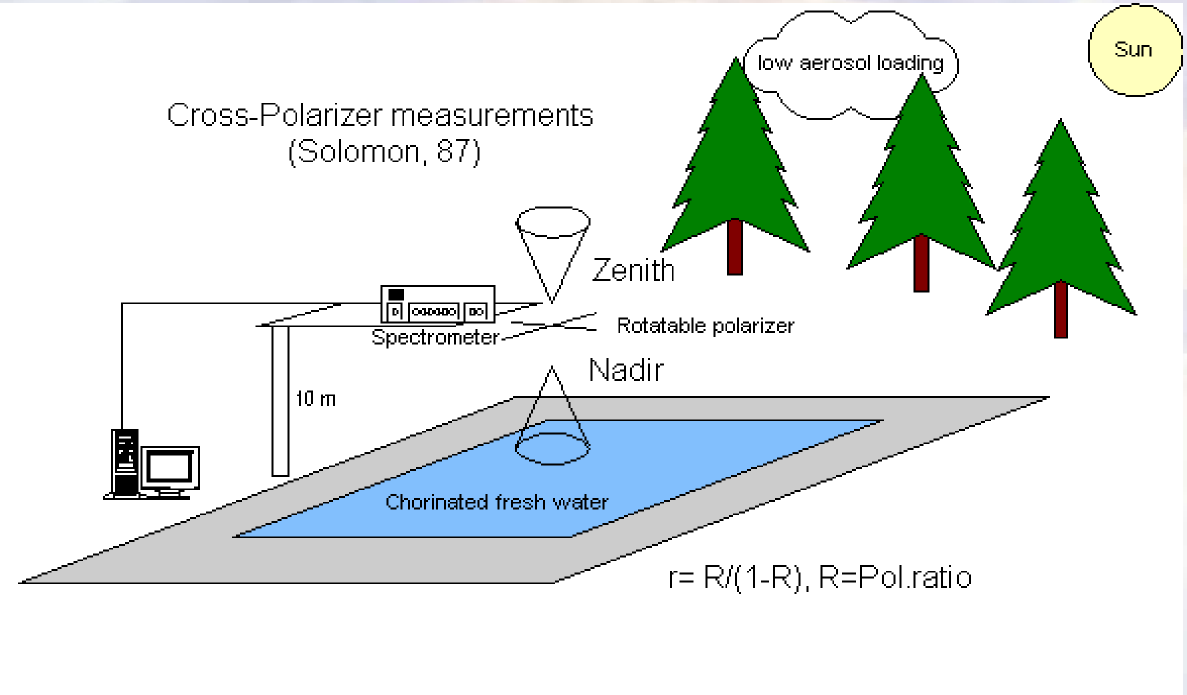
SeaWiFS Chlorophyl 1-28 FEB 1999



- Significant correlation of large residuals and low chlorophyll-a concentration (derived from SeaWiFS).
- ➢ Spectral structures induced by **water inherent properties???**

Water Ring: Historical Background II

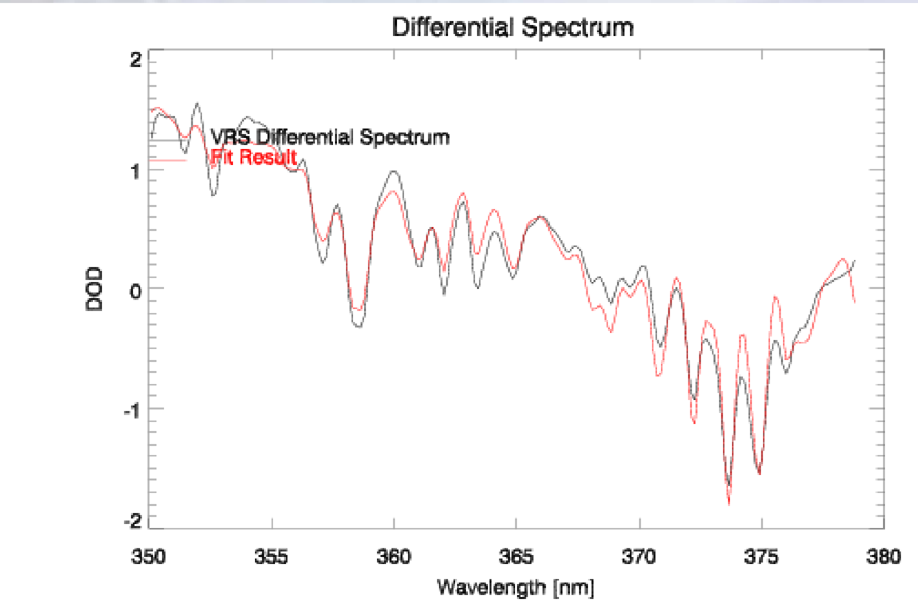
- ➢ Experiment was set up. On-ground measurements in Bremen
- Grating spectrometer:
  - The spectral resolution ~ GOME; spectral range covered 344-388 nm.

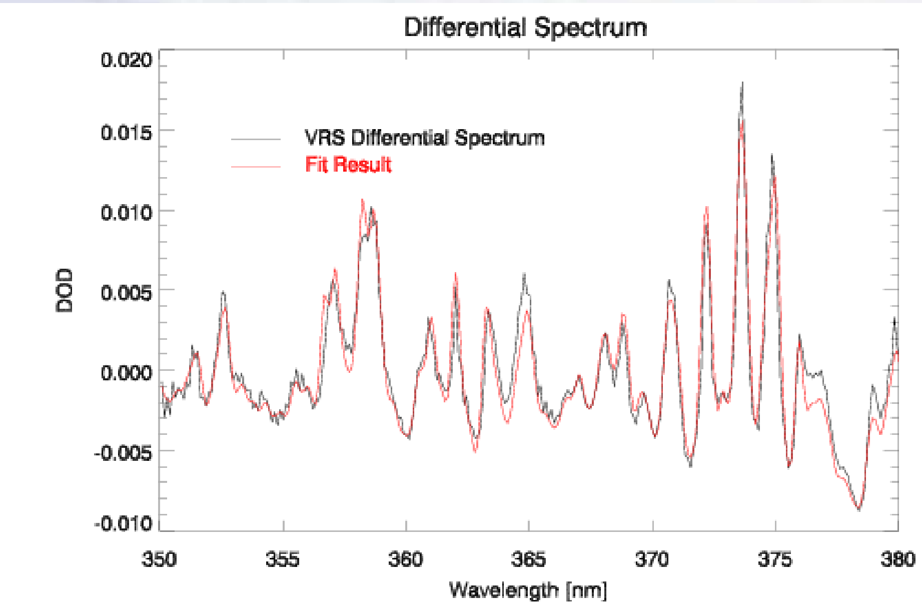


➢ Typical „Ring structure“ for Zenith measurements, insignificant structure for Nadir

Water Ring: Historical Background III

- Swimming pool residual
- **GOME residual**



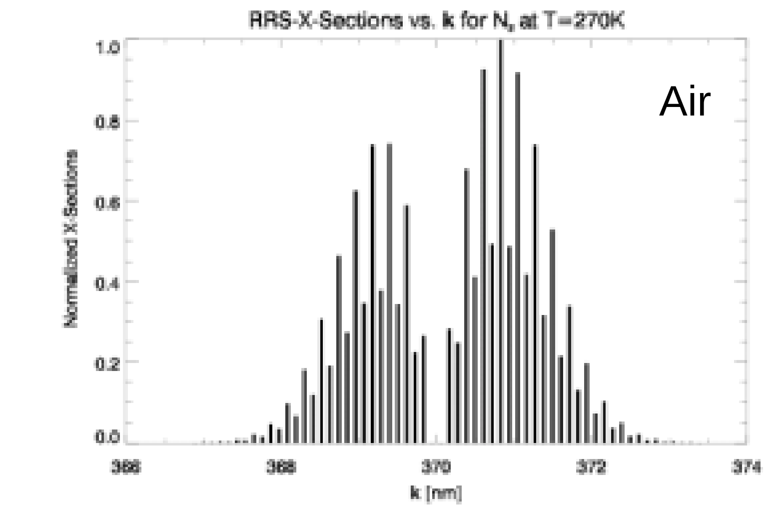


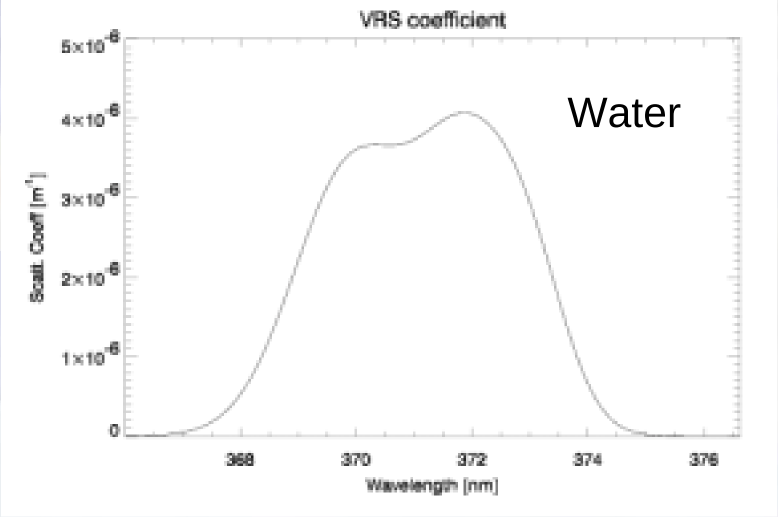
- Overall agreement between swimming pool spectrum and GOME residual.
- Reasons for this structure seem to be water-inherent:
  - Emission, Absorption or
  - Redistribution (inelastic scattering)???

Water Ring: Raman Scattering

- **From experience with the *atmospheric* Ring effect we know that Raman scattering can be an efficient photon redistributor.**
- **In liquid water rotational transitions are suppressed, vibrational not!**

➢ **Vibrational Raman Scattering (VRS) could play a role!**





- At typical oceanic temperatures there are not enough molecules excited

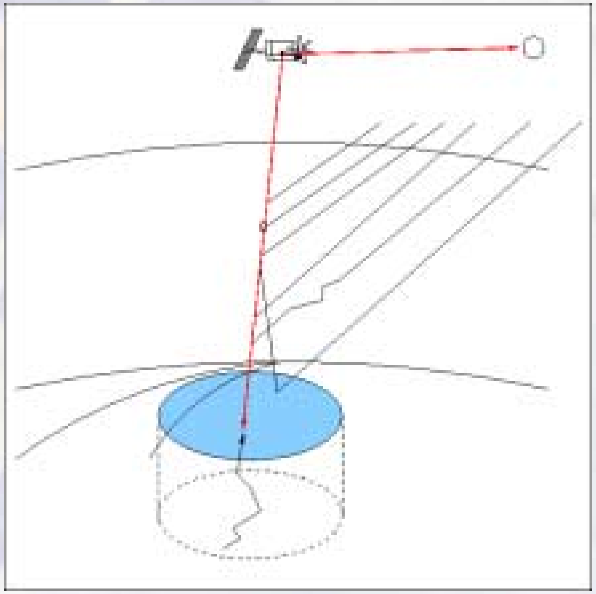
➢ Only Stokes-transitions are possible.

Modelling

- Photon´s fate in Earth´s Atmosphere and Ocean requires:

A coupled Atmosphere-Ocean Radiative Transfer Model

- Atmospheric radiative transfer code SCIATRAN (V1.2) comprises lots of features:
  - Absorption, and elastic&inelastic scattering in a pseudo-spherical atmosphere.
  - Ground-Reflection is included as Lambertian Refl.

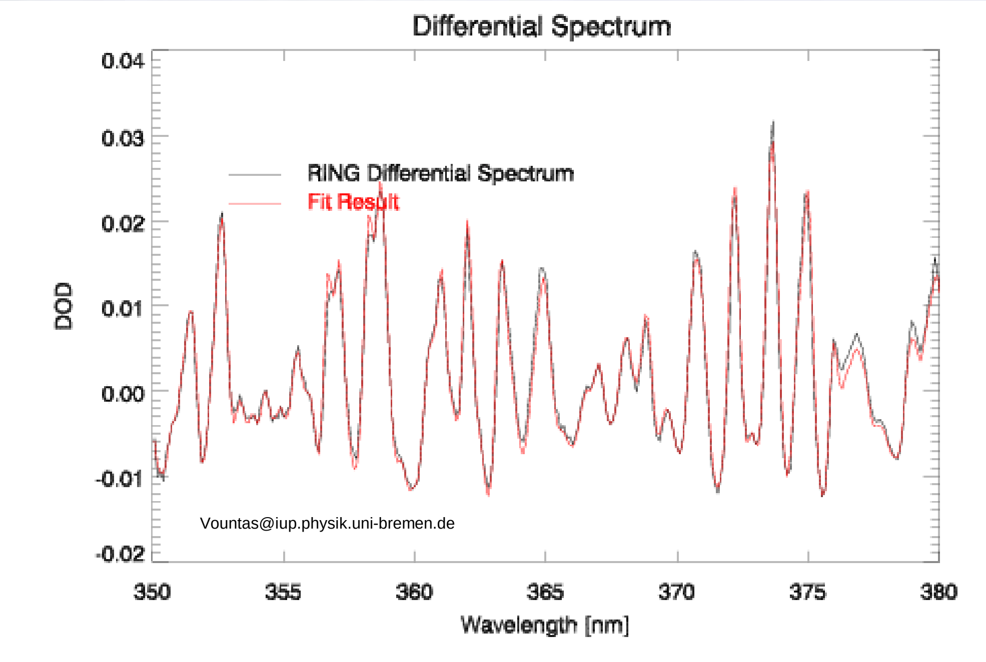


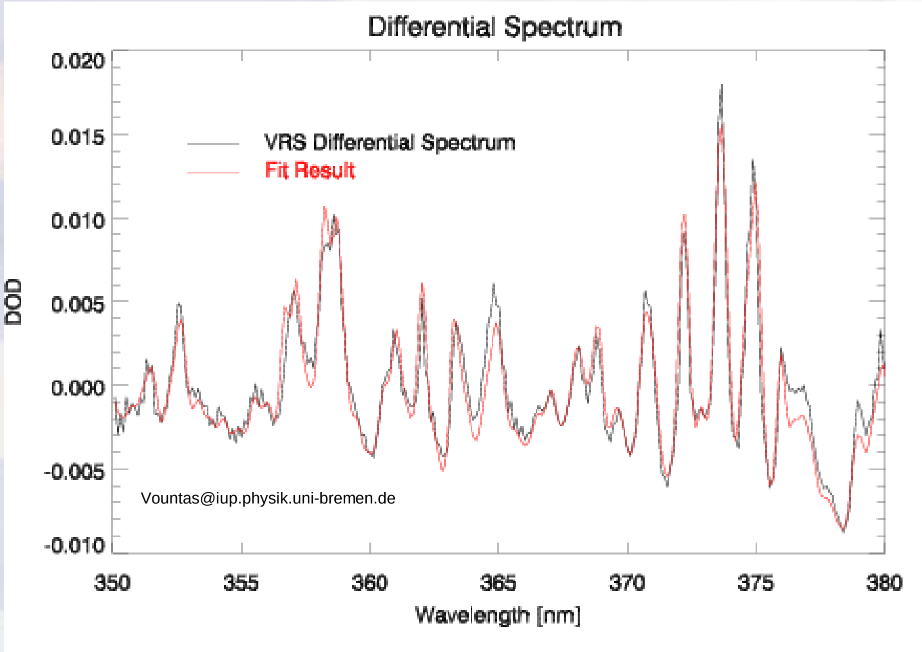
➢ Idea: Coupling of RT in Atmosphere and Ocean via spectral Reflection function

➢ Sathyendranath & Platt (1998) proposed such a reflection function using an adaption of Gordon´s QSSA-Approach (Gordon, 1973)

Application

- Fitting model results within GOME DOAS-Retrievals leads to promising results:





DOAS fits of clear-sky GOME data (lv1: 90208175).

Ocean Reflectance

Ocean Reflectance 1

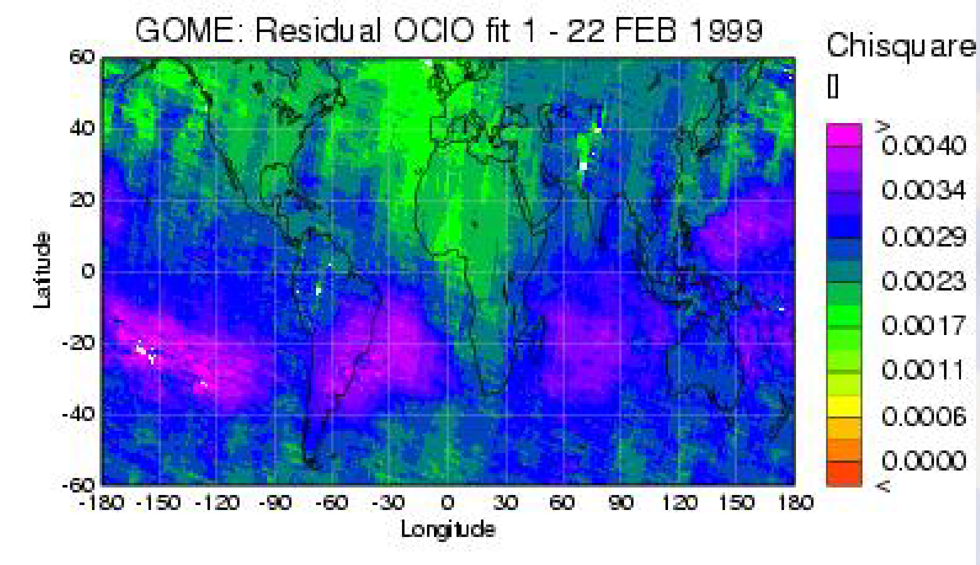
- Nadir observations from air-or spacecraft are influenced by the reflectance of water.
- The reflectance is a function of the scattering and **absorption coefficient** of the water body.
- The total **absorption coefficient** **a** of any water body can be expressed by: $a=a_{ph}+a_{CDOM}+a_d+a_w$

Coefficient	Absorption due to
a_{ph}	**phytoplankton (mainly seen by Chlorophyll-a)**
a_d	**Detritus (including inorganic suspended matter)**
a_{CDOM}	**Chromomorphic Dissolved Organic Matter (CDOM or Gelbstoff-Yellow Substance)**
a_w	**Water itself**

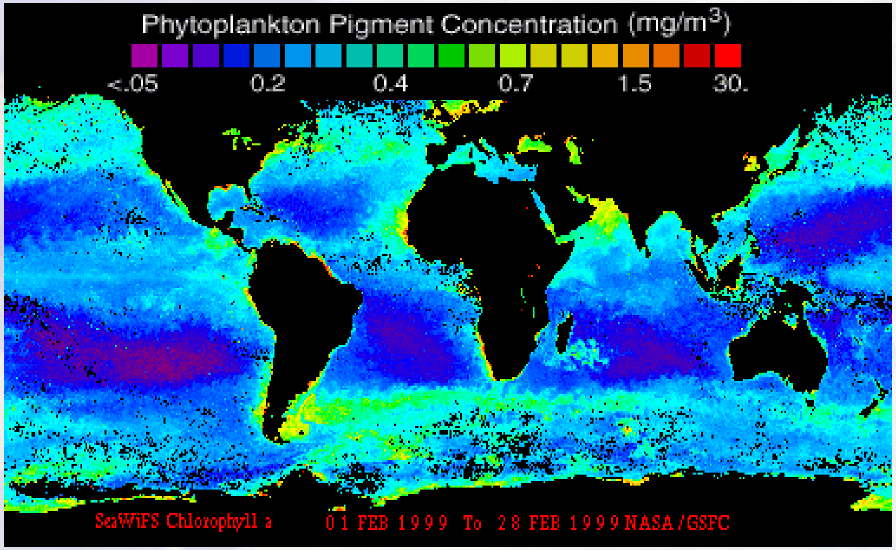
- With significantly strong and variable spectral features in the ocean reflectance we will have the possibility to retrieve **Chlorophyll-a concentrations**.

Ocean Reflectance 2

- Using GOME data we could indirectly produce such a spectral signature („Water Ring“):



SeaWiFS Chlorophyl 1-28 FEB 1999



- Significant correlation of large residuals and low chlorophyll-a concentration (derived from SeaWiFS).
- Modulation of the size of residual with chlorophyll-a concentration!
- ➢ Retrieval of chlorophyll-a using the residual information. Study is ongoing!

Retrieval Experiments

- Radiative transfer model to simulate radiance spectra

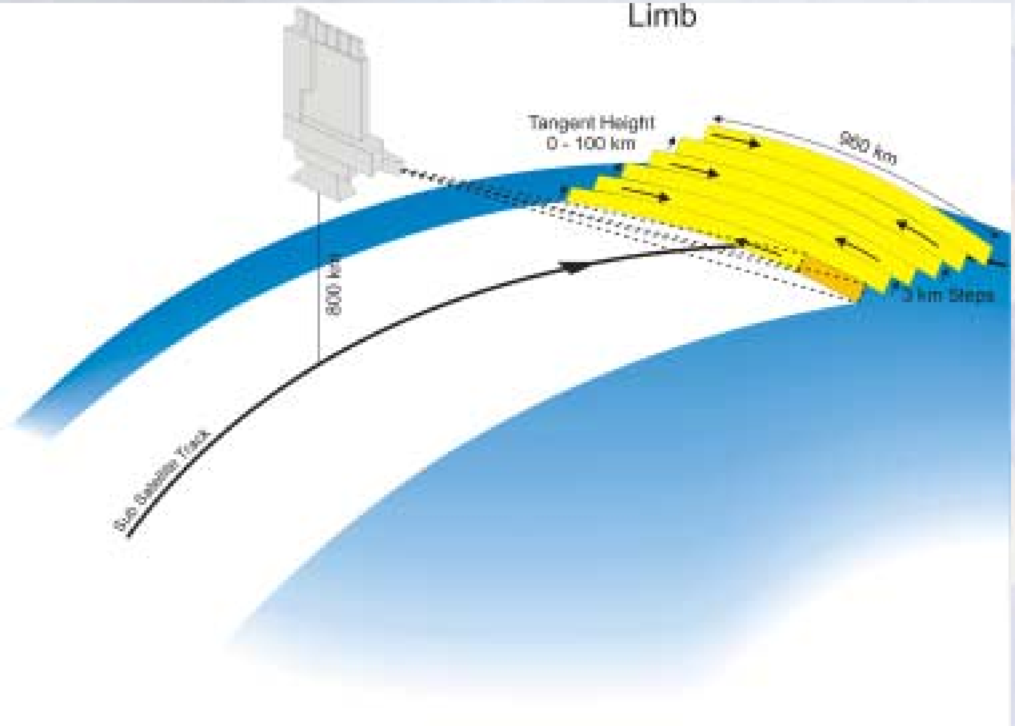
- Instrument model

- ➢ Simulated limb measurements

- Optimal estimation retrieval formalism

- ➢ Theoretical retrieval precisions for trace gases from diagonal elements of the retrieval covariance matrix

Limb Scattering Theoretical Precisions

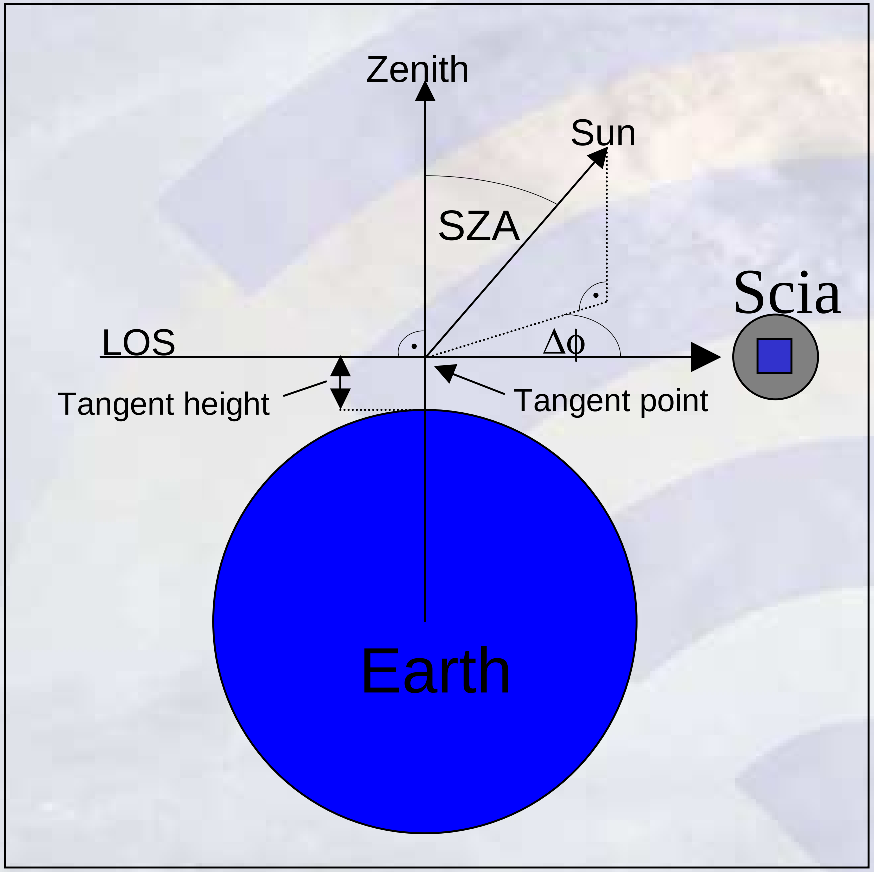


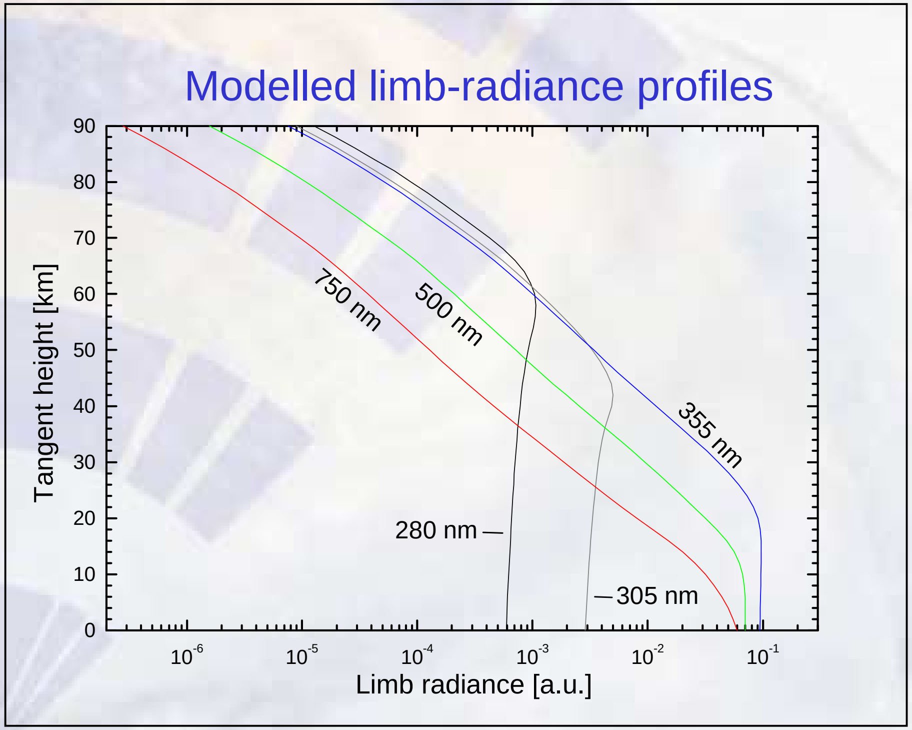
- **vertical res.: 3 km**
- **horizontal resolution in azimuth: 240 km (120 km min.)**
- **horizontal resolution in flight direction: approx. 400 km**
- **Observation optimised to match limb with nadir measurements**
- **Duration of Limb sequence: 60 sec.**
- **Global coverage: 6 days at the equator**

The theoretical precision for a given instrument configuration is the limit of accuracy determined by random or stoichastic noise.

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

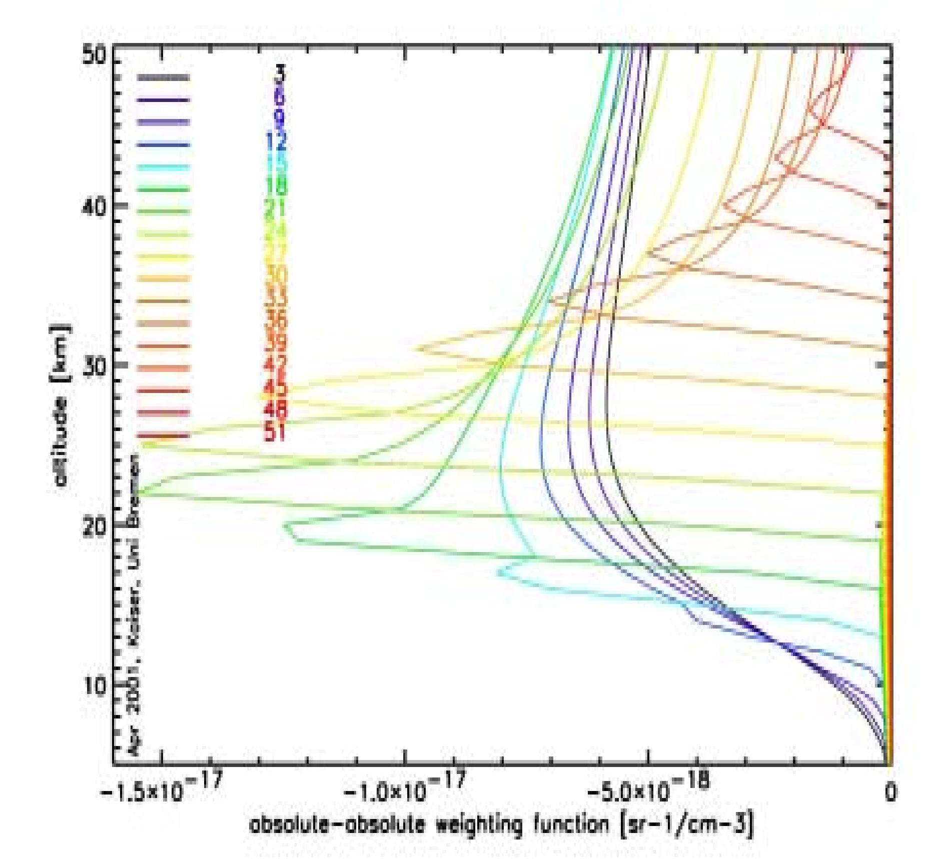


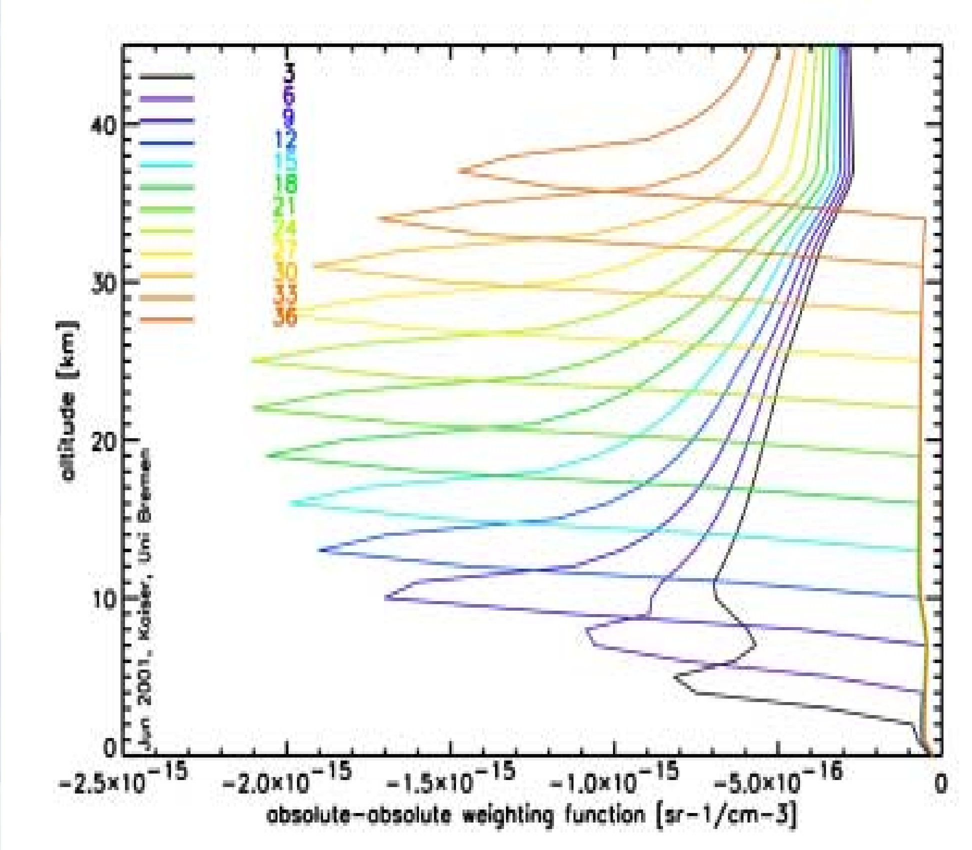


Modelling the Radiative Transfer

Requirements UV-VIS-SWIR RTM Limb	SCIATRAN/CDIPI (A. Rozanov 2001)	SCIARAYs (Kaiser 2001)
Refraction	☺	☺
Full Sphericity	☺	☺
Multiple Scattering	☺	😐 (double scattering)
Ground Reflection	☺	☺
Rayleigh, Mie-Scattering	☺	☺
Analytical Weighting Functions	😐 (In progress)	☺
Computational fast for global analysis of data	☹	☺
Occultation included	☺	☺

O_3 Weighting Function for Limb



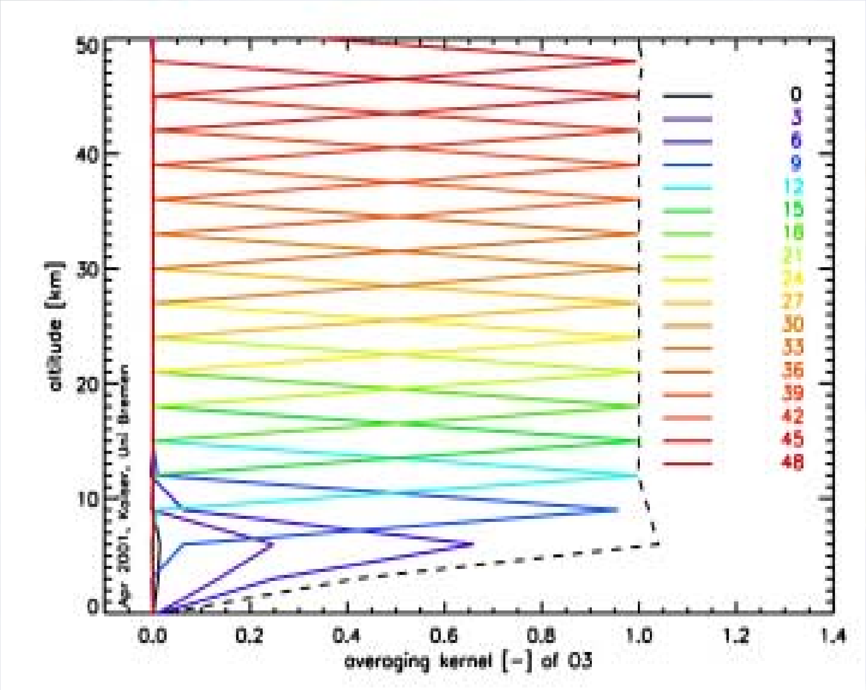


- **360 nm** **790 nm**
- **Light path is wavelenght dependence => multi spectral advantage**

Averaging Kernels Limb

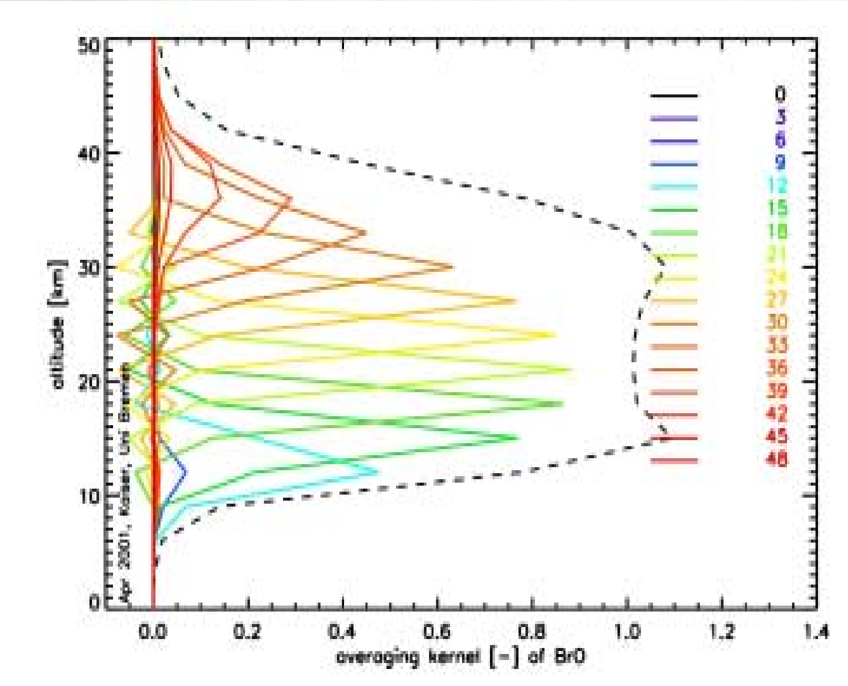
- **300 –370 nm**

Ozone



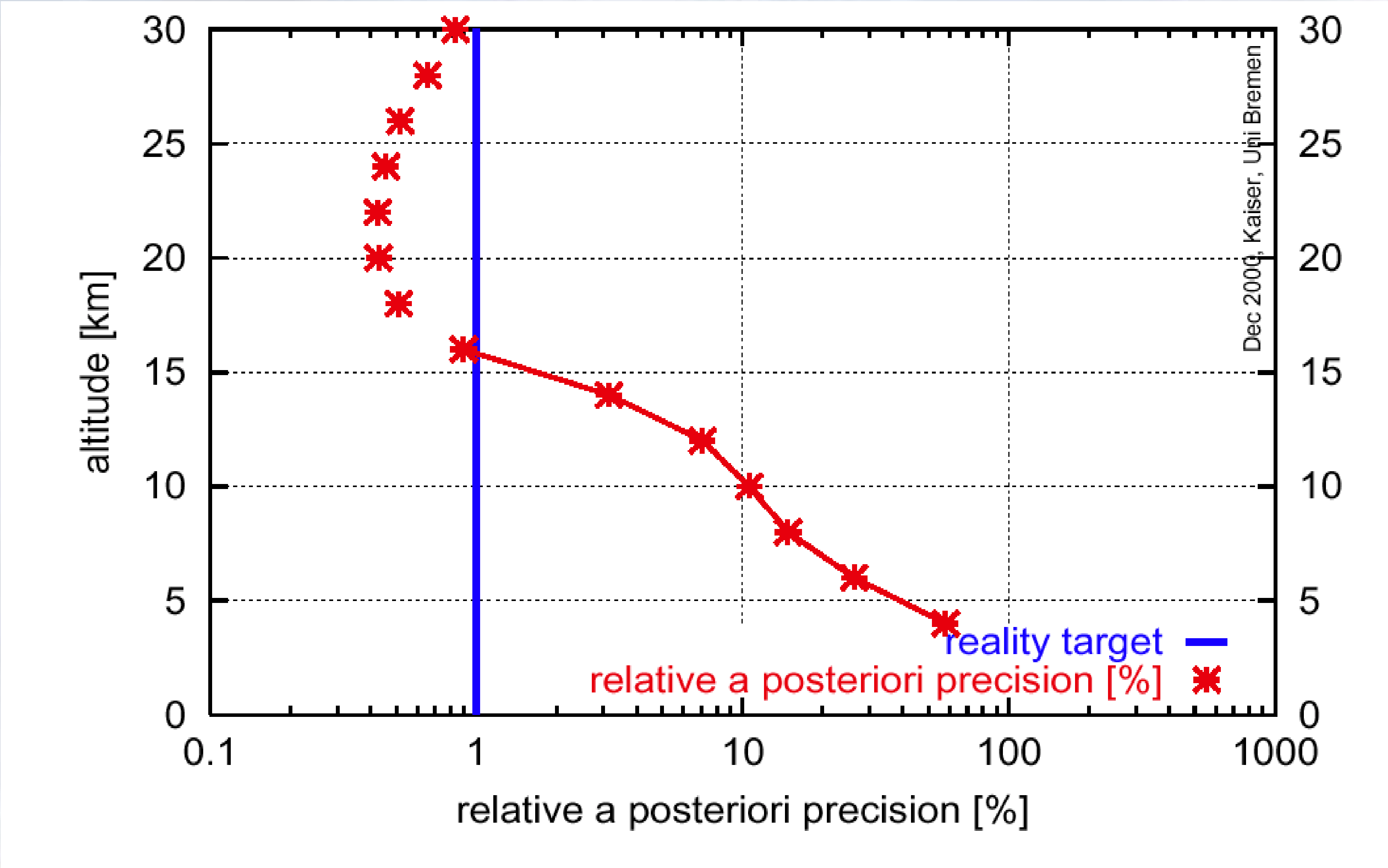
- **Useful height range: 5—50 km**
- **Above 12 km all information comes from the measurement**
- **No smoothing**

- **BrO**

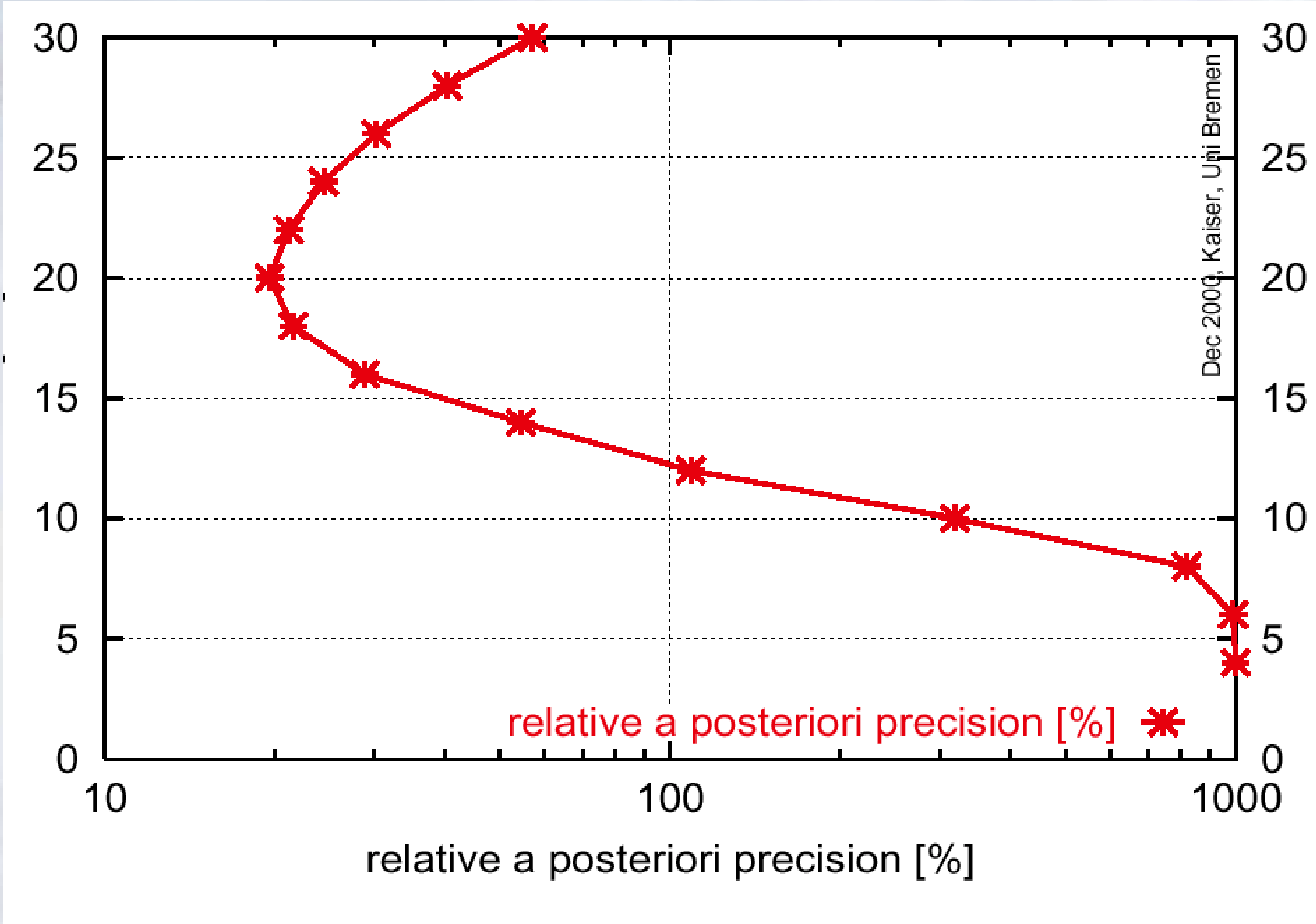


- **Useful height range: 15—30 km**
- **Information determined by the measurement**
- **some smoothing**

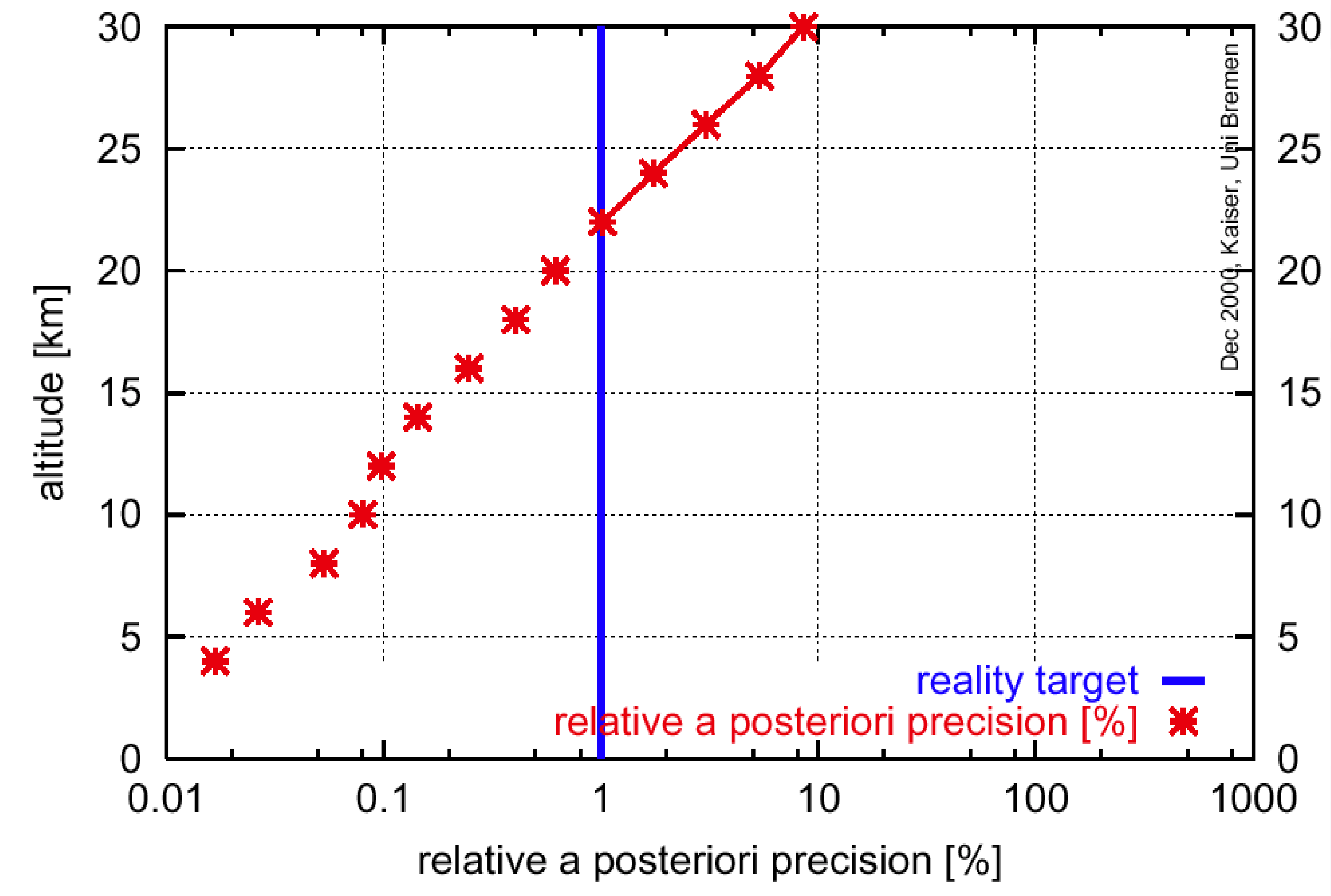
Limb: NO_2 Precision



Limb: BrO Precision



Limb: H_2O Precision



Summary

- Radiative Transfer in the solar region, UV, Visible and NIR discussed
- Single and Multiple scattering significant
- Particle scattering significant.