

Remote sensing in the UV-vis

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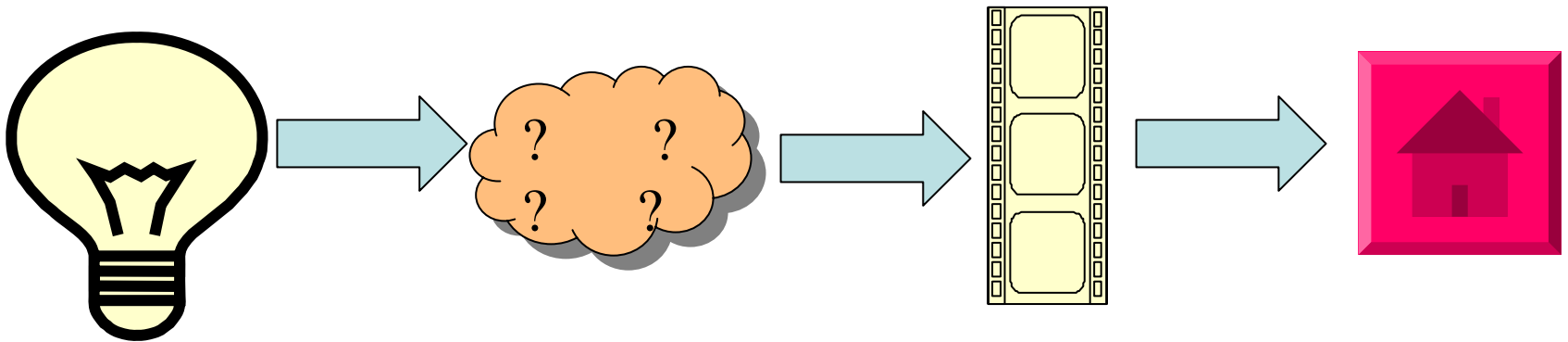
The Netherlands

Overview

- Remote sensing by satellites
- The inversion problem
- The forward model
- DOAS technique

Passive remote sensing

Sun > Earth > Satellite > Scientist



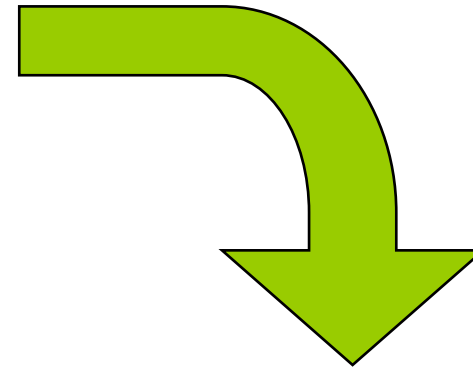
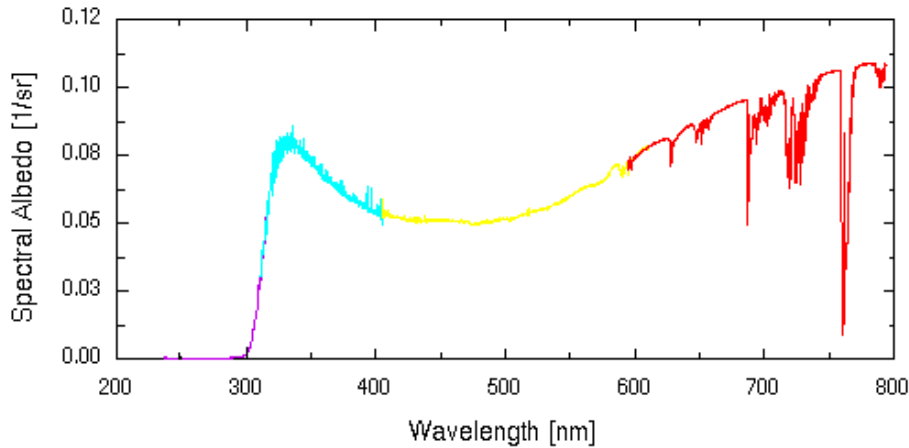
Lamp > Object > Detector > Analysis

> measure radiation

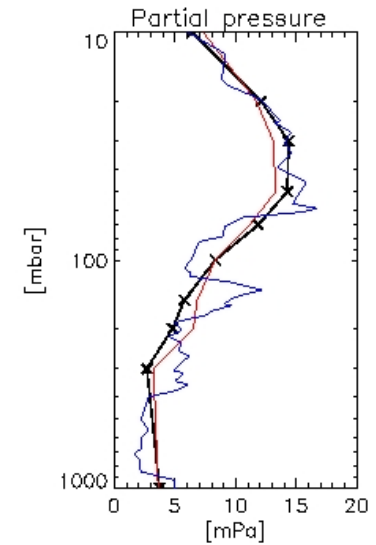
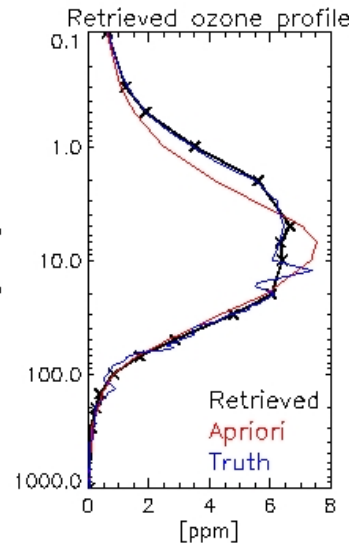
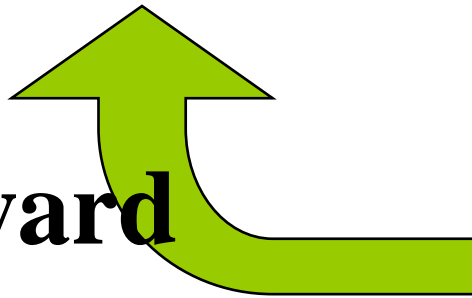
> infer information on quantities that affect the radiation

The inversion problem in the retrieval

Inversion



Forward Model



Retrieval

$$\mathbf{y} = F(\mathbf{x})$$

\mathbf{y} : vector, measured, \mathbf{x} : vector, to be derived

F: forward model

Auxiliary information:

- Measurement error: S_y
- Best guess for \mathbf{x} : \mathbf{x}_0

Default method

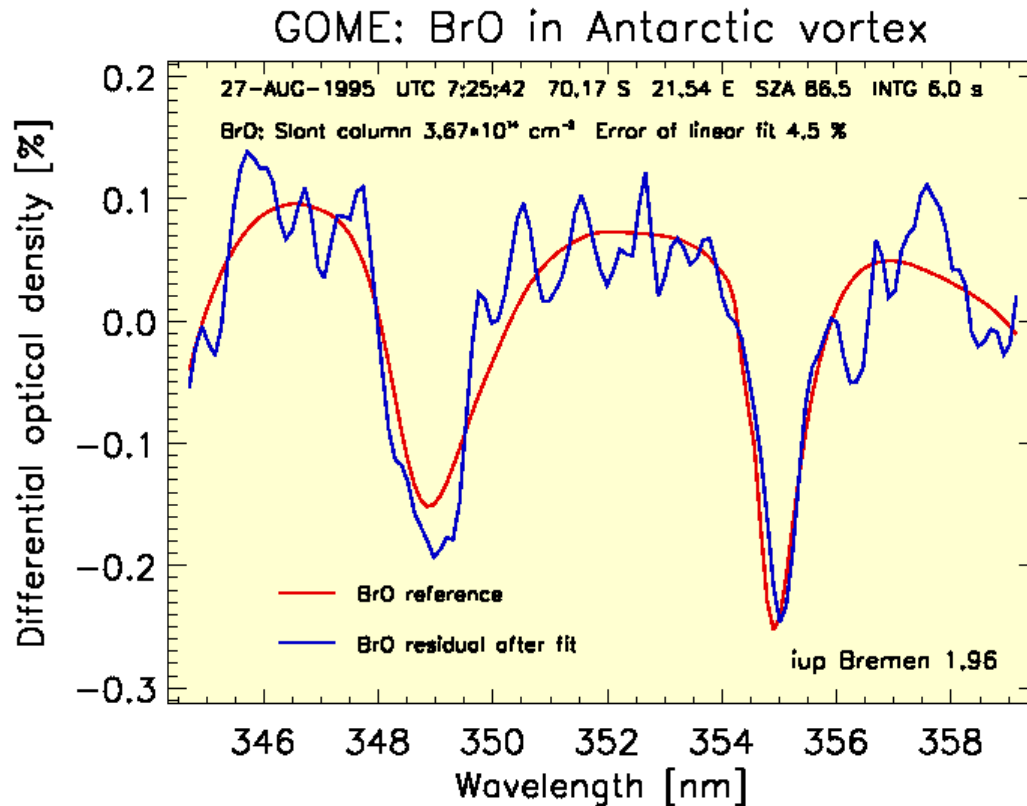
Non-linear least squares - iteratively find minimum of cost function:

$$CF = (\mathbf{y} - F(\mathbf{x}))^T S_y^{-1} (\mathbf{y} - F(\mathbf{x}))$$

(Levenberg-Marquardt)

Well-posed problems

total column retrieval



Differential Optical Absorption Spectroscopy: fitting absorption structures

Ill-posed problems

Profile retrieval

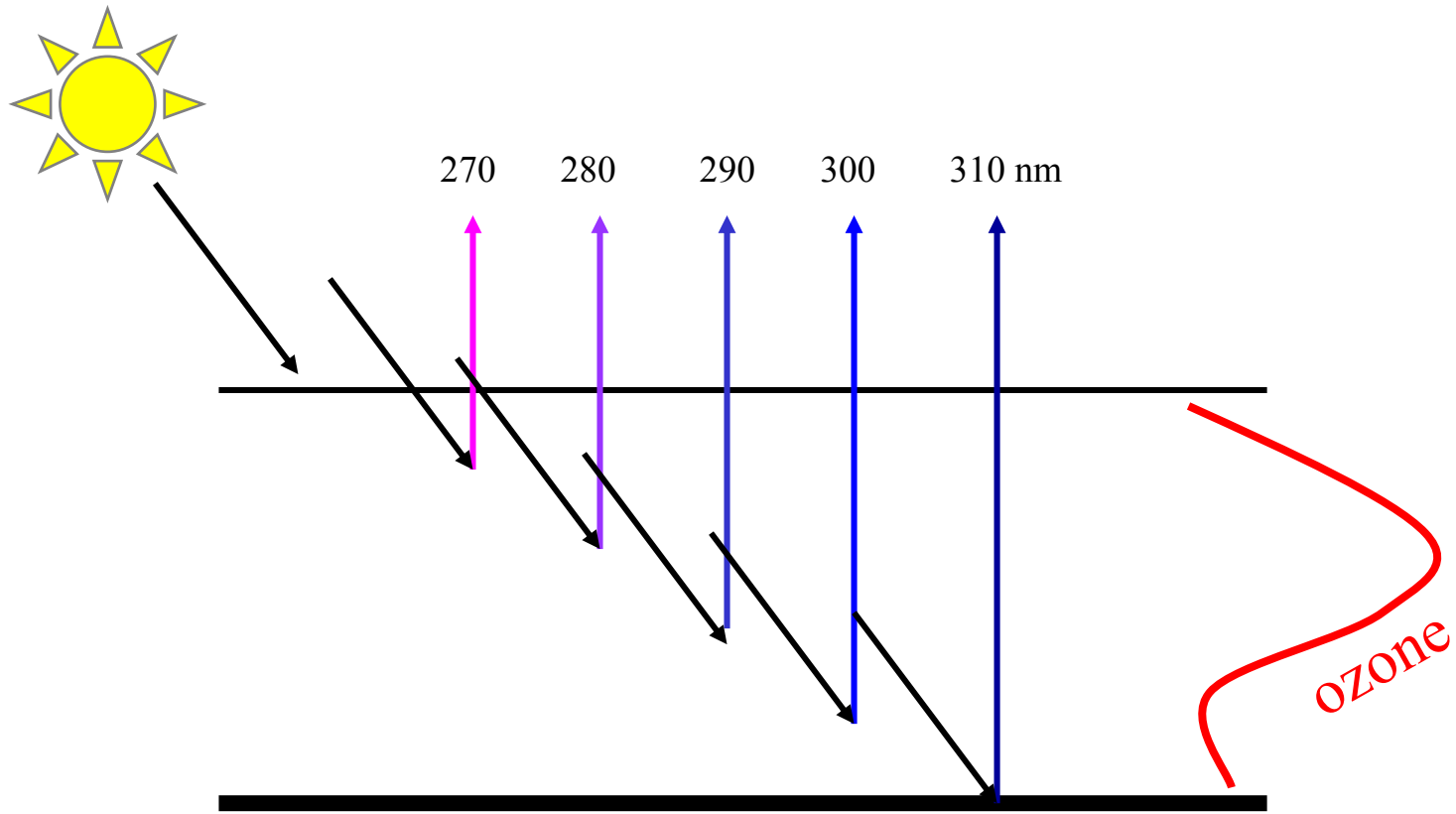
> more information requested as available

Least squares gives problems > noise
amplification

Example

Nadir ozone profile retrieval

Ozone profile from nadir



Noise amplification

Simple two layer model:

$$\lambda_1 \quad : \quad 1.00 x_1 + 1.00 x_2 = I_1 \pm \Delta I$$

$$\lambda_2 \quad : \quad 0.99 x_1 + 1.01 x_2 = I_2 \pm \Delta I$$

Pick numbers:

$$x_{1,2} = 10; \quad I_{1,2} = 20; \quad E(\Delta I) = 1$$

Solution:

$$x_1 + x_2 = 20 \pm 1 \quad x_1 - x_2 = 0 \pm 141$$

Solution: regularisation

Extra term in cost function

Optimal Estimation

$$(y - F(x))^T S_y^{-1} (y - F(x)) + (x - x_a)^T S_a^{-1} (x - x_a)$$

x_a : a-priori, S_a : a-priori error covariance

- Damps unrealistic solutions
- Based on Bayes theorem: $P(x|y) = P(x)P(y|x)/P(y)$
P probability density function

See e.g. Rodgers Inverse Methods for atmospheric sounding

Optimal Estimation

Linear forward model (linearize $y = F(x)$)

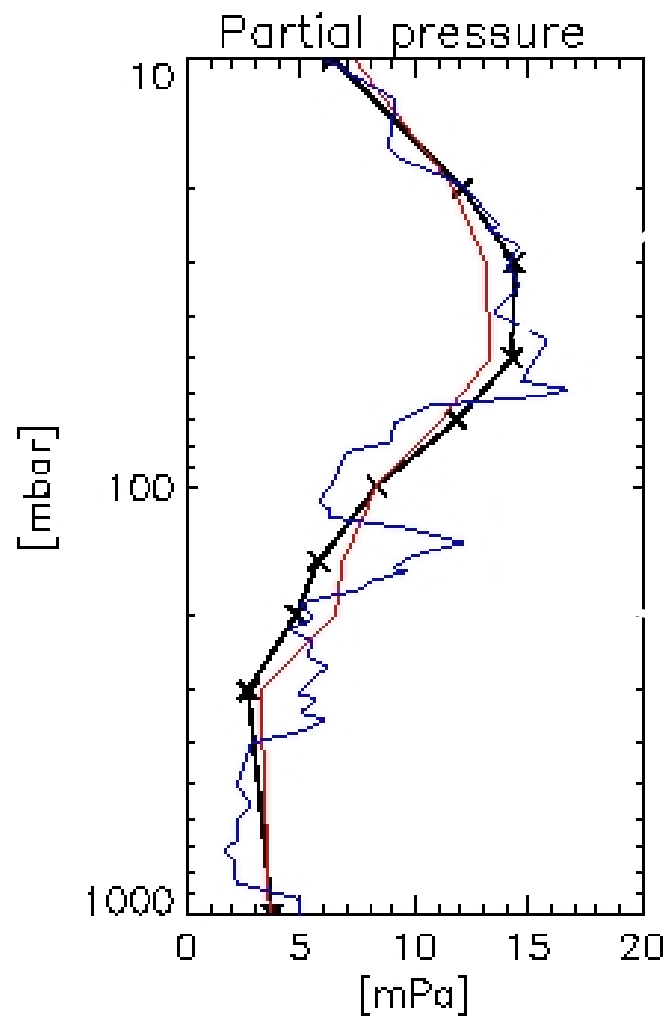
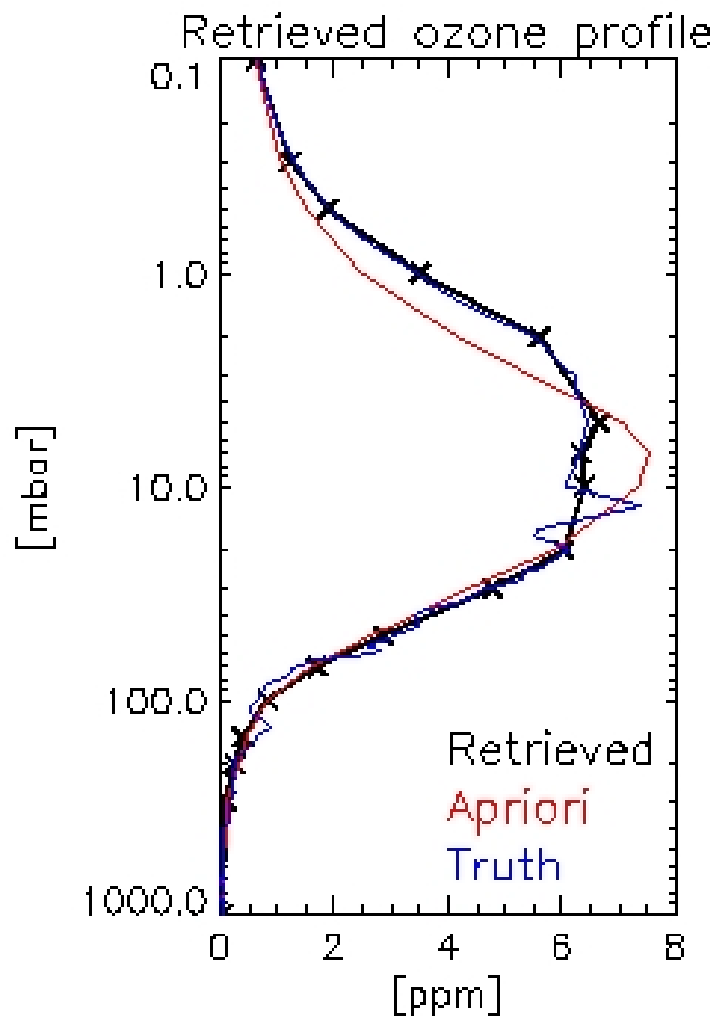
$$\mathbf{y} = \mathbf{K}\mathbf{x}$$

Analytic solution for CF minimum:

$$\hat{x} = x_a + S_a K^T (K S_a K^T + S_y)^{-1} (y - K x_a)$$

Moderately non-linear case: apply iteratively

Information from a-priori  Information from measurement



GOME

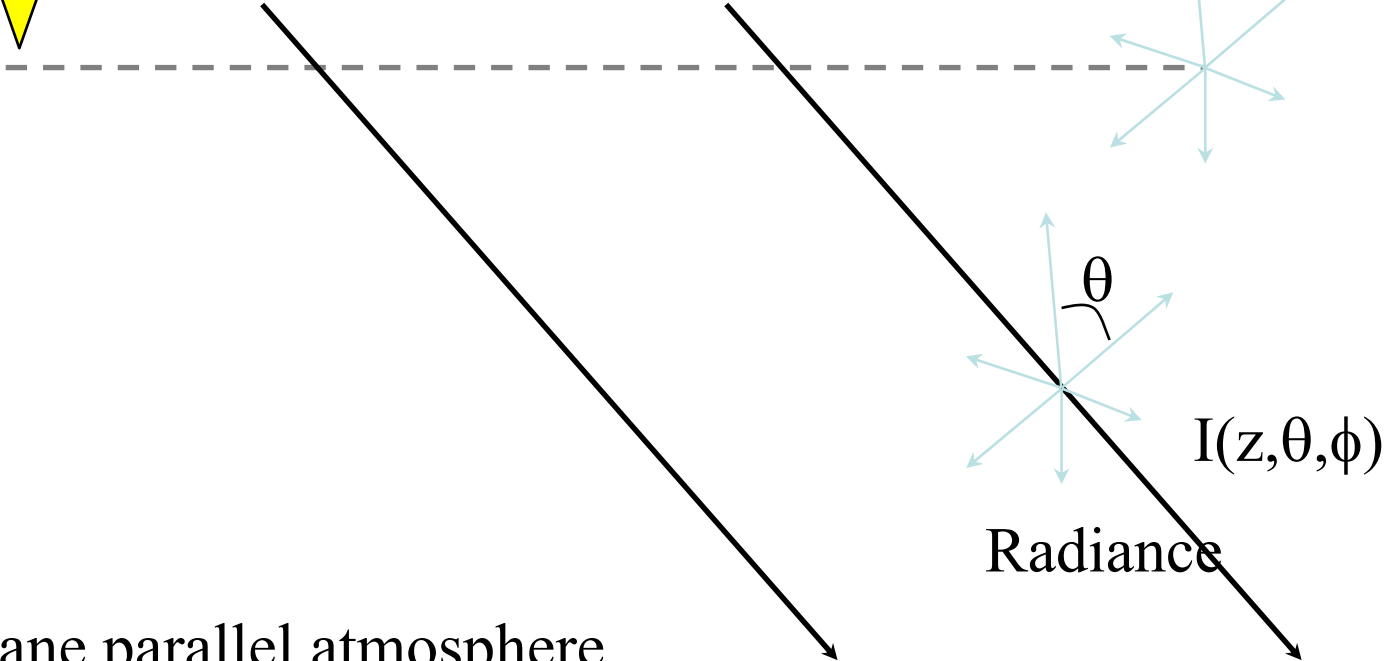
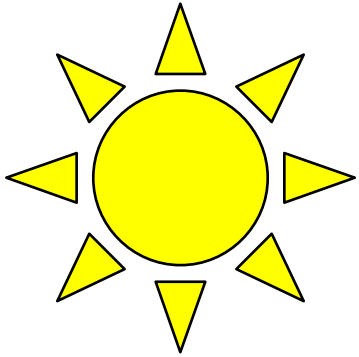
Balloon

Forward Model

Atmospheric Radiation Transfer

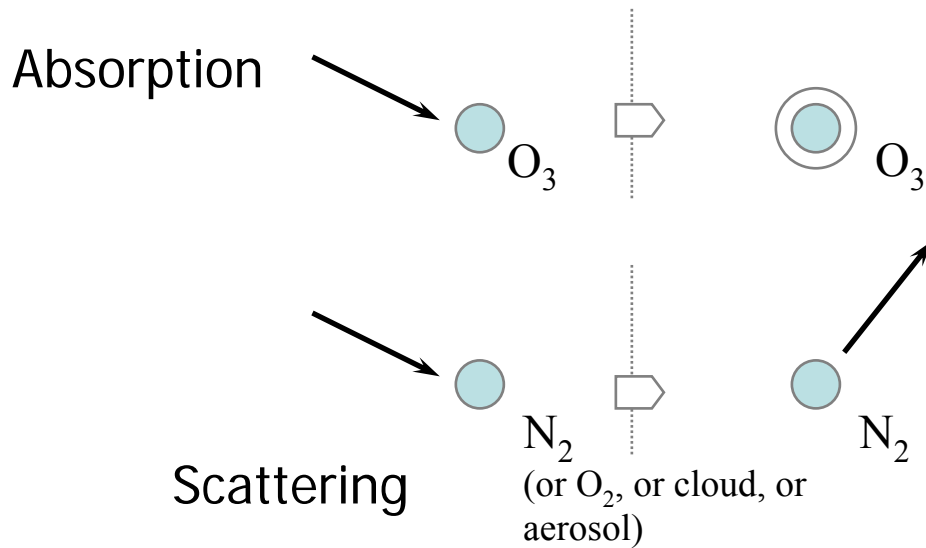
(UV-VIS nadir)

The stage...



Plane parallel atmosphere

Radiation transfer: processes



$$\text{Extinction} = \text{Absorption} + \text{Scattering}$$

Radiation Transfer Equation

Optical depth:

$$d\tau = -\text{ext } dz = -(\text{abs} + \text{scat}) dz$$

TOA: $\tau = 0$, Surface: $\tau = \tau^*$

$$\mu \frac{dI}{dz} = -eI + sJ,$$

$$\mu \frac{dI}{d\tau} = I - \omega J, \quad \omega = s/e$$

$$J = (\text{Source}) = \int d\Omega' P(\Omega', \Omega) I(\Omega),$$

$$P = (\text{scattering function}) = P(\cos \theta_s),$$

θ_s = scattering angle,

$$\mu = \cos \theta$$

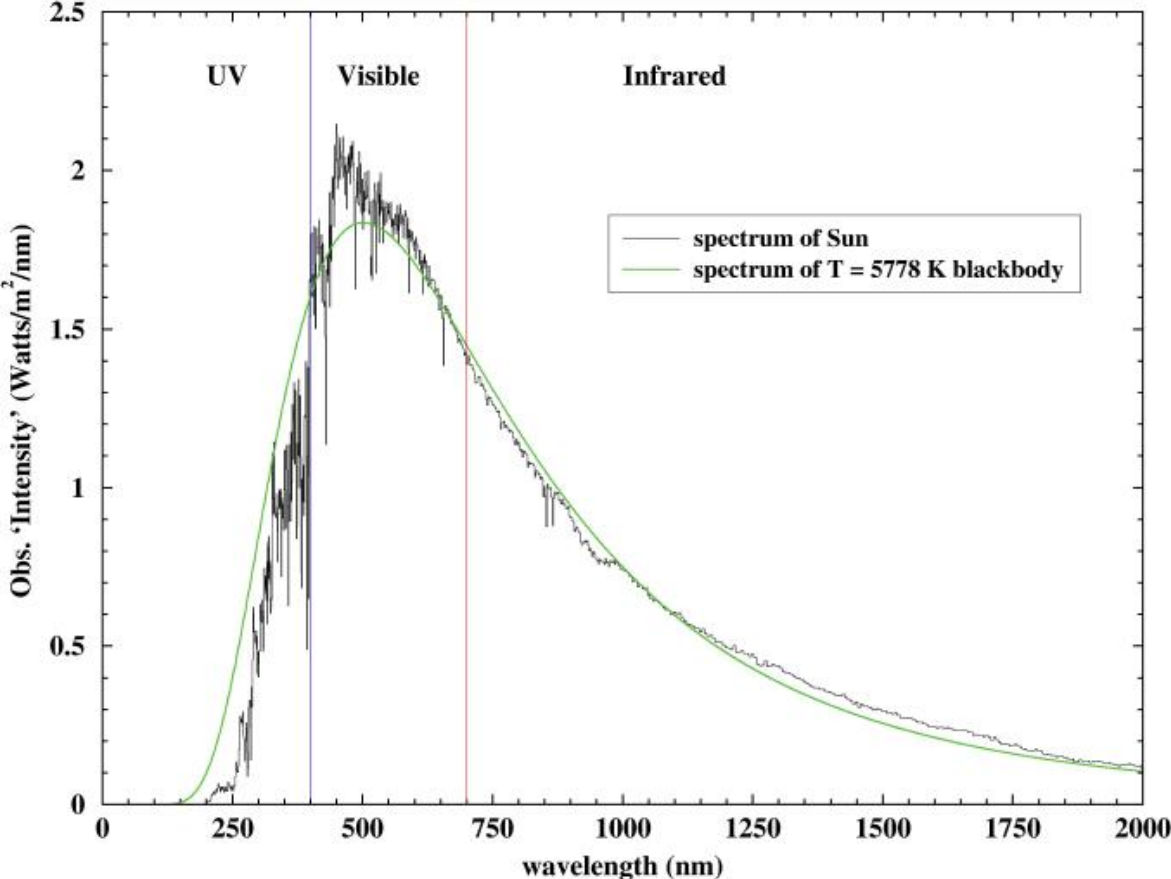
Passive remote sensing in the solar spectral range

The source of light is the sun:

- Solar spectrum: 0.2 – 3.0 μm , consisting of the:
- Ultraviolet: **UV** < 400 nm
- Visible: 400 nm < **VIS** < 700 nm
- Near-Infrared: 700 nm < **NIR** < 3 μm .

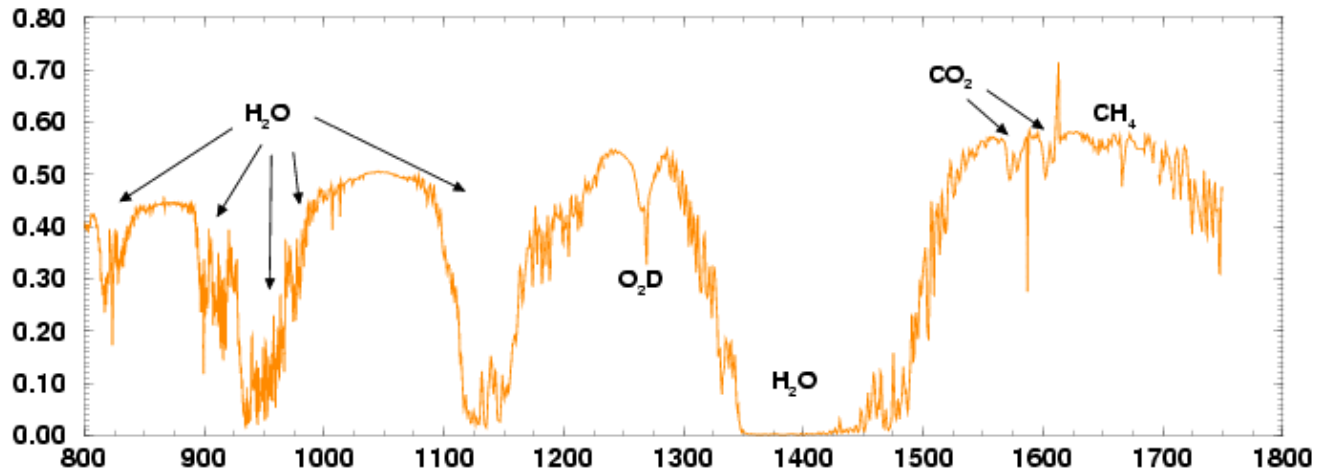
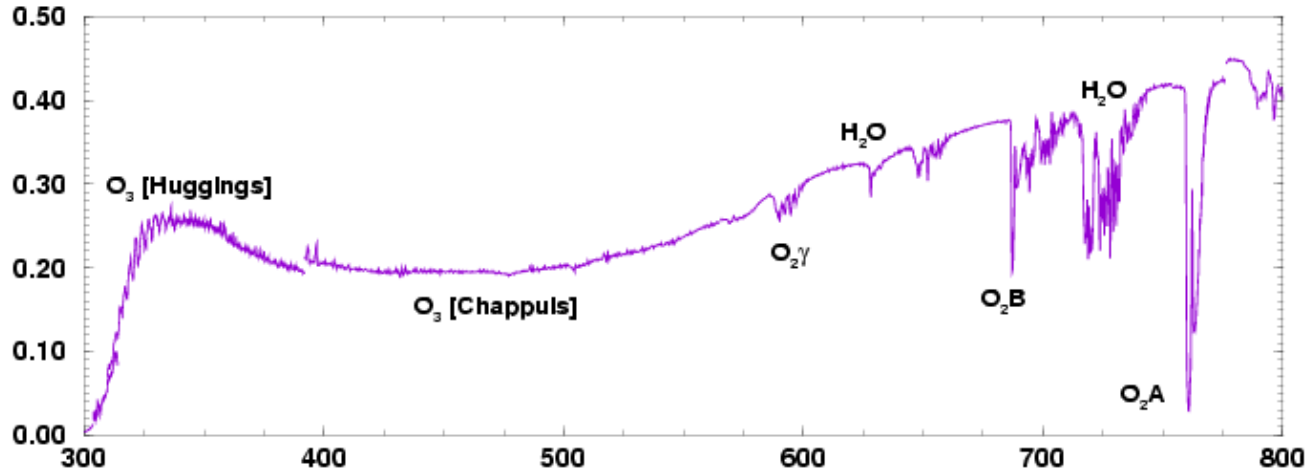
Solar Spectrum vs. Blackbody

$T_{BB} = 5778 \text{ K}$



Earth reflectance spectrum (cloudfree Sahara scene measured by SCIAMACHY)

SCIAMACHY over the Sahara (Aug 23, 2002)



Approach for remote sensing of atmospheric composition

Choose a quantitative “*signature*” = unique identification of the quantity of interest:

To detect absorbers: use spectral features

- Trace gases have spectral absorption lines

To detect scattering particles: use

brightness + colour + angular features

- Clouds: brightness, whiteness, fractal shape, rainbow
- Aerosols: colour, polarization

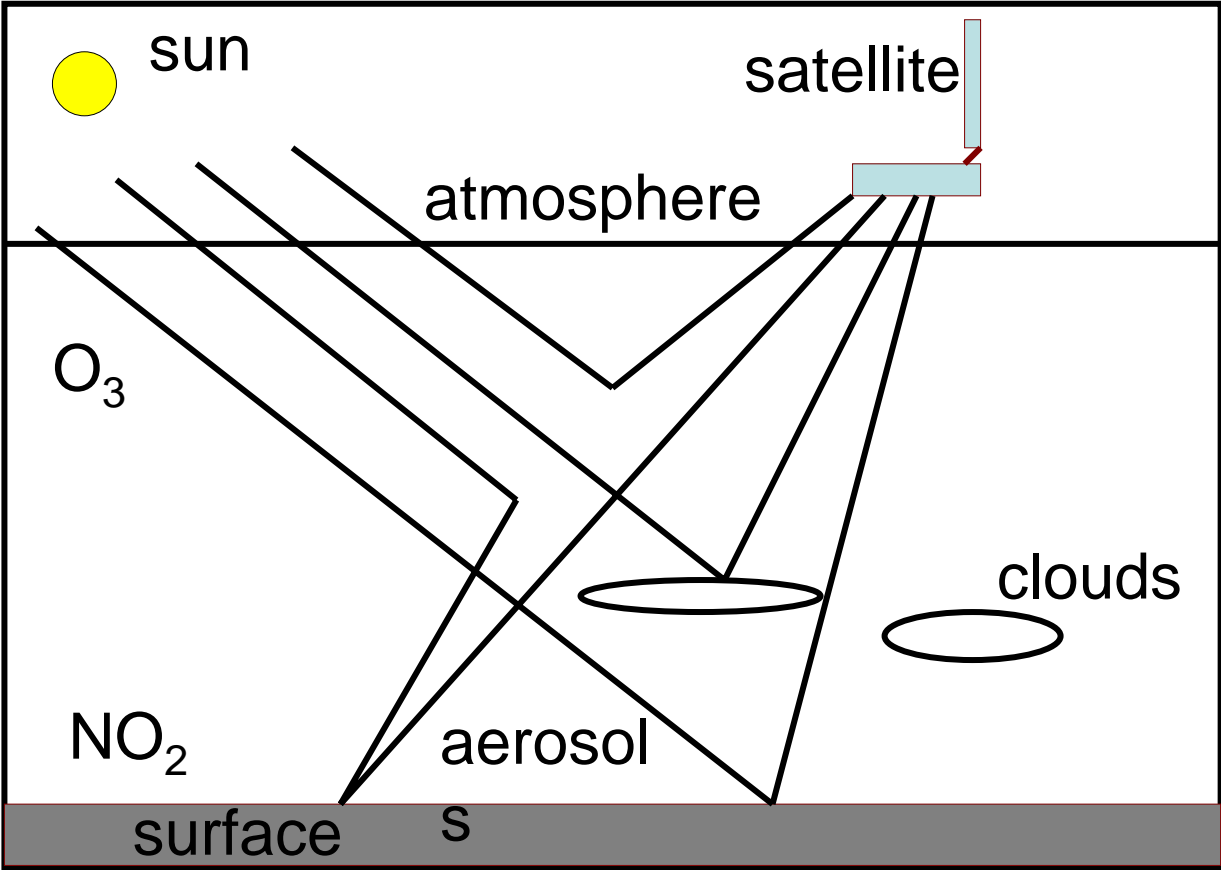
Detection of trace gases

- Trace gases are most easy to detect, because the absorption lines of a molecule are its unique signature.
- From the absorption lines the amount of trace gas can be determined.
- The deeper an absorption line in the atmospheric spectrum, the more gas there is.
- The precise quantitative determination of the total amount of gas depends on:
 - Vertical distribution of the gas (not known).
 - Interference with clouds, aerosols.

Detection of scatterers: clouds and aerosols

- Clouds and aerosols give usually a brighter scene, because they scatter more light than the clear atmosphere.
- But they are difficult to quantify precisely, because they usually do not have unique scattering features.
- Sometimes their angular scattering pattern is unique:
 - Spherical droplets have rainbows, which are depending on particle size.

Interaction of solar radiation with the atmosphere



Radiation-matter interaction processes

- Rayleigh scattering by air
- Absorption by trace gases
- Scattering and absorption by aerosol particles
- Scattering and absorption by cloud particles
- Reflection by the surface.

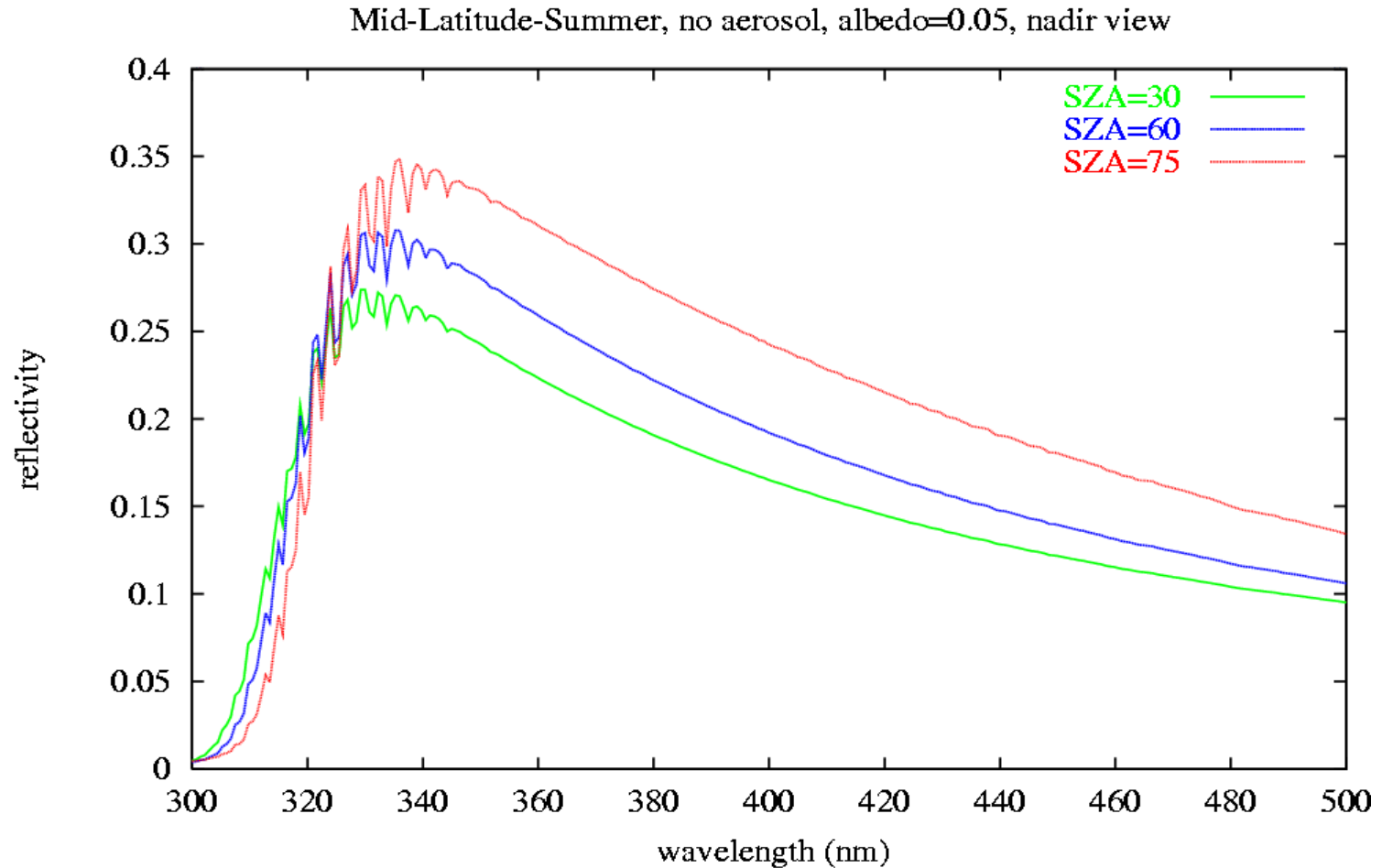
Analysis of satellite measurements

Requirement:

radiative transfer model of the atmosphere

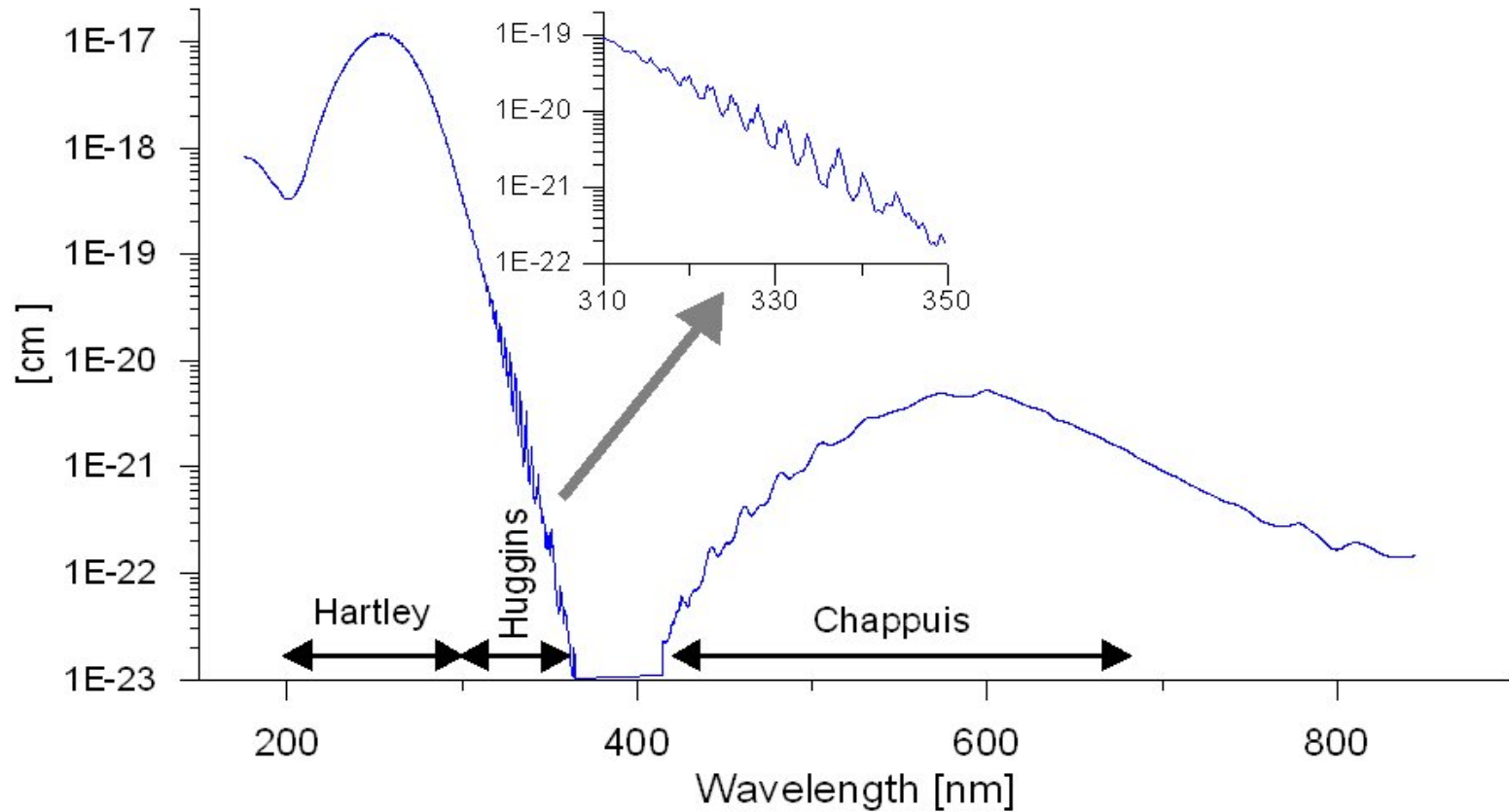
= a formula (or a computer code) for describing the transport of sunlight passing through the atmosphere, absorbed by trace gases, scattered by air molecules, clouds and aerosols, reflected by the surface, and finally arriving at the satellite.

Calculated reflectance spectrum in the UV-VIS

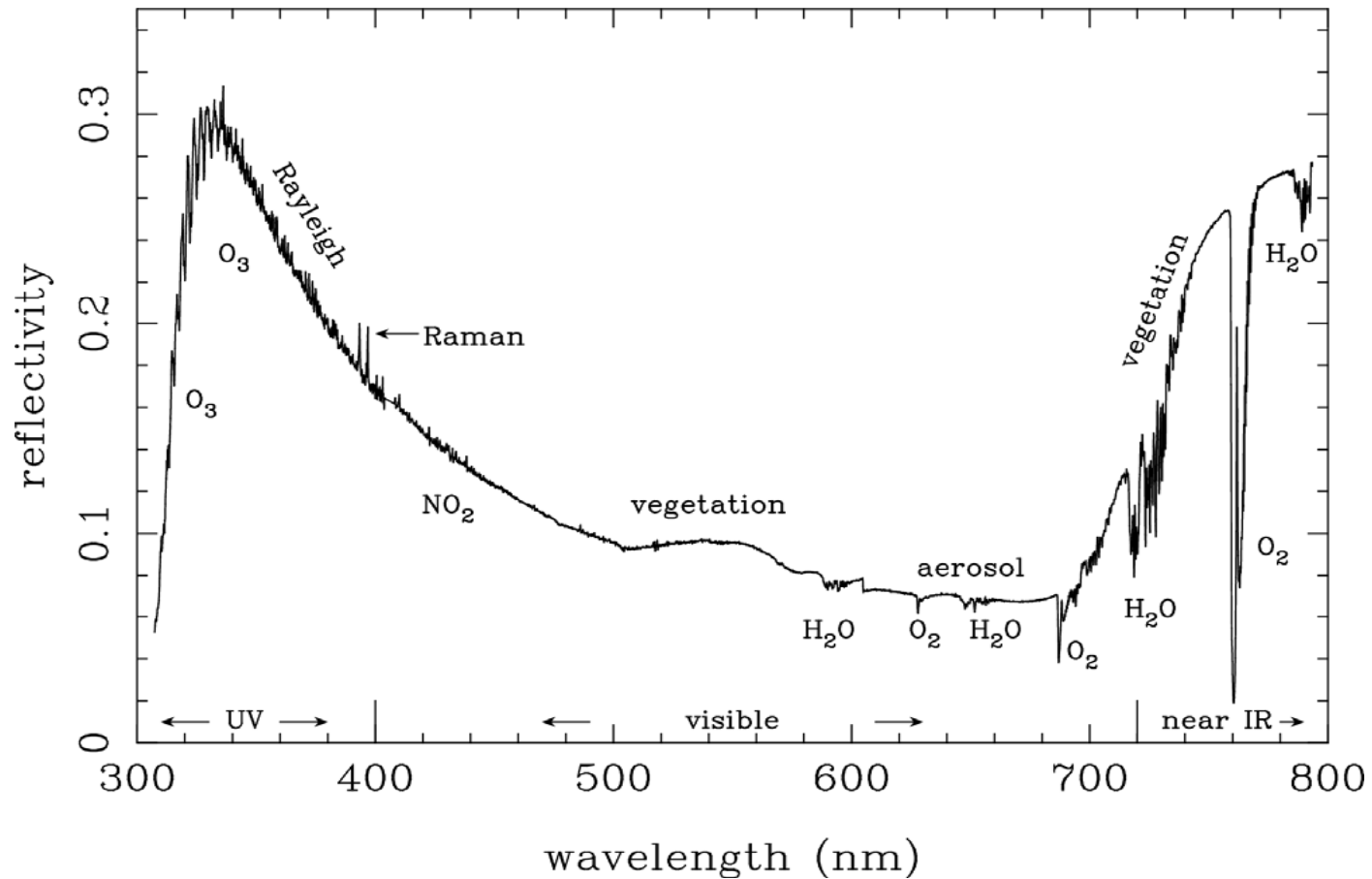


Ozone

Ozone absorption spectrum measured in the laboratory

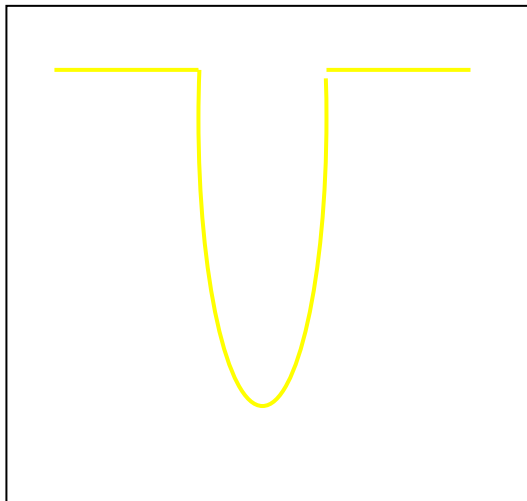


Reflectance spectrum of the Netherlands (cloudfree) measured by GOME



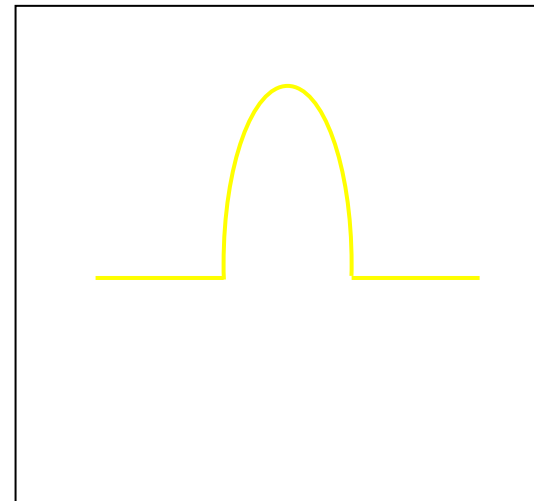
Absorption line in spectrum of reflected light

Spectrum of atmospheric radiation

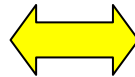


λ

Spectrum of absorption cross-section per molecule



λ

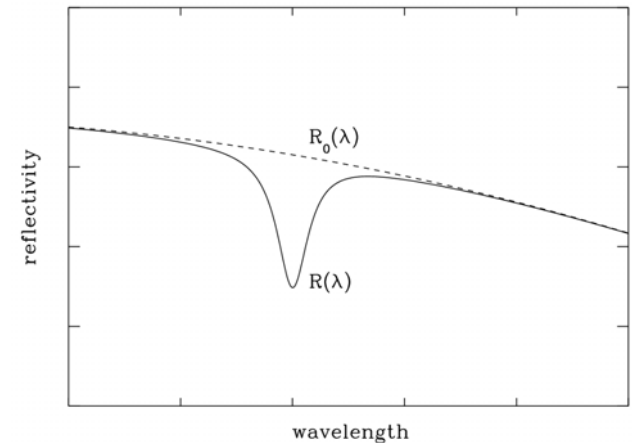


Differential Optical Absorption Spectroscopy = DOAS

Fit the absorption cross-section spectrum $\sigma(\lambda)$ to the logarithm of atmospheric reflectance spectrum $R(\lambda)$, to find the vertical column density N of the trace gas.

Assumption is:

$$R(\lambda) = R_0(\lambda) \exp(-\tau_s(\lambda))$$



where:

$R(\lambda)$: reflectance with the trace gas

$R_0(\lambda)$: reflectance without the trace gas

$\tau_s(\lambda)$: slant optical thickness of trace gas

DOAS formula:

$$R(\lambda) = R_0(\lambda) \exp(-\tau_s(\lambda))$$

$$\Leftrightarrow \ln R(\lambda) = \ln R_0(\lambda) - \tau_s(\lambda)$$

$$\Leftrightarrow -\ln R(\lambda) + \ln R_0(\lambda) = N_s \sigma(\lambda)$$

where:

$\ln I_0(\lambda)$: low-order polynomial in λ

N_s : slant column density of trace gas

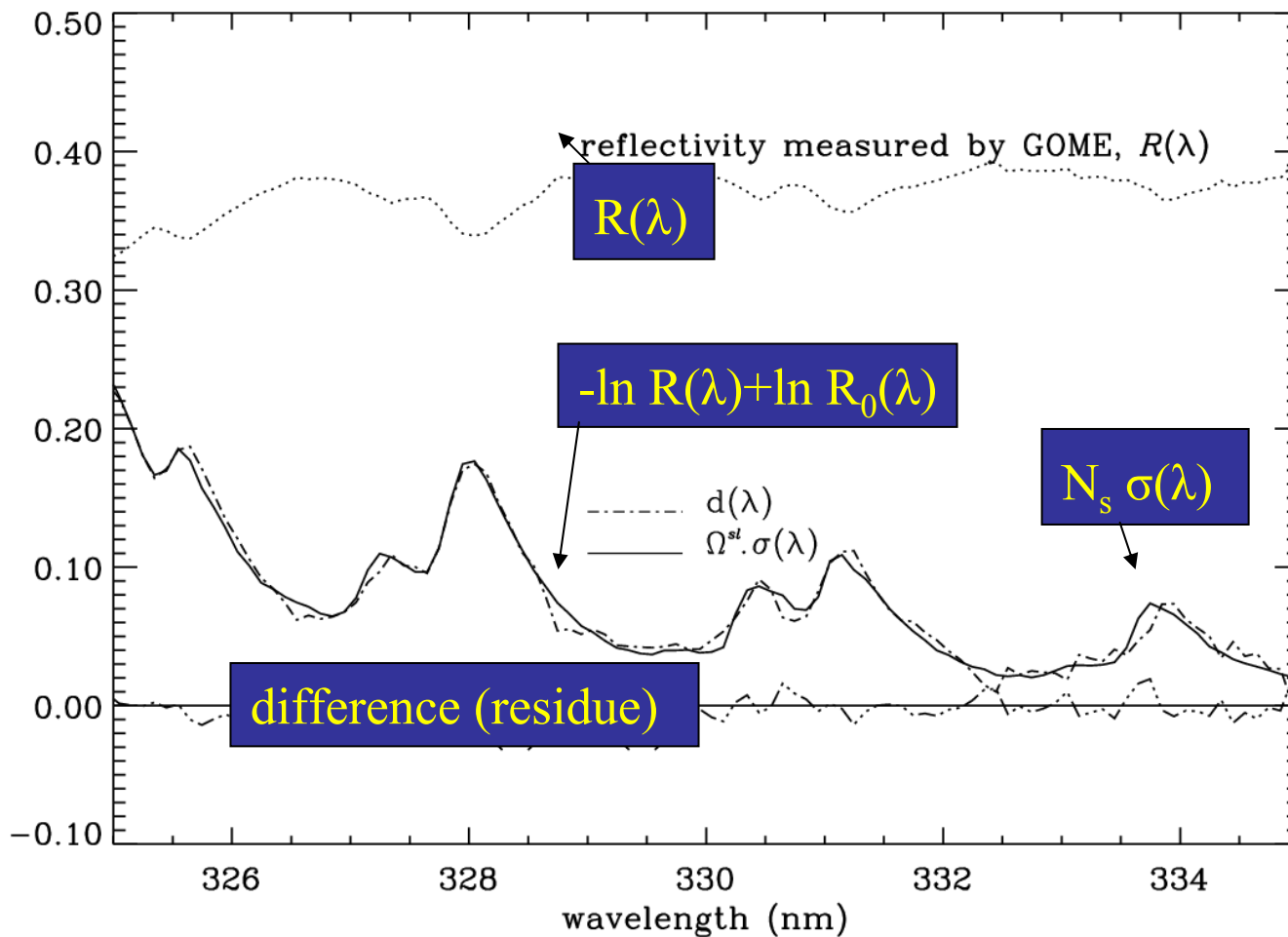
$N = N_s / M$: vertical column density of trace gas

M = air mass factor

Geometric path approximation:

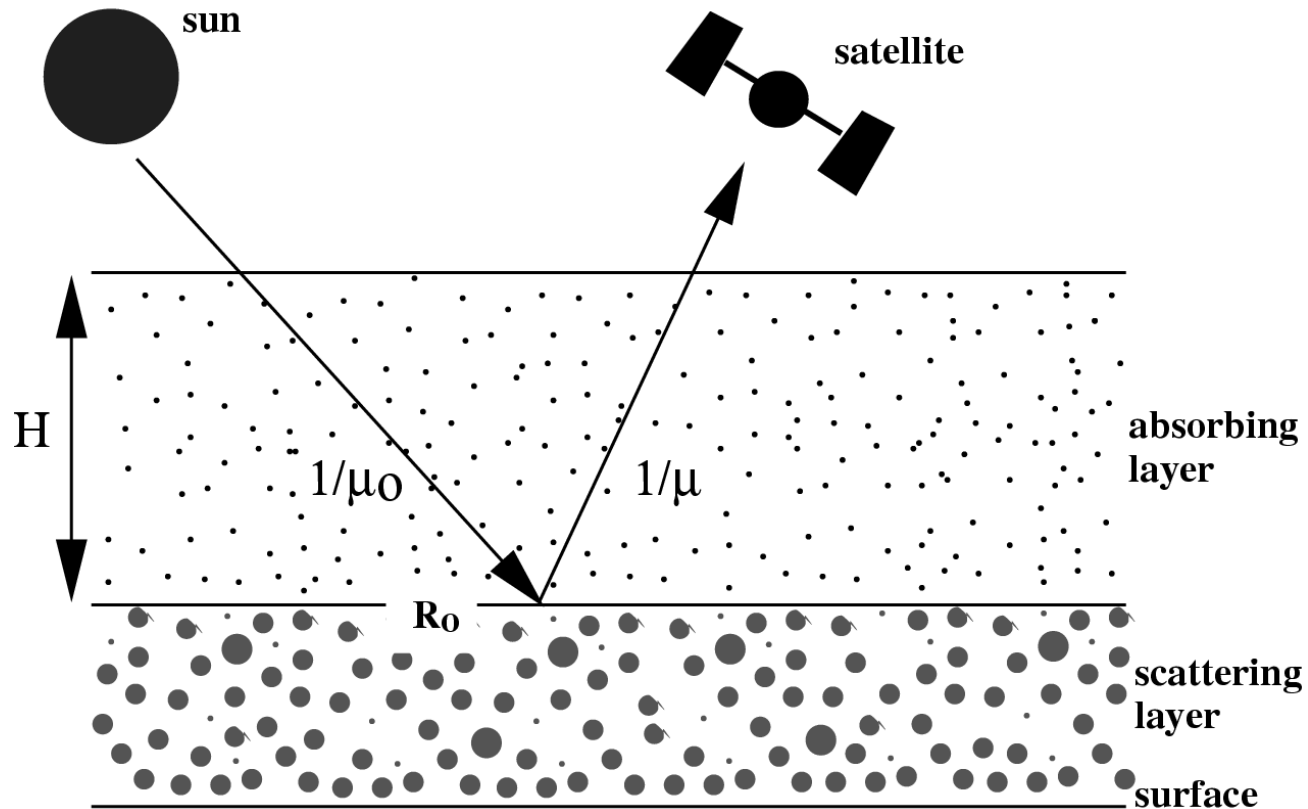
$$M \cong 1/\cos \theta + 1/\cos \theta_0 = 1/\mu_0 + 1/\mu$$

DOAS spectral fit of ozone

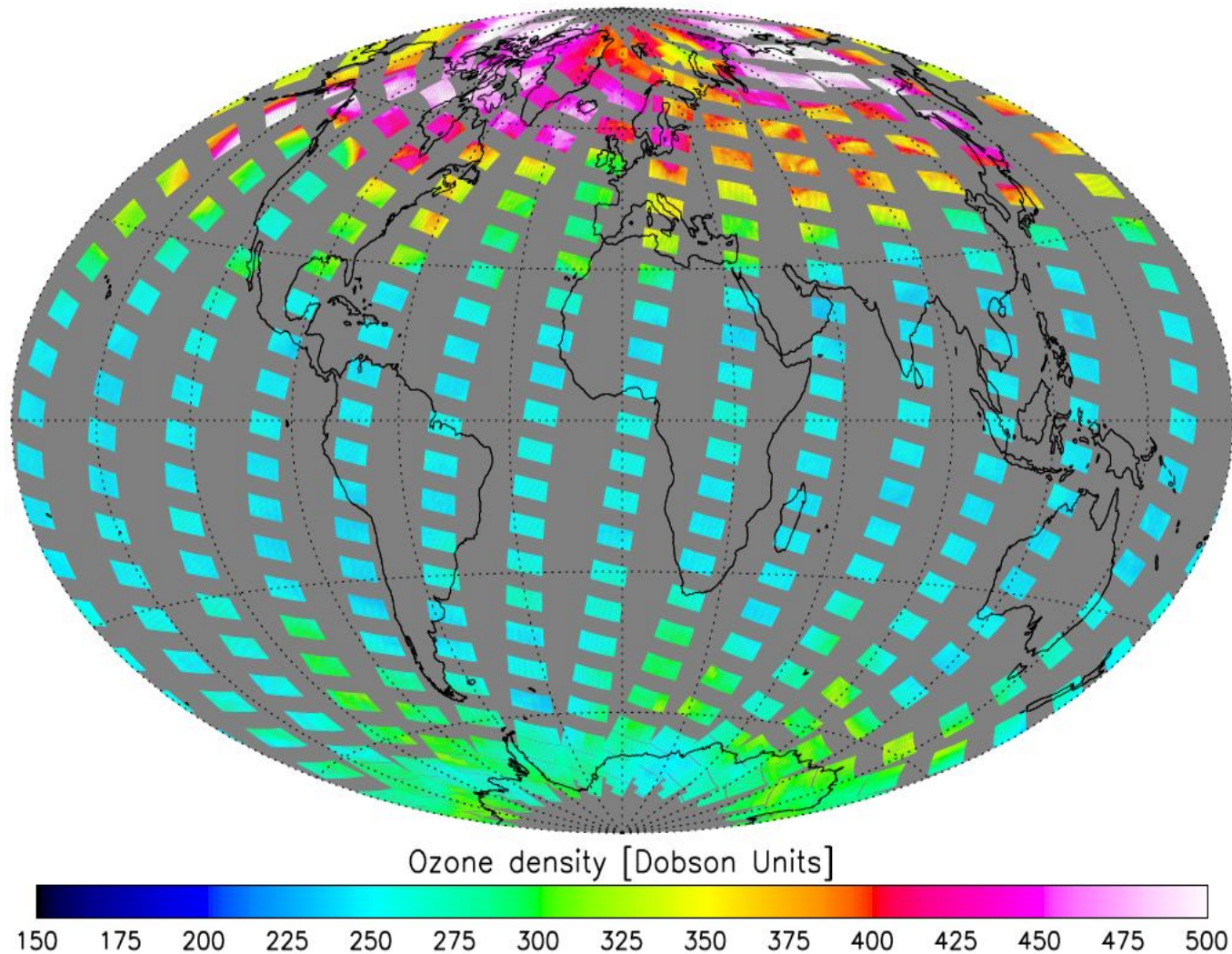


Air Mass Factor for ozone

Approximation: $N = N_s / M = 1/\mu_0 + 1/\mu$



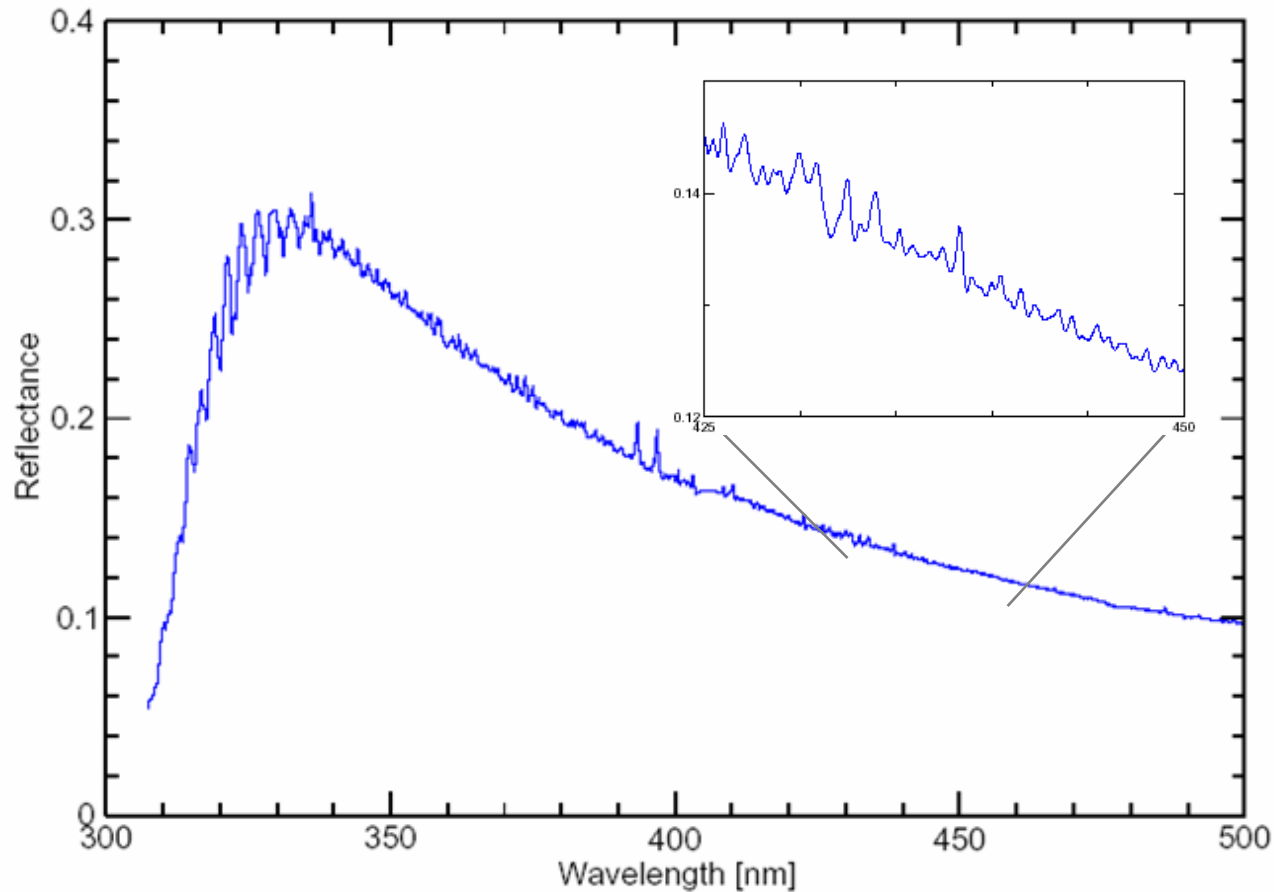
Ozone measurements by SCIAMACHY



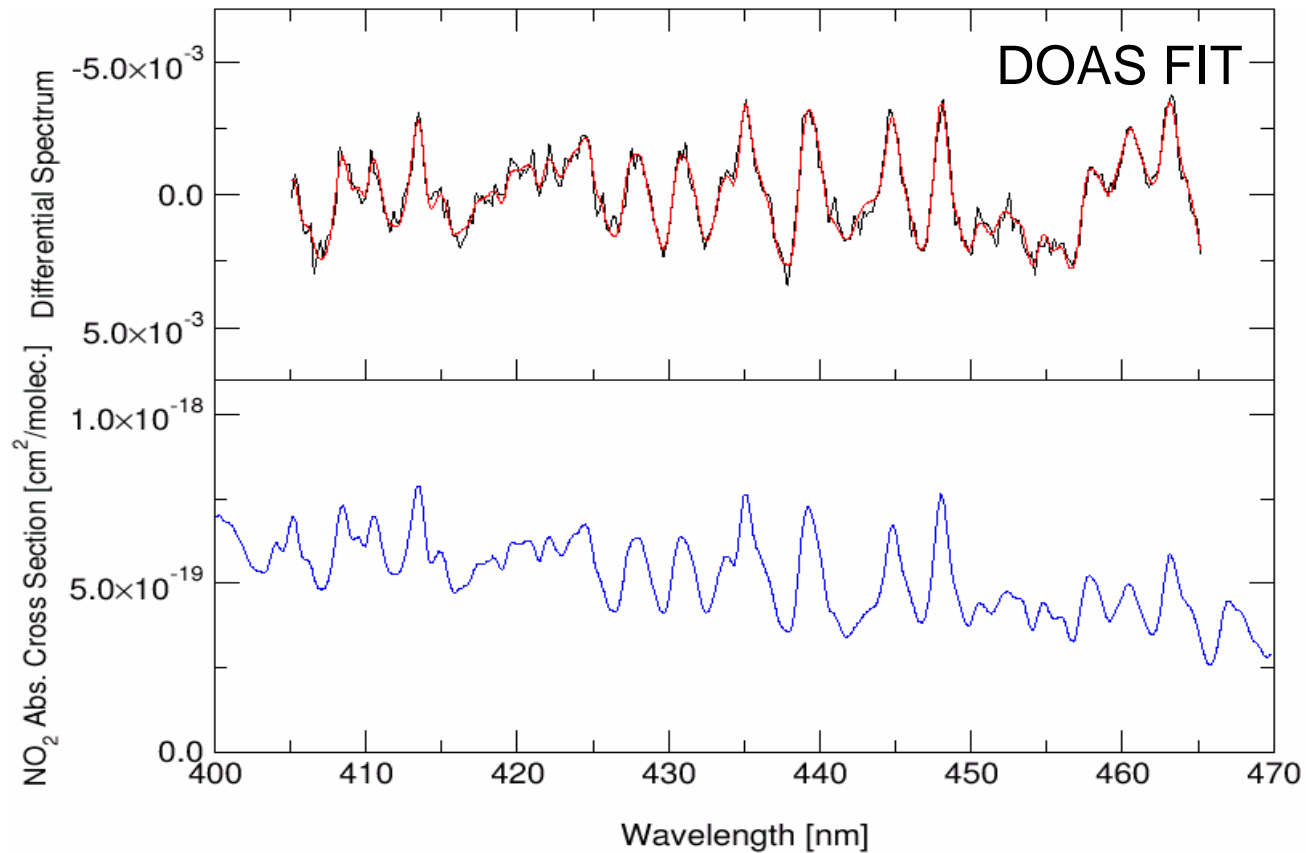
NO₂

How to measure NO₂ from the reflectance spectrum ?

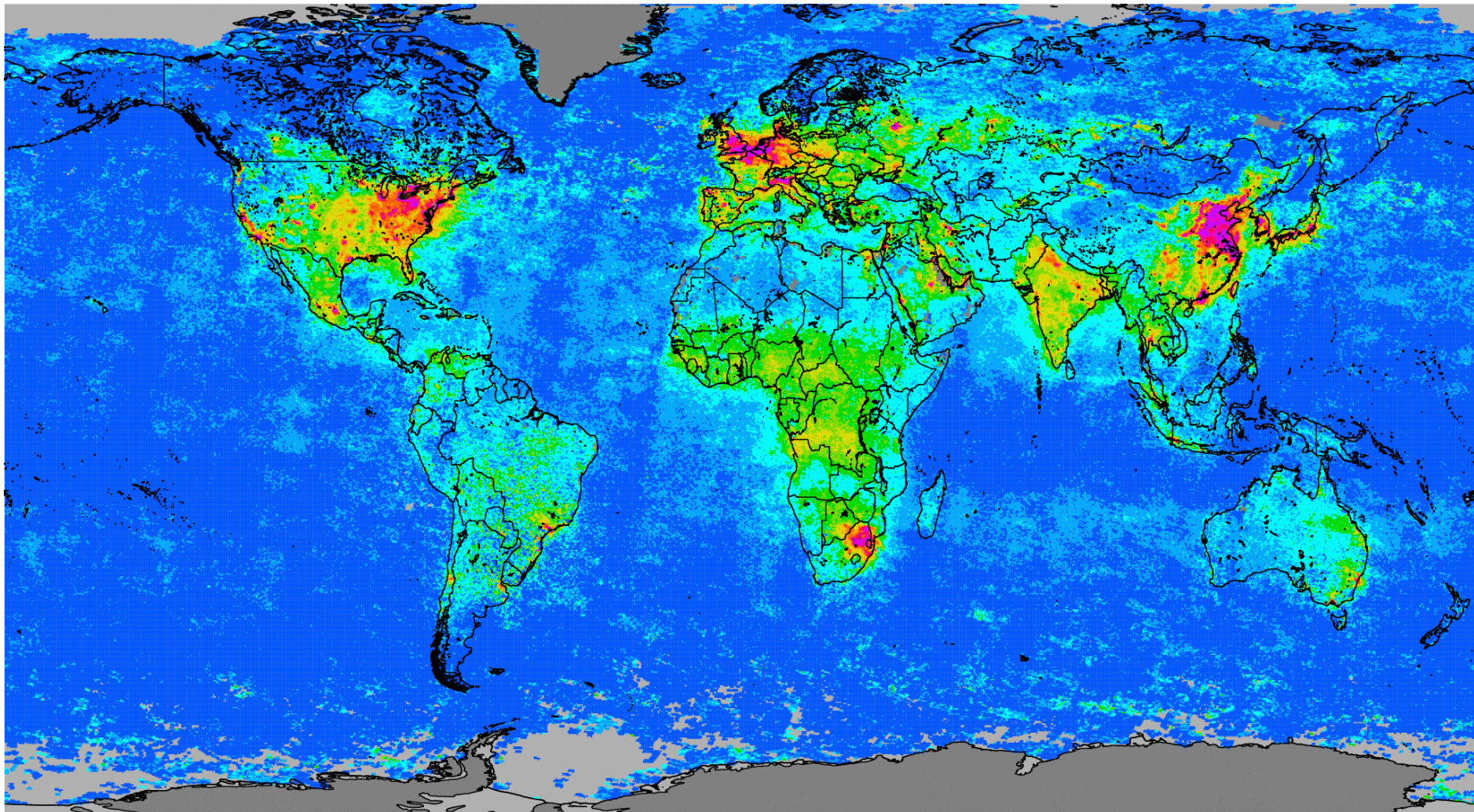
GOME, 25 July 1995, The Netherlands



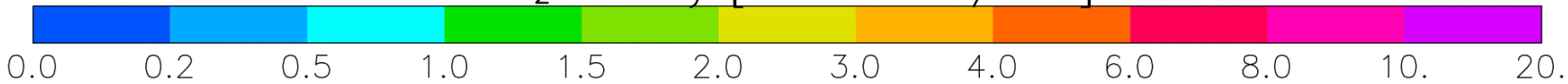
DOAS spectral fit of NO₂



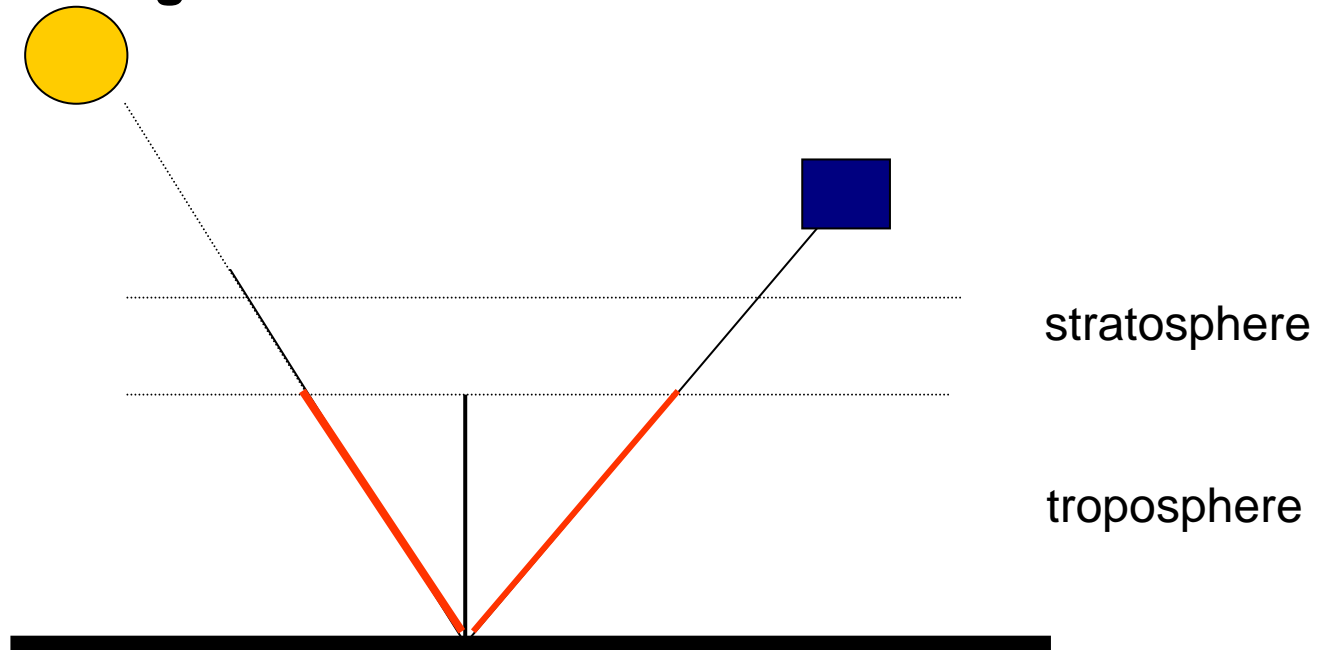
-> Slant column of NO₂



NO₂ density [10^{15} molec/cm²]

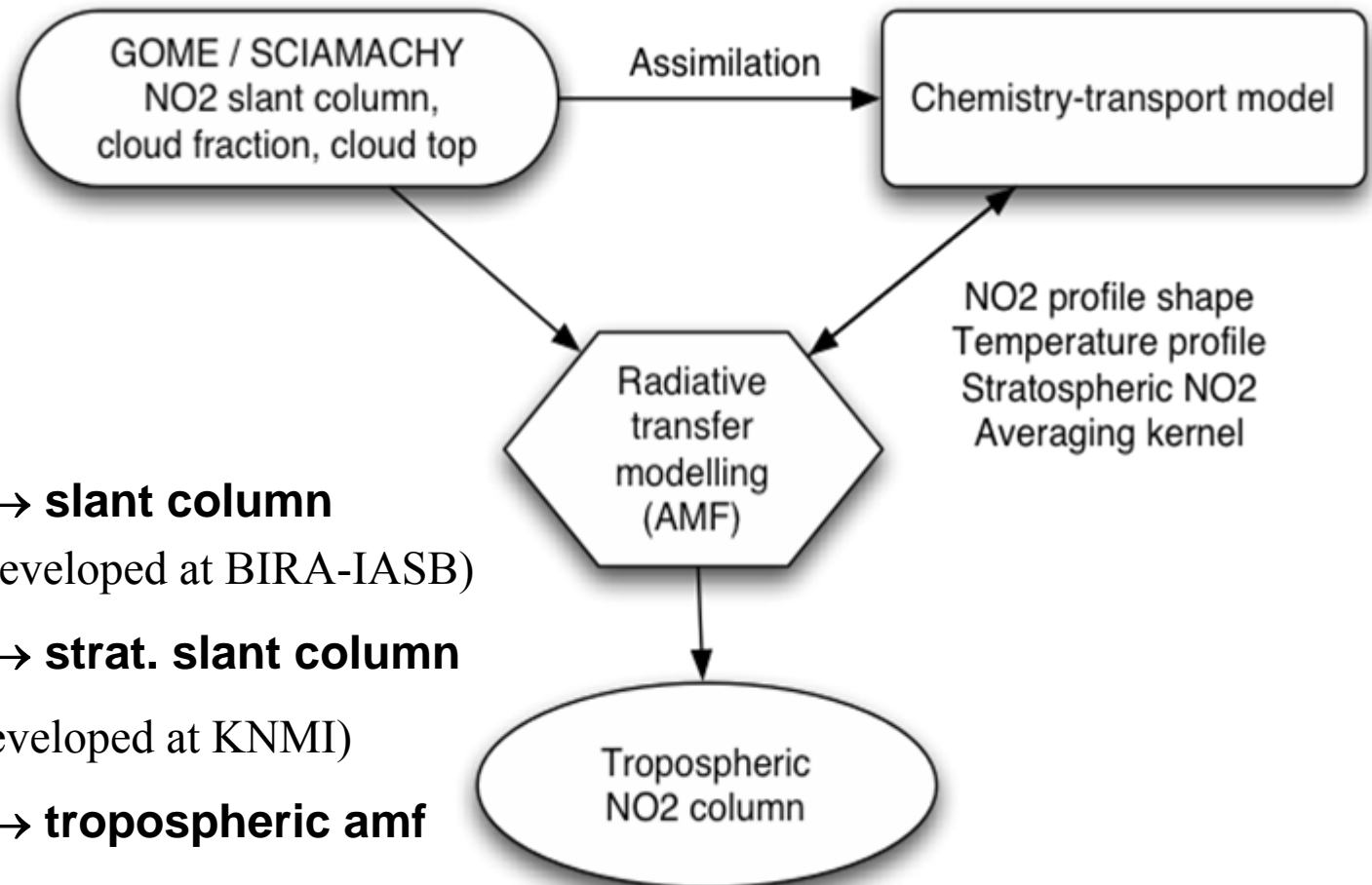


Retrieval using model information and satellite measurements



$$N_{\text{trop vertical}} = \frac{N_{\text{total slant}} - N_{\text{strat slant}}}{M_{\text{airmass trop}}}$$

Tropospheric NO₂



- 1. DOAS** → **slant column**
(GwinDOAS, developed at BIRA-IASB)
- 2. Assimilation** → **strat. slant column**
(TM4-DAM, developed at KNMI)
- 3. Modelling** → **tropospheric amf**
(DAK, developed at KNMI)

Summary

- UV-VIS spectrometry is preferred method to detect trace gases like ozone and NO₂.
- A radiative transfer model (including scattering) is needed to interpret these spectra.
- There are suitable spectrometers in space: GOME, SCIAMACHY, OMI.
- These instruments show important geophysical phenomena: ozone hole, tropospheric pollution.