Lecture 10.

Applications of passive remote sensing using extinction and scattering: Remote sensing of trace gases (ozone) and aerosols in the UV region.

1. The principles of Differential Optical Absorption Spectroscopy (DOAS).
2. Determination of total ozone concentration from ground–based measurements. The Dobson method.
3. TOMS (Total Ozone Mapping Spectrometer). Theoretical foundation of the TOMS ozone retrieval algorithm. Aerosol Index.

Required reading:

S: 6.2.1, 6.5

Richter A., Differential optical absorption spectroscopy as a tool to measure pollution from space. http://www.doas-bremen.de/paper/spec_euro_06_richter.pdf

Additional reading:

TOMS web site: http://toms.gsfc.nasa.gov/index.html

OMI web site: http://aura.gsfc.nasa.gov/instruments/omi/index.html

OMI ozone product –Algorithm Theoretical Basis Document (ATBD): http://eospso.gsfc.nasa.gov/eos_homepage/for_scientists/atbd/docs/OMI/ATBD-OMI-02.pdf

GOME, GOME-2, SCIAMACHY: http://www.iup.uni-bremen.de/gome/ http://www.doas-bremen.de/index.html

Advanced reading:

Platt**,** U., Stutz**,** J., Differential Optical Absorption Spectroscopy: Principles and Applications. Springer Berlin Heidelberg, 2008.

1. The principles of Differential Optical Absorption Spectroscopy (DOAS).

Recall Table 4.6 that shows gaseous species retrieved from satellite sensors. Retrievals in the UV/visible spectrum are performed by using the DOAS method (e.g., TOMS, OMI, GOME, GOME-2, SCIAMACHY).

The concept of DOAS: DOAS is a method to determine concentrations of trace gases by measuring their specific narrow band absorption structures in the UV and visible spectral region. In this spectral radiances measured from ground or satellites contain the "smooth" spectral contribution from molecular scattering, aerosol scattering and absorption, and surface reflection where as absorption by gases have fine spectral feature. DOAS separates the trace gas absorption cross sections into low and high frequency parts by specific numerical filtering methods, as well as separate via low filtering the smooth spectral contributions.

Examples of absorption cross-session: see Figure 4.10 for O_3 and O_2

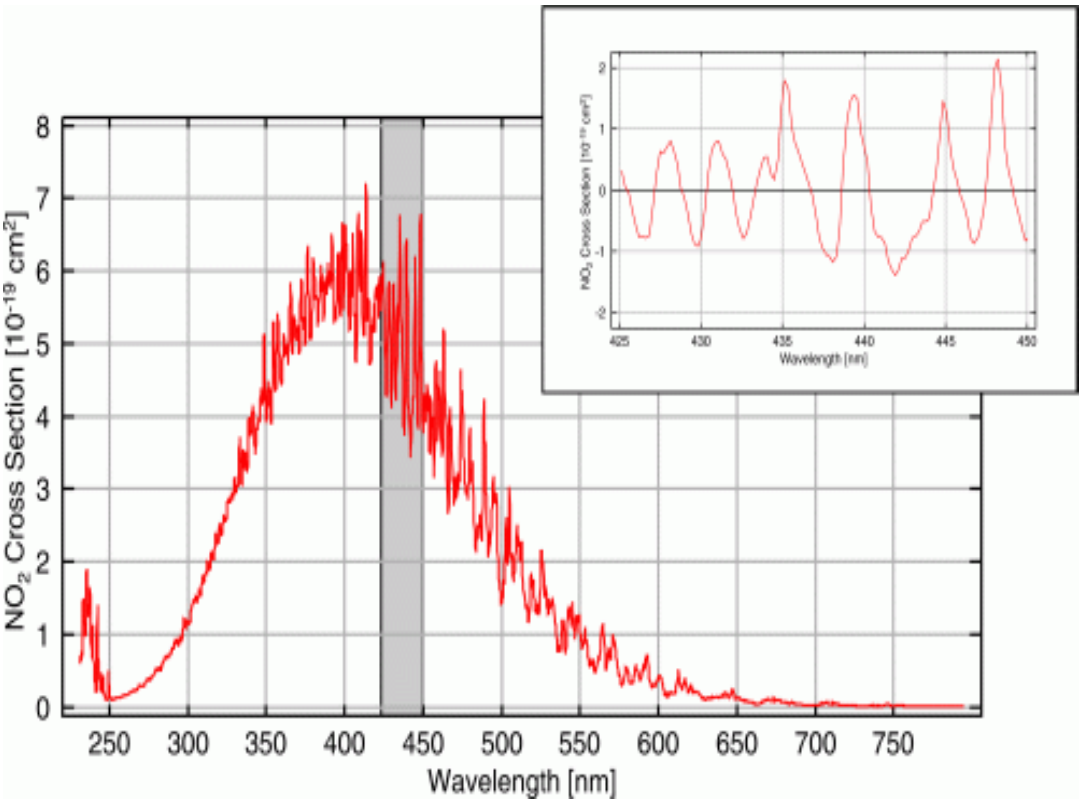
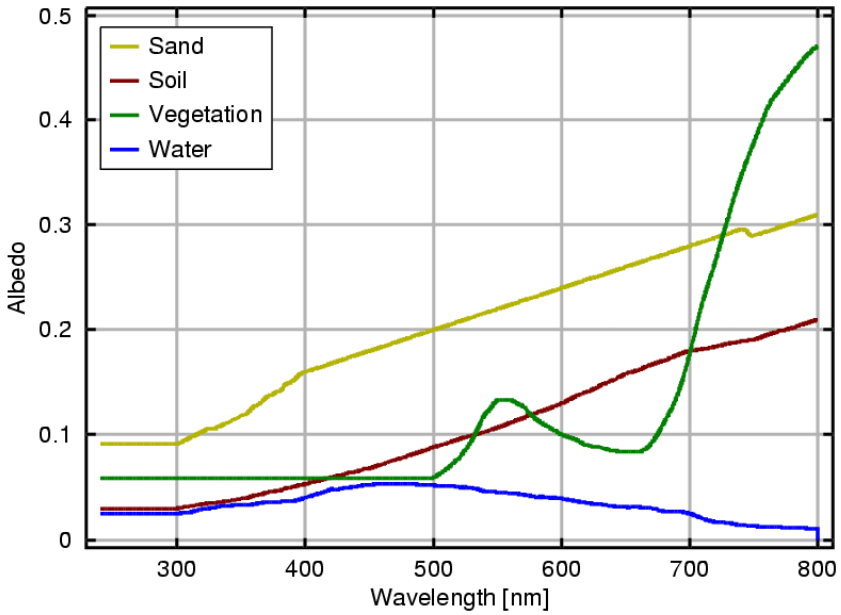
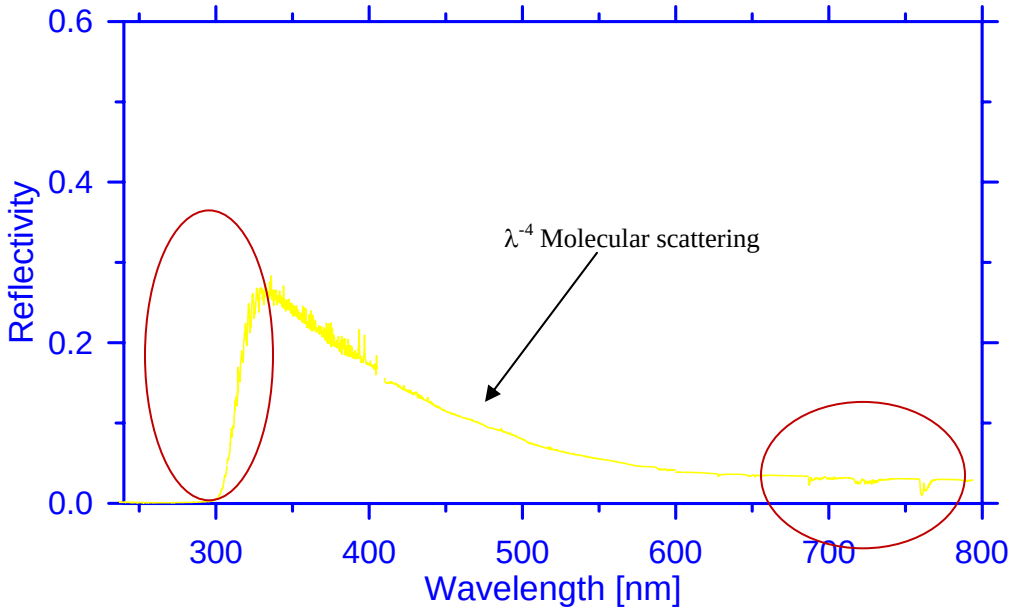


Figure 10.1 The absorption cross-section of NO_2 in the wavelength range covered by GOME and in the region often used for NO_2 retrieval (inset). The latter is already high pass filtered to highlight the differential structures which are used to separate absorption by trace species and extinction by scattering.

Surface reflectance in the UV: many natural surfaces have low albedo, exept snow and ice, and exibit a „smooth“ wavelength dependence



Example of TOA reflectivity observed by GOME over ocean (cloud- and aerosol free conditions): Red cicles show the spectral range of O3, H2O and O2 absorption, the



Consider the direct radiation:

$$I(\lambda,\Theta) = I_{ref}(\lambda)\exp\{-\int(\sum_{j=1}^{J}\sigma_j(\lambda)\rho_j(s) + \sigma_{Mie}(\lambda)\rho_{Mie}(s) + \sigma_{Ray}(\lambda)\rho_{Ray}(s))ds\}$$

$$I(\lambda,\Theta) = I_{ref}(\lambda)\exp\{-\sum_{j=1}^{J}\sigma_j(\lambda)u_j + \sigma_{Mie}(\lambda)u_{Mie} + \sigma_{Ray}(\lambda)u_{Ray}\}$$

$$\ln(I(\lambda,\Theta)/I_{ref}(\lambda)) = -\sum_{j=1}^{J}\sigma'_j(\lambda)u_j + \sum_p b_p^*\lambda^p$$

Air mass factor: is the ratio of the amount of a species measured in the slant column (SC) to that in the vertical column (VC):

$$AFM = \frac{SC}{VC} = \frac{\int \rho_j(s)ds}{\int \rho(z)dz}$$

The AMF depends on a variety of parameters such as

- wavelength
- geometry
- vertical distribution of the species (vertical profile must be known to compute AFM)
- clouds
- aerosol loading
- surface albedo

NOTE: An interactive calculator of air mass factor
http://www.doas-bremen.de/airmassfactors.htm

NOTE: There significant problems in the presence of clouds and aerosols.

2. Determination of total ozone concentration from ground –based measurements. The Dobson's method.

Principle: The Dobson's method uses measurements of direct solar radiation for pairs of wavelength in the Harltley-Huggins UV ozone bands (see Fig. 4.10 in Lecture 4): one pare where ozone UV absorption is strong and a second where absorption is weak. At each wavelength, the measured direct solar radiation obeys the Extinction law:

$$I^{\downarrow}_{dir,\lambda} = I_{0,\lambda} \exp(-\tau^{*}_{\lambda} / \mu_0)$$

where τ^{*}_{λ} is the optical depth of the entire atmospheric column

$$\tau^{*}_{\lambda} = \tau^{O3}_{a,\lambda} + \tau^{M}_{s,\lambda} + \tau^{A}_{\lambda} \qquad [10.1]$$

where $\tau^{O3}_{a,\lambda}$ is the optical depth due to O3 absorption; $\tau^{M}_{s,\lambda}$ is the optical depth due to molecular (Rayleigh) Scattering and τ^{A}_{λ} is the optical depth due to aerosol extinction. The difference between two adjacent wavelengths is

$$\Delta = \log(I^{\downarrow}_{dir,\lambda 1} / I^{\downarrow}_{dir,\lambda 2}) - \log(I_{0,\lambda 1} / I_{0,\lambda 2}) = -[\Delta\tau^{O3}_{a} + \Delta\tau^{M}_{s} + \Delta\tau^{A}] / \mu_o \qquad [10.2]$$

In Eq.[10.2], the differential aerosol optical depth, $\Delta\tau^{A}$, is the most uncertain => subtract the differences for two pairs of wavelengths

$$\Delta^{AD} = \Delta^{A} - \Delta^{D} \qquad [10.3]$$

Assuming that differences of aerosol optical depth are the same for each pair, we have

$$\Delta^{AD} \approx -[\Delta\tau^{A,O3}_{a} - \Delta\tau^{D,O3}_{a}] / \mu_0 - [\Delta\tau^{A,M}_{s} - \Delta\tau^{D,M}_{s}] / \mu_0 \qquad [10.4]$$

The ozone optical depth is the product of the ozone absorption coefficient and the column integrated ozone amount, X_0, then from Eq.[10.4] we have

$$X_0 = [\mu_0\Delta^{AD} - (\Delta\tau^{A,M}_{s} - \Delta\tau^{D,M}_{s})] / [\Delta k^{A,O3}_{a} - \Delta k^{D,O3}_{a}] \qquad [10.5]$$

or

$$X_0 = \frac{\mu_0\Delta^{AD}}{a} - b \qquad [10.6]$$

where the coefficients ***a*** and ***b*** are determined from known absorption coefficients and the Rayleigh scattering.

A Dodson spectrometer operating at the WMO network has two pairs of wavelengths:

A=(0.3055 μm, 0.3254 μm) and D= (0.3176 μm, 0.3398 μm)

For these two pairs:

$$a = \Delta k_a^{A,O3} - \Delta k_a^{D,O3} \approx 1.388(atm\ cm)^{-1} \qquad [10.7]$$

$b \approx 0.009 P_{sur}$, where P_{sur} id the surface pressure (in atm)

X_0 from Eq.[10.6] is in **Dobson units** (milli atm–cm)

Dobson Unit (DU) is a vertical thickness of atmosphere in thousandths of a centimeter that is occupied by O3 when concentrated into a uniform layer of pure gas at the STP.

3. TOMS (Total Ozone Mapping Spectrometer). Theoretical foundation of the TOMS ozone retrieval algorithm. Aerosol Index.

- **TOMS on board of the NIMBUS-7 Satellite (TOMS/ NIMBUS-7):**
  data from October 1978 to May 1993
- **TOMS on board of the Earth Probe Satellite (EP TOMS):**
  data from July 1996 to present

NOTE: TOMS also has flown on the ADEOS and Meteor-3 Satellites

EP TOMS measures both incoming solar energy and backscattered UV radiation at six different channels: 360.4 ± 0.2 nm, 331.3 ± 0.1 nm, 322.4 ± 0.1 nm, 317.6 ± 0.1 nm, 312.6± 0.1 nm, and 308.6 ± 0.1 nm.

TOMS ozone retrieval algorithm:

Consider an atmosphere bounded below by a Lambertian surface of reflectivity R_{sur}.
The radiance measured by a TOMS instrument at the top of the atmosphere (TOA), I_{TOA}, can be represented as the sum of purely atmospheric backscattered radiance, I_A, and reflection from the incident radiation from the reflecting surface, I_s,

$$I_{TOA}(\lambda,\theta,\varphi,\theta_0,\varphi_0,u_{o3},P_0,R_{sur}) = I_A(\lambda,\theta,\varphi,\theta_0,\varphi_0,u_{o3},P_0) + I_s(\lambda,\theta,\varphi,\theta_0,\varphi_0,u_{o3},P_0,R_{sur}) \quad [10.8]$$

where

λ is the wavelength (central value of a particular TOMS channel); (θ, φ) is the satellite viewing angle; (θ_0, φ_0) is solar angle*;* $\boldsymbol{P_o}$ is the surface pressure and $\boldsymbol{u_{03}}$ is the column ozone amount.

The surface reflection term can be expressed as follows

$$I_s(\lambda,\theta,\varphi,\theta_0,\varphi_0,u_{o3},P_0,R_{sur}) = \frac{R_{sur} I_{dd}(\lambda,\theta,\varphi,\theta_0,\varphi_0,u_{o3},P_0) f(\lambda,\theta,\varphi,P_0)}{1 - R_{sur} S_b(\lambda,u_{o3},P_0)} \quad [10.9]$$

where

$\boldsymbol{S_b}$ is the fraction of radiation reflected from surface that atmosphere reflects back to space;

$\boldsymbol{I_{dd}}$ is the total amount of direct and diffuse radiation reaching the surface at $\boldsymbol{P_o}$;

$\boldsymbol{f}$ is the fraction of radiation reflected toward satellite in the direction (θ, φ) that reaches the satellite.

NOTE: The denominator in the above equation accounts for multiple reflection between the ground and the atmosphere.

<u>Steps of TOMS ozone retrieval algorithm:</u>

a) Using a radiative transfer code, pre-calculate N-values at TOMS channels that should be measured for different ozone amounts, given the location of the measurement, viewing conditions, and surface properties.

The **N-value** is defined as

$$N = -100 \log_{10}\left(\frac{I_{TOA}}{F}\right) \quad [10.10]$$

b) The initial estimate of O_3 is derived from N-values of a pair of wavelengths (one with strong O_3 absorption and another without O_3 absorption).

c) Construct **the residues** as $\Delta N = N_{meas} - N_{calc}$. Using the **residues** at a properly chosen **triplet wavelength**, it is possible to simultaneous solve for the <u>ozone amount</u> and for contribution to the radiances that is linear with wavelengths (e.g.,

from wavelength dependence of the surface reflectivity or instrument calibration).

Table 10.1 Pair/triplet wavelength of EP-TOMS

Pair/Triplet designation	O3 sensitive Wavelength (nm)	O3 insensitive Wavelength (nm)	Reflectivity wavelength (nm)
A	312.6	331.3	360.4
B	317.6	331.3	360.4
C	322.4	331.3	360.4

To carry out the above calculations (i.e., to calculate $I_{TOA,}$ I_A, I_{dd} , f and S_b in Esq.[10.8]-[10.9]), the following information is required:

1) Ozone absorption coefficients as a function of temperature at the TOMS wavelengths;

2) Rayleigh scattering coefficients;

3) Climatological temperature profiles;

4) Climatological ozone profiles (TOMS retrieval algorithms uses 26 O_3 profiles. Each standard profile represents a yearly average for a given total ozone and latitude based on ground-based and ozonesonde data; Profiles have been constructed for three latitude bands: low latitude (15^0)- 6 profiles, mid-latitude (45^0) - 10 profiles, and high latitude (75^0) – 10 profiles (total 26 O_3 profiles).

5) Solar position, satellite viewing angle and IFOV

(EP/TOMS makes 35 measurements every 8 seconds, strung along a line perpendicular to the motion of the satellite. This results in an instantaneous satellite field of view (or a footprint) of 39x39 km at nadir to 70x140 km at the extreme off-nadir)

6) Pressure at the reflecting surface

- ***Effects of aerosols on O3 retrievals***

Atmospheric aerosols can scatter and absorb the UV-radiation in addition to molecular scattering and hence affect the ozone retrieval.

UV-absorbing aerosols: dust, carbonaceous, some organics, volcanic ash

- Aerosol effects on UV radiation depend on aerosol type (refractive index and particle size distribution, optical depth, and aerosol layer height.
- The presence of UV-absorbing aerosols result in the underestimation of the TOMS retrieved ozone

Aerosol Correction Scheme:

Assumes the linear relationship between ozone retrieval errors and TOMS Aerosol Index

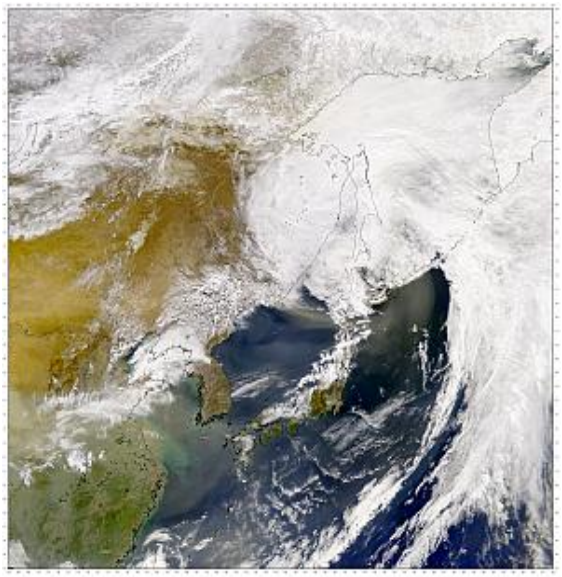
TOMS **Aerosol Index (AI) is** defined as

$$AI = -100[\log_{10}\left(\frac{I_{331}}{I_{360}}\right)_{meas} - \log_{10}\left(\frac{I_{331}}{I_{360}}\right)_{cal}] \qquad [10.11]$$

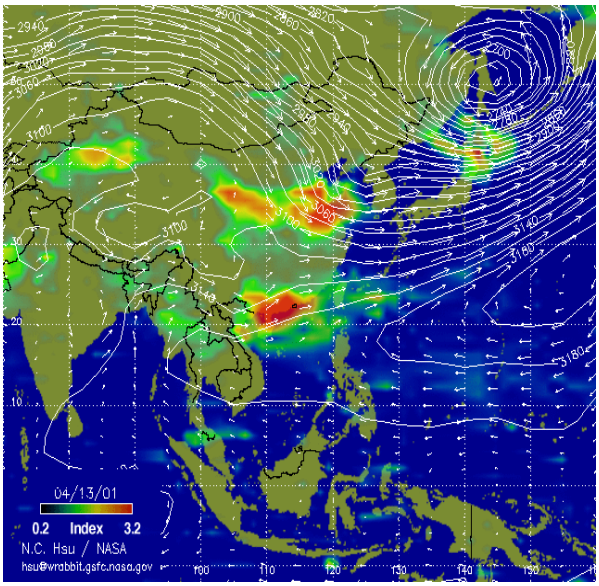
AI is defined in such a way that positive values correspond to absorbing aerosol, while small positive and negative for nonabsorbing aerosols and clouds. AI is a qualitative characteristic to detect the presence of aerosols absorbing in the UV (such as dust and soot).

Example: Dust storm and biomass burning of April 13, 2001

SeaWiFS image (true color image)



TOMS AI



Other products from TOMS:

Volcanic SO2 (see Krueger A.J. et al., Volcanic sulfur dioxide measurements from the total ozone mapping spectrometer instruments, Journal of Geophysical Research (1995), v. 100, 14,057-14,076 .

OMI (Ozone Monitoring Instrument)

launched on the Aura Satellite on 25 July 2004.

OMI's features:

- OMI employs hyperspectral imaging in a push-broom mode to observe solar backscatter radiation in the visible and ultraviolet. The Earth will be viewed in 740 wavelength bands along the satellite track with a swath large enough to provide global coverage in 14 orbits (1 day). The nominal 13 x 24 km spatial resolution can be zoomed to 13 x 13 km for detecting and tracking urban-scale pollution sources. The hyperspectral capabilities will improve the accuracy and precision of the total ozone amounts.
- Continue global total ozone trends from satellite measurements beginning in 1970 with BUV on Nimbus-4.
- OMI maps ozone profiles at 36 x 48 km, a spatial resolution never achieved before.
- OMI measures key air quality components such as NO_2, SO_2, BrO, OClO, and aerosol characteristics.
- OMI maps global distribution and trends in UV-B radiation.
- A combination of algorithms including TOMS version 7, Differential Optical Absorption Spectroscopy (DOAS), Hyperspectral BUV Retrievals and forward modeling will be used together to extract the various OMI data products.
- Near Real Time (NRT) production of ozone and other trace gases.