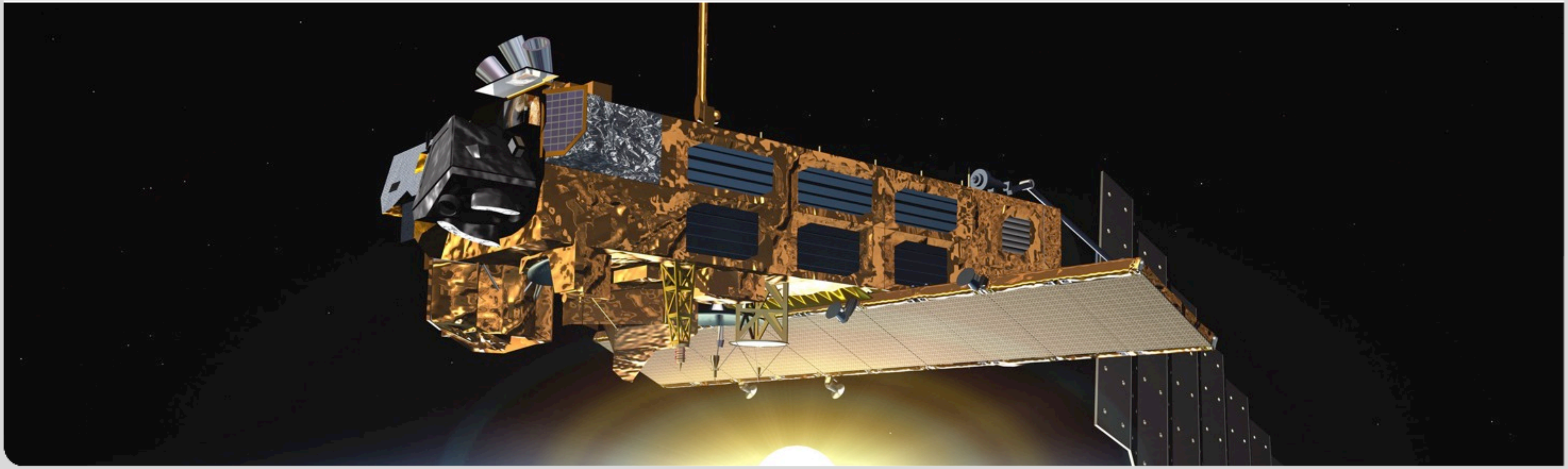
Karlsruhe Institute of Technology

Satellite remote sensing of trace gases – Limb sounding geometry

Gabriele Stiller

Institute of Meteorology and Climate Research



Outline

- Characteristics of the limb observation geometry
  - Solar, lunar and stellar occultation
  - Limb emission sounding
  - Limb scattering
- Spectroscopy and Radiative transfer
  - Physical basis – molecular absorption, emission, and scattering
  - Radiative transfer equations for various observation geometries and wavelength ranges
- Wavelength ranges and related instruments
  - Trace species
  - Coverage
- Retrieval theory
- Examples of trace species distributions from different instruments
- Data availability and download

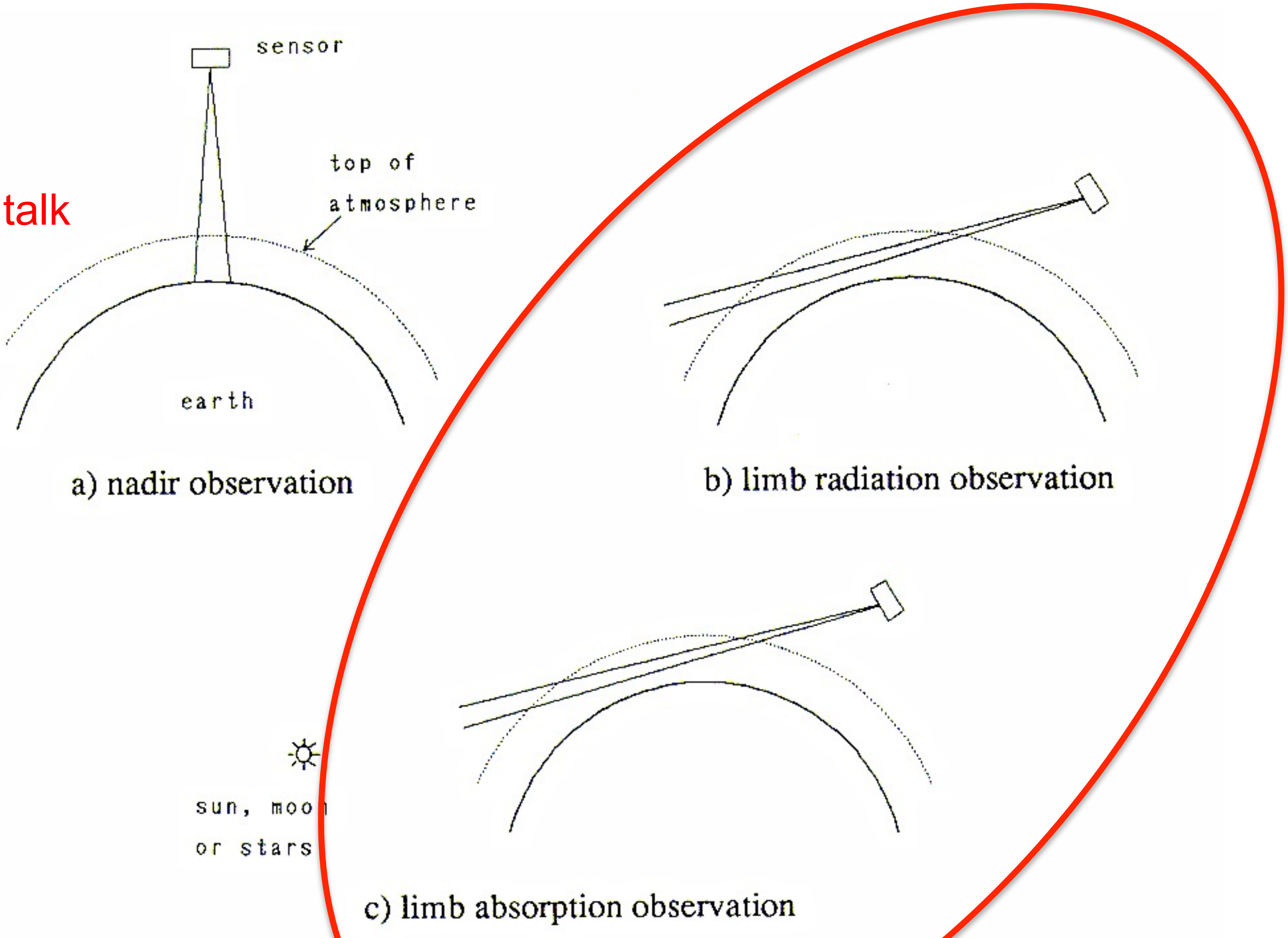
What is remote sensing from satellites?

- Satellite instruments do not measure at the position of the atmosphere the scientists are interested in **– remote**
- The instruments do not measure the composition or other physical parameters directly **- indirect**
- The measurement technique makes use of the interaction of the atmosphere's constituents with electromagnetic fields – absorption, emission or scattering of photons
- All satellite instruments measure the spectral distribution of photons arriving at the instrument and deduce from this the distribution of constituents in the atmosphere

How? This is the content of this talk

Characteristics of the limb sounding observation geometry

Cathy's talk



a) nadir observation

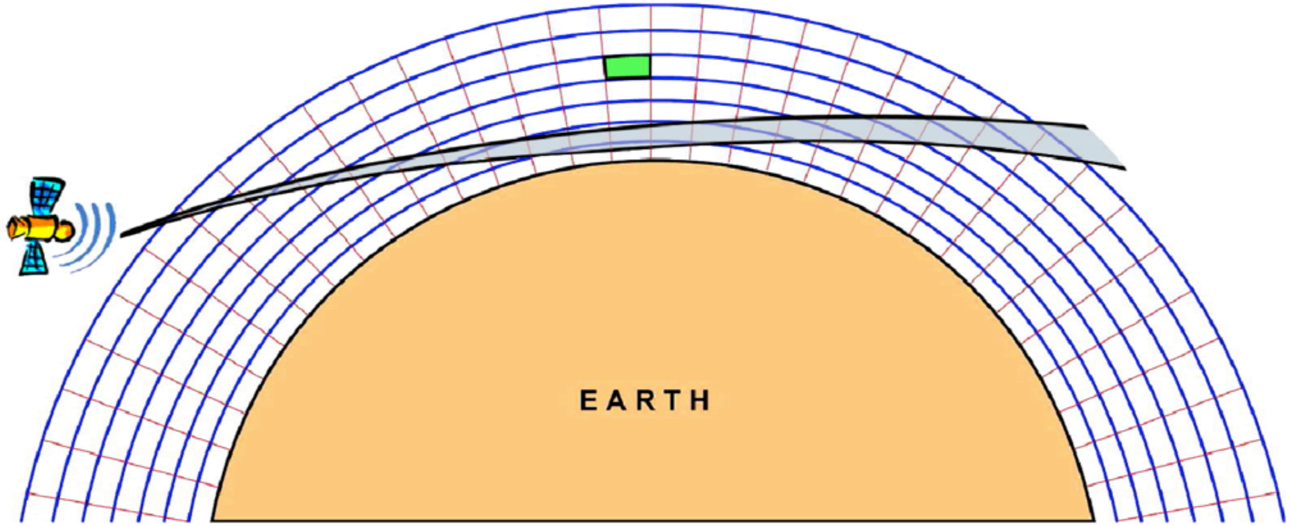
b) limb radiation observation

c) limb absorption observation

Figure 2.13.1 Direction of atmospheric observation

Figure source: http://wtlab.iis.u-tokyo.ac.jp/~wataru/lecture/rsgis/rsnote/cp2/cp2-13.htm

Limb viewing geometry

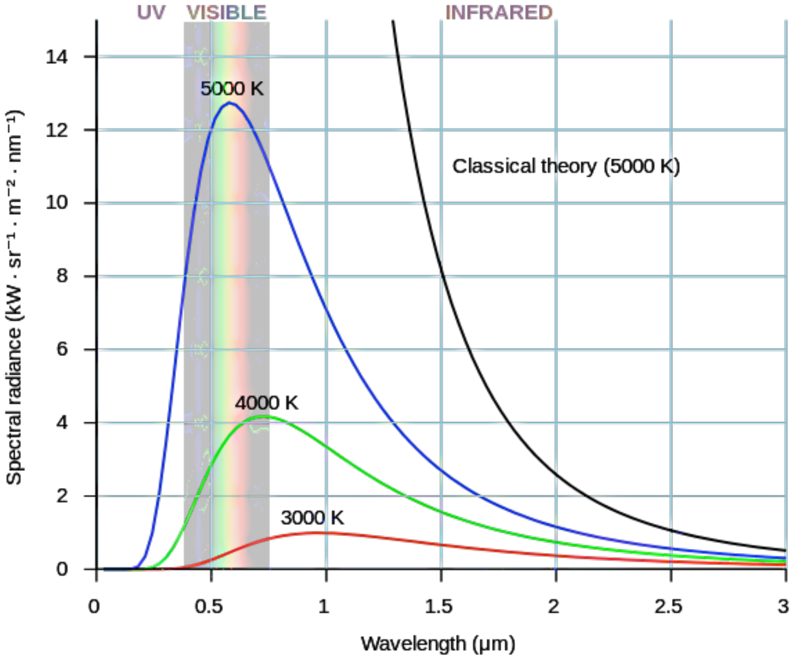


- Long Long way through the atmosphere – very sensitive to low abundances
- Atmosphere usually becomes too dense at low altitudes – covers atmosphere down to upper troposphere only
- Observations at different viewing angles provide profiles with good vertical resolution

Figure by Carlotti and Magnani, Optics express, Vol. 17, Issue 7, pp. 5340-5357 (2009)
http://www.osapublishing.org/oe/fulltext.cfm?uri=oe-17-7-5340

Solar, stellar and lunar occultation

- Satellite instruments looks through the atmosphere to a bright radiation source; very good signal-to-noise ratio
- The radiation of the source is attenuated by the atmosphere
- The absorption signatures contain the information on the atmosphere
- The Planck function of the incoming radiation is determined by temperature of emitter: Sun ~ 5700 K, moon ~ 270 K , stars: like the sun, or hotter/colder
- Along the orbit of a satellite, the instrument can measure only a few times:
  - For solar/lunar occultation for example: one sun/moon-rise and one sun/moon-set
  - For stellar occultation: depends on the number of stars used

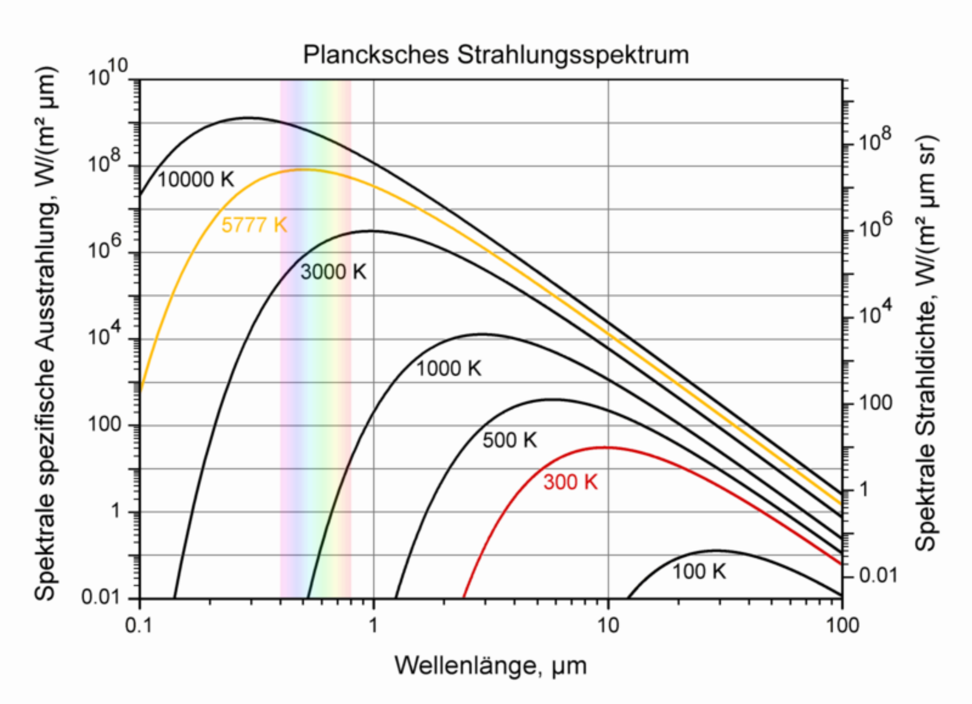


http://upload.wikimedia.org/wikipedia/commons/1/19/Black_body.svg

By Darth Kule (Own work) [Public domain], via Wikimedia Commons

Limb emission sounding

- No background radiation source, the Earth's atmosphere itself is the radiation emitter.
- Due to lower temperatures of the atmosphere compared to stars, the Planck function's peak is far lower, and the peak position is shifted to higher wavelengths (infrared to microwave); lower signal-to-noise ratio.
- The measurements do not depend on the satellite position relative to the radiation source: day and night time measurements over the full globe (depending on inclination angle) are possible.



http://upload.wikimedia.org/wikipedia/commons/0/0e/BlackbodySpectrum_loglog_150dpi_de.png

By Sch (Own work) [GFDL (http://www.gnu.org/copyleft/fdl.html) or CC-BY-SA-3.0 (http://creativecommons.org/licenses/by-sa/3.0/)], via Wikimedia Commons

Limb scattering

- Sunlight scattered by the gaseous atmosphere or particles (clouds, aerosols) towards the satellite position is measured
- Makes use of the radiation maximum of the sun: VIS-UV
- Complicated radiative transfer due to (multiple) scattering
- Independent of satellite position wrt sun, but only daytime measurements possible

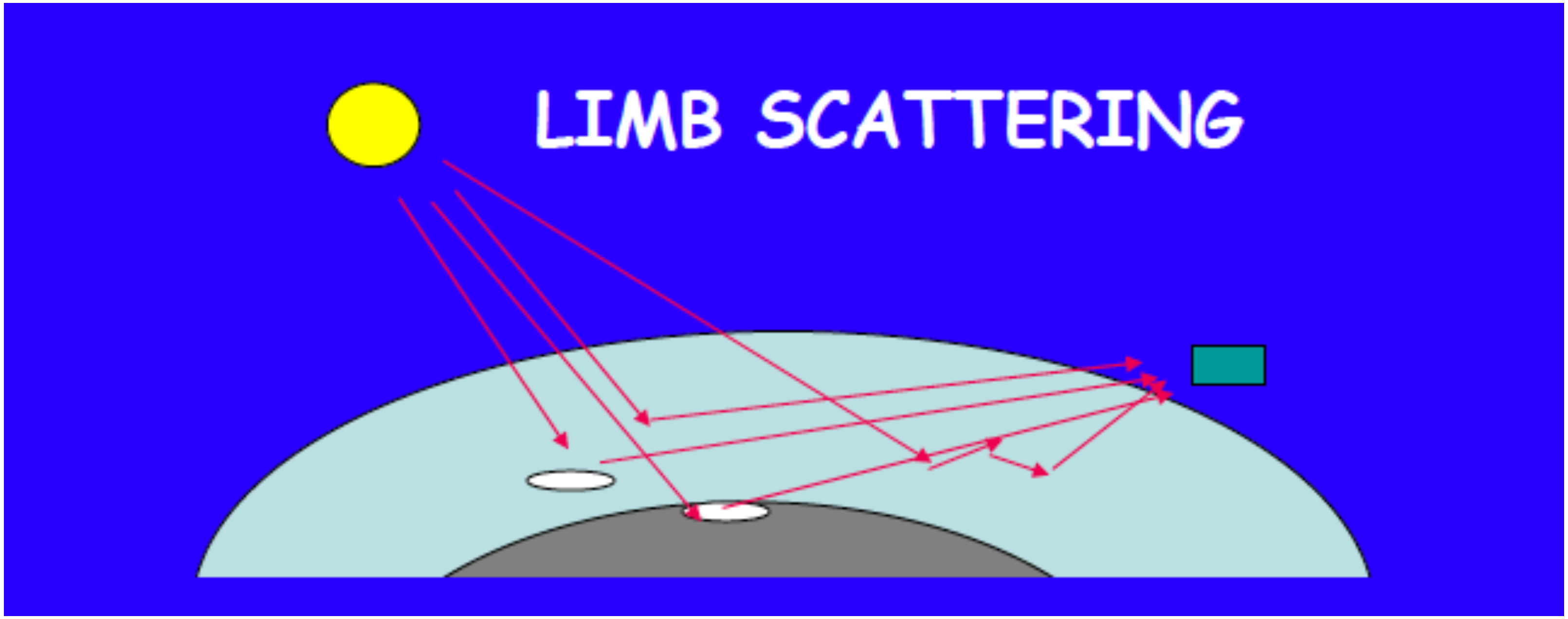
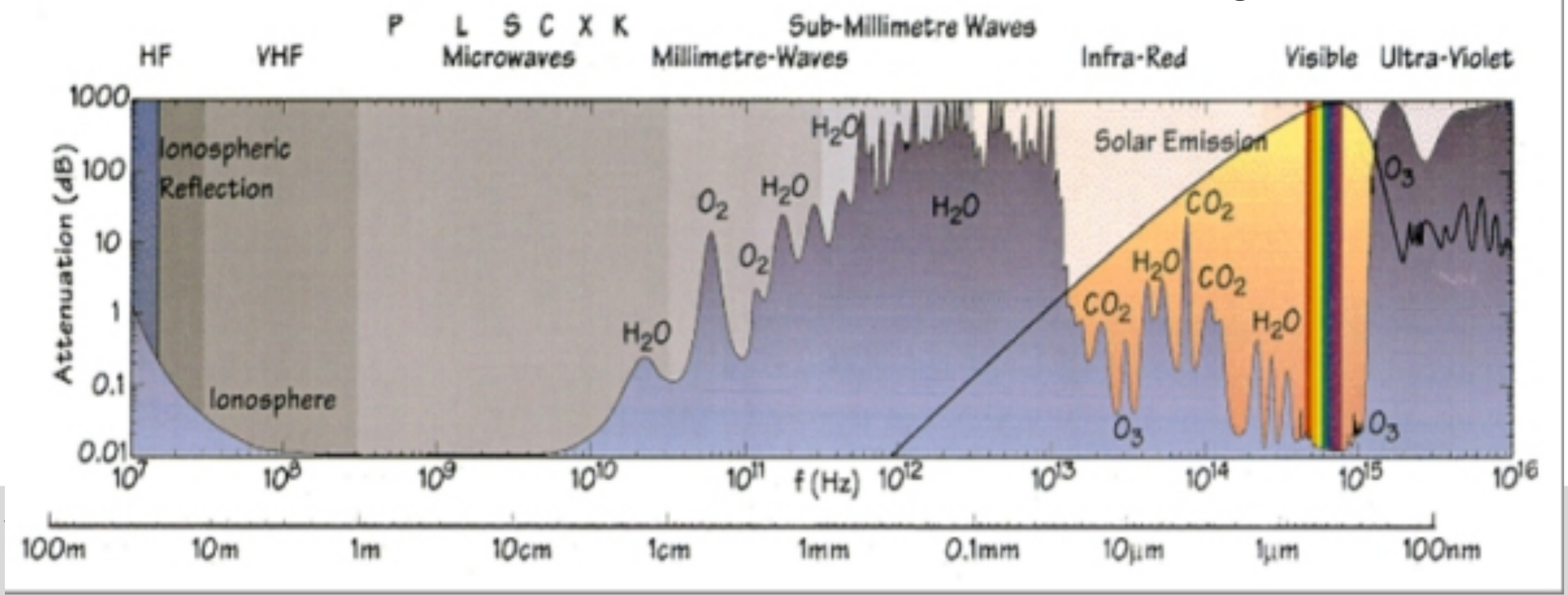


Figure from E. Kyrölä, https://earth.esa.int/dragon/D3_L3_Kyrola.pdf

Spectroscopy and Radiative transfer – the physical basis

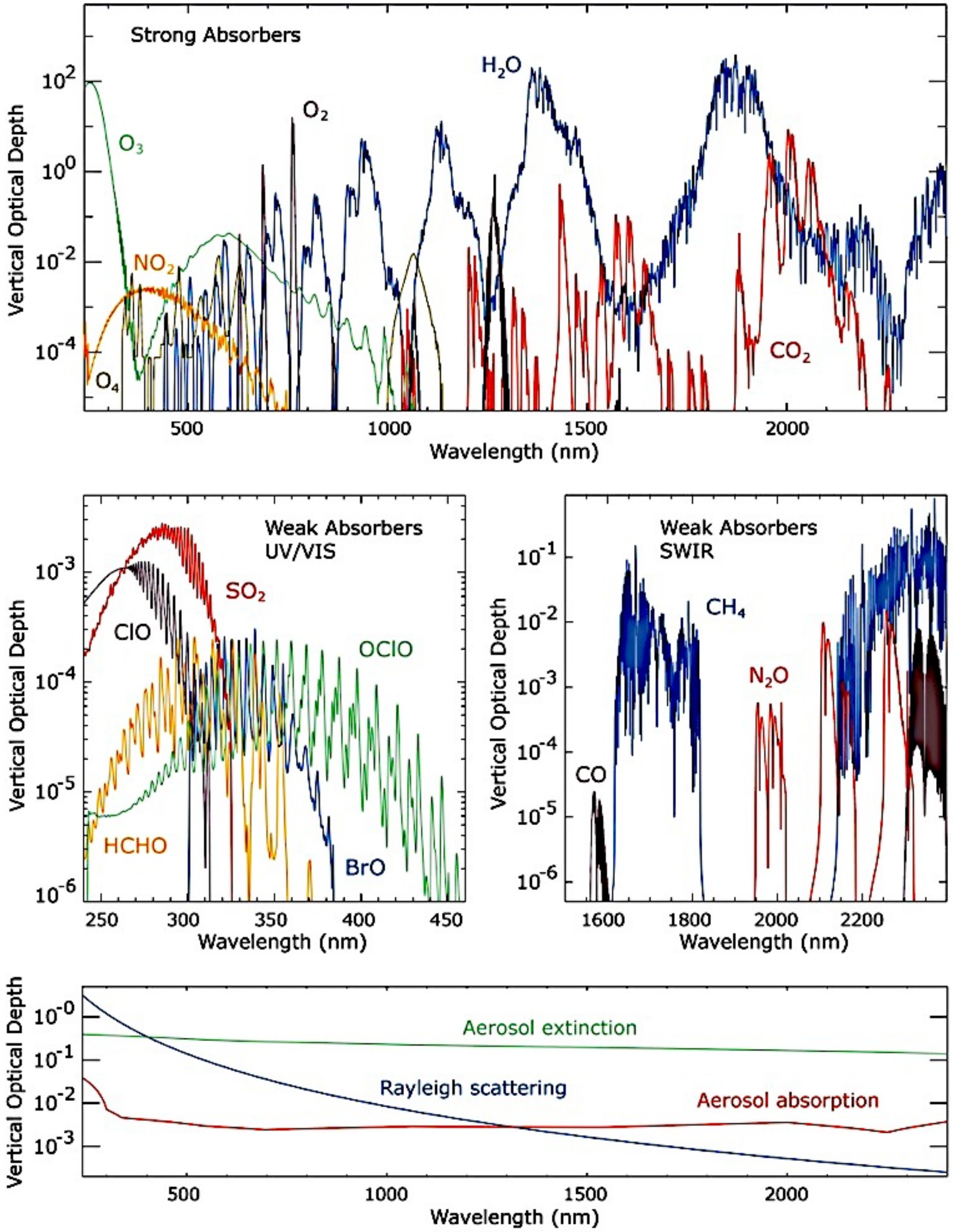
- The electromagnetic spectrum of the atmosphere (absorption or emission) results from the interaction of molecules and particles with the electromagnetic field
- Wavelength ranges: UV, Visible, Near-infrared, infrared, far infrared, sub-millimeter wave, millimeter wave, microwave
- In the following:
  - UV, vis, NIR
  - mid-infrared
  - FIR, Sub-millimeter, millimeter and microwave

Figure credits: ESA

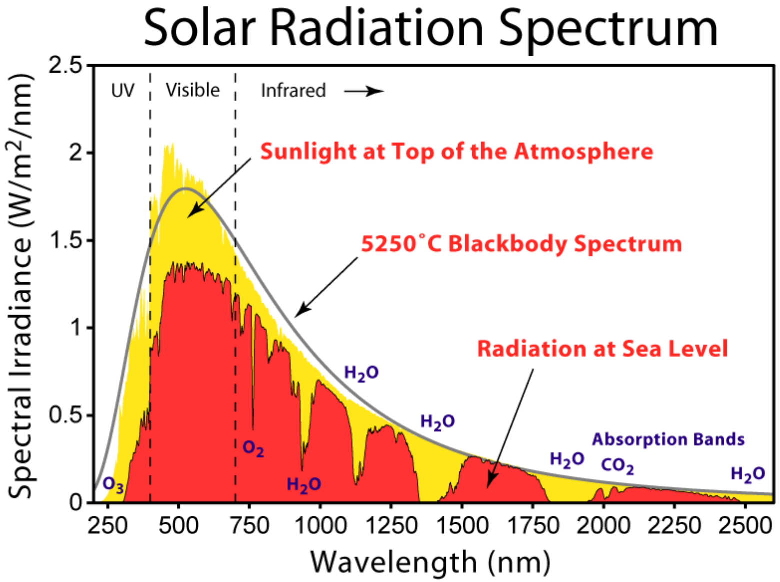


Spectroscopy and radiative transfer – UV/vis and NIR (SWIR)

- Relevant processes: absorption and emission of electronic states, scattering of radiation at molecules (molecular size and wavelength is similar!)
- Examples: ozone Huggins band at 320-360 nm, Hartley bands between 200 and 300 nm, Chappuis band 375 to 650 nm

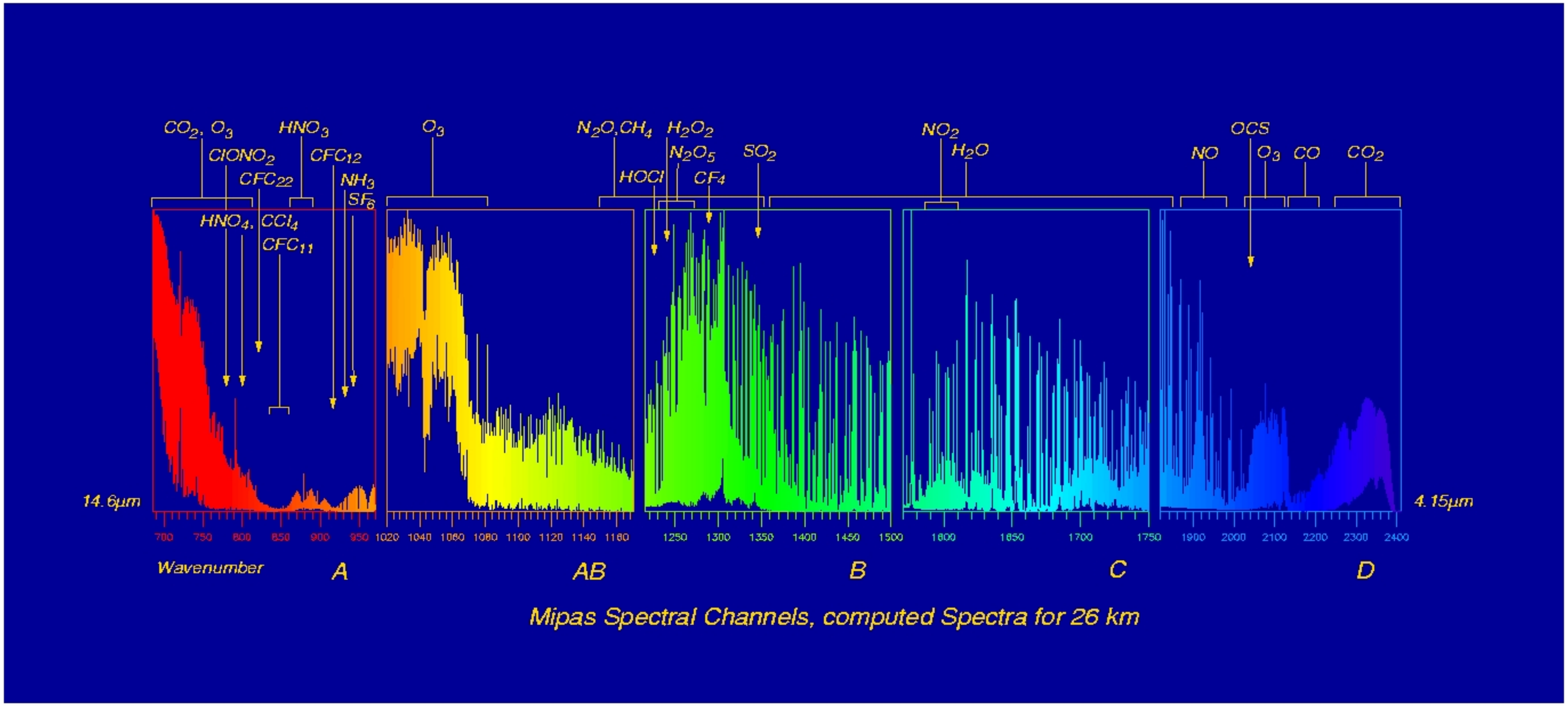


http://atmos.caf.dlr.de/projects/scops/sciamachy_book/sciamachy_book_figures_springer/chapter_7_figures_springer.html



Spectroscopy and radiative transfer – mid-IR (~4 to 15 µm = 2500 to 667 cm^{-1})

- Relevant processes: Absorption and emission by molecular states (rotation-vibration states)
- Scattering relevant for particles only (clouds, aerosols)
- Spectra are line spectra
- All molecules with a permanent dipole moment emit or absorb (not O2, N2)



Mipas Spectral Channels, computed Spectra for 26 km

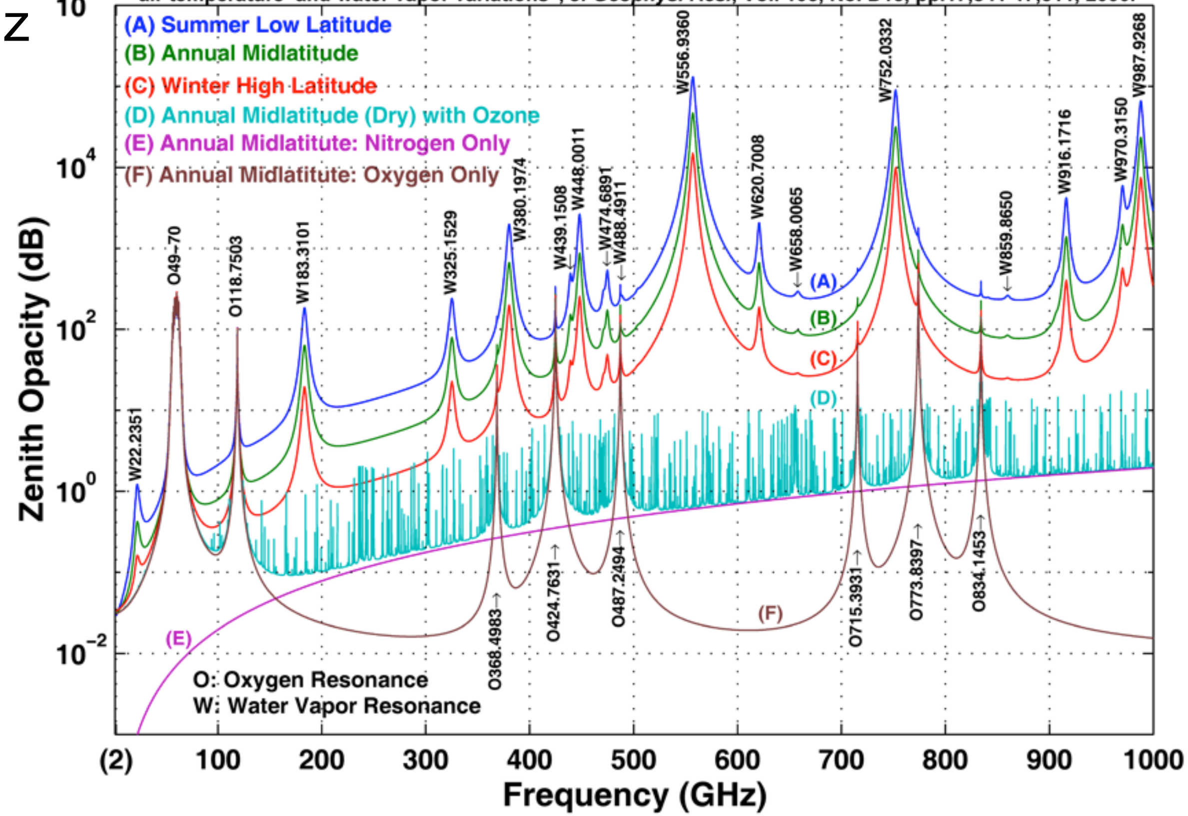
Spectroscopy and radiative transfer – FIR, mm, sub-mm and microwave (15µm to 1cm; 20 THz to 30 GHz)

- Relevant processes: absorption and emission by rotational states of molecules
- (Almost) no sensitivity for particles (clouds, aerosols)
- FIR and sub-millimeter:

  15 µm – 1 mm (20 THz to 300 GHz)
- microwave: > 1 mm

  (< 300 GHz)

Klein, M., A.J. Gasiewski: "Nadir sensitivity of passive millimeter and submillimeter wave channels to clear air temperature and water vapor variations", *J. Geophys. Res.*, Vol. 105, No. D13, pp.17,841-17,511, 2000.



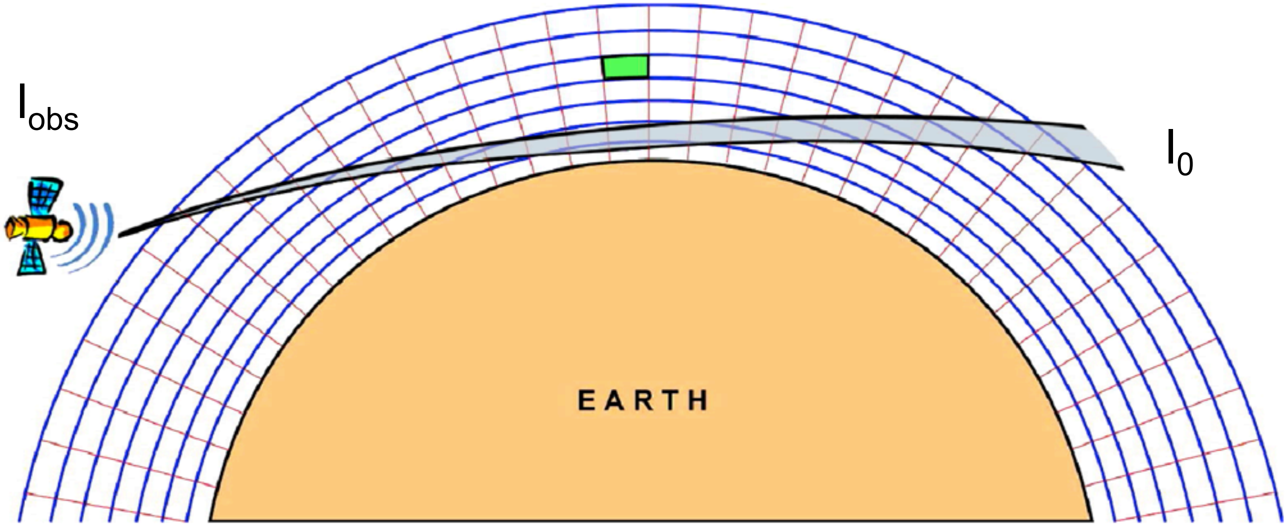
Spectroscopy and Radiative Transfer – Radiative transfer calculations

- Chandrasekhar’s radiative transfer equation:

$$S_\Theta(\nu, l_{obs}) \;=\; S_\Theta(\nu, l_o)\,\tau(\nu, l_{obs}, l_o) \;+\; \int\limits_{l_{obs}}^{l_o} J(\nu, l)\,\sigma^{Vol}_{a,total}(\nu, l)\,\tau(\nu, l_{obs}, l)\,dl$$

S_Θ	spectral radiance for the viewing angle Θ
J	source funktion
$\tau(\nu, l_1, l_2)$	transmission between l_1 and l_2 for wavenumber ν
dl	path element (see Section 2.1)
$\sigma^{Vol}_{a,total}$	absorption coefficient including gases and aerosols (per volume)
l_{obs}	position of the observer
l_o	position of background radiative source
ν	wavenumber
l	path coordinate

Schematic view of the observation geometry



$$S_\Theta(\nu, l_{obs}) = \boxed{S_\Theta(\nu, l_o)\,\tau(\nu, l_{obs}, l_o)} + \int_{l_{obs}}^{l_o} \boxed{J(\nu, l)}\,\boxed{\sigma^{Vol}_{a,total}(\nu, l)}\,\boxed{\tau(\nu, l_{obs}, l)}\,dl$$

Background radiation S_Θ attenuated by transmittance τ through entire atmosphere

Plus, for each path element:

Source function (= Planck function for T) at each point l along the line of sight

modulated by the emission characteristics of the composition of this path element

and transmitted through the rest of the atmosphere from l to l_{obs}

Figure by Carlotti and Magnani, Optics express, Vol. 17, Issue 7, pp. 5340-5357 (2009)
http://www.osapublishing.org/oe/fulltext.cfm?uri=oe-17-7-5340

The information we want to derive is in σ and τ:

$$\tau(\nu, l_1, l_2) = \exp - \left\{ \int_{l_1}^{l_2} \sigma^{Vol}_{a,gas}(\nu, l)\, dl \; + \underbrace{\int_{l_1}^{l_2} \sigma^{Vol}_{e,aerosol}(\nu, l)\, dl}_{\text{Aerosol}} \right\}$$

Volume absorption coeff. for gases

$$= \exp - \left\{ \sum_{g=1}^{G} \int_{l_1}^{l_2} \sigma_{a,g}(\nu, l)\, \frac{\partial m_g(l)}{\partial l}\, dl \; + \underbrace{\int_{l_1}^{l_2} \sigma^{Vol}_{e,aerosol}(\nu, l)\, dl}_{\text{Aerosol}} \right\}$$

$$\sigma^{Vol}_{a,gas}(\nu, l) = \sum_{g=1}^{G} \sigma_{a,g}(\nu, l) \cdot \rho_g(l)$$

$$\rho_g(l) = \boxed{C_{V,g}} \cdot \frac{N_{avo}}{R} \cdot \frac{p(l)}{T_{kin}(l)}$$

$m_g(l)$ = slant path column amount of gas g

$\sigma_{a,g}$ (ν,l) = absorption coefficient of gas g

$C_{V,g}$ = volume mixing ratio of gas g

Further terms:

- If scattering plays a role, we need an additional source term for the scattering of radiation **into** the line of sight:

$$J_s(\nu, l) = \frac{\Omega_o}{4\pi} \int\int p(\Omega, \Omega') S(\Omega, \Omega')\, d\Omega'$$

- $\sigma_{a,g}$ (v,l) is calculated from data bases containing spectroscopic information on the gases (position, intensity, width of spectral signatures) and quantum mechanical laws regulating the dependence on temperature and pressure of these
- Databases: e.g. HITRAN, GEISA, etc.

- A detailed description of a radiative transfer model for the mid-infrared can be found at:

  http://www.imk-asf.kit.edu/english/312.php (KOPRA)

Wavelength ranges and related contemporary limb instruments: UV/vis/NIR/SWIR

Instrument	GOMOS	MAESTRO	OSIRIS	SCIAMACHY
Type	Star occultation	Solar occultation	Limb scattering	Limb scattering and lunar occultation
Wavelength range	250 – 950 nm	400-545 and 525-1010 nm	274 nm to 810 nm	240 nm to 1700 nm and selected regions between 2.0 µm and 2.4 µm.
Altitude range	~ 10 – 100 km	2.5 – 23 km	~ 7 – 65 km	Cloud top – 100 km
Mission duration	4/2002 – 4/2012	2004 - …	2002 - …	4/2002 – 4/2012
Species	O3, NO2, Aerosol	Aerosol, O3, H2O, NO2	Aerosol, O3, NO2	O3, NO2, H2O, BrO, CO2, CH4,
Vertical resolution	2 – 3 km (O3) 4 km (other)	1 – 2 km	1 – 3 km	~ 3 km

Previous instruments: POAM, SAGE

Wavelength ranges and related contemporary limb instruments: mid-IR

Instrument	ACE-FTS	HIRDLS	MIPAS	SABER
Type	Solar occultation	Limb emission spectrometer	Limb emission spectrometer	Limb emission radiometer
Wavelength range	2.2 – 13.3 µm	6 – 17 µm	4.15 – 14.6µm	1.27 – 17 µm
Altitude range	~ 6 – 100 km	~ 5 – 30 km	~ 6 – 70 km	~ (10) 20 – (180)100 km
Mission duration	2004 - …	2004 - …	4/2002 – 4/2012	2002 - …
Species	More than 60 species, temp	O3, H2O, CH4, N2O, NO2, HNO3, N2O5, CFC11, CFC12, ClONO2, and aerosols;	More than 30 species, temp, clouds	O3, CO2, H2O, O, H, NO, OH, …
Vertical resolution	2 – 4 km (worse at higher altitudes)	1 – 2 km	~ 3 km (becoming worse with altitude)	5 - 9 km

Earlier instruments: ATMOS, CLAES, CRISTA, HALOE, ILAS

Role of spectral resolution for mid-IR observations

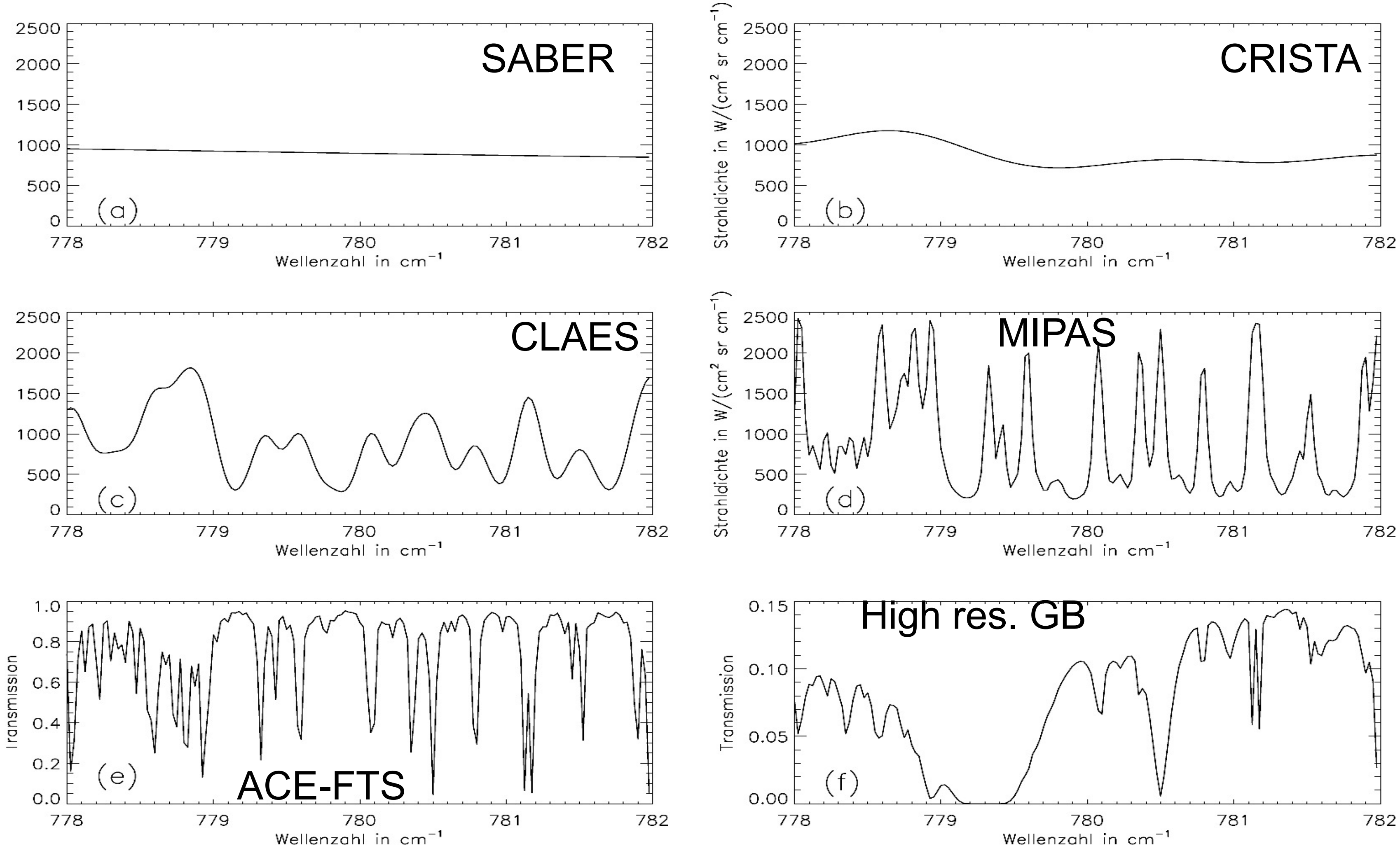


Figure: T. von Clarmann, 2015

Wavelength ranges and related contemporary limb instruments: FIR/mm/sub-mm/microwave

Instrument	Aura/MLS	Odin/SMR	SMILES
Type	Limb emission	Limb emission	Limb emission
Wavelength range	Bands centered around 118, 190, 240, 640 and 2500 GHz	118.25–119.25 GHz, 486.1–503.9 GHz und 541.0–580.4 GHz	624 – 650 GHz
Altitude range	~ 300 – 0.001 hPa depending on species	~ 7 – 75 km	~ 10 – 60 km
Mission duration	2004 - …	2001 - …	9/2009 – 4/2010
Species	~ 20 species	O3, H2O, N2O, HNO3, CO	O_3, HCl, ClO, CH_3CN, HOCl, HNO_3, O_3isotopes
Vertical resolution	1.5 – 6 km dep. on species and altitude range	3 – 4 km	~ 3 km

Earlier instruments: UARS/MLS

Retrieval theory

Linearization of the problem:

$$\mathbf{y} = f(\mathbf{x}) + \boldsymbol{\varepsilon} = f(\mathbf{x_0}) + \mathbf{K}(\mathbf{x} - \mathbf{x_0}) + \boldsymbol{\varepsilon} = \mathbf{y_0} + \mathbf{K}(\mathbf{x} - \mathbf{x_0}) + \boldsymbol{\varepsilon}$$

y = vector of radiance measurements by the instrument, dimension m

x = vector of atmospheric parameters to be determined, for example volume mixing ratio of gas g, dimension n

f = radiative transfer equation

K = Jacobi matrix : $\partial y_m / \partial x_n$

Assuming the errors of **y** follow a Gaussian distribution, the probability density distribution of **y** for a given **x** is

$$\mathrm{pdf}(y) = c \exp -[\tfrac{1}{2}(y-F(x))^T S_y^{-1}(y-F(x))] \approx$$
$$\approx c \exp -[\tfrac{1}{2}(y- y_0-K(x-x_0))\ ^T S_y^{-1}(y- y_0-K(x-x_0))]$$

With $\mathbf{S_y}$ = covariance matrix of **y** (diagonals are variances of **y**)

The most likely **x** maximizes pdf (**y**); i.e. derivative of this expression wrt **x** is zero:

$$x_{ml} = x_0 + (K^T S_y^{-1} K)^{-1} K^T S_y^{-1}(y-F(x_0))$$

This is the Maximum Likelihood solution of the problem

T. von Clarmann, 2015

Bayesian solution = maximum a posteriori solution = optimal estimation

- Some *a priori* knowledge is available, e.g. climatologies
- This information is introduced in Bayesian sense: the best estimate is the weighted mean of the measurement and the a priori knowledge, both weighted with their inverse covariance matrices

$$\mathrm{pdf} = c_1 \exp-[½(y-F(x))^T S_y^{-1}(y-F(x))]\ c_2 \exp -[½(x-x_a)^T S_a^{-1}(x-x_a)]$$
$$= c_3 \exp-[½(y-F(x))^T S_y^{-1}(y-F(x) + (x-x_a)^T S_a^{-1}(x-x_a)\ ]$$

$$x_{map} = x_a + (K^T S_y^{-1} K + S_a^{-1})^{-1} K^T S_y^{-1}(y-F(x_a))$$

- (Rodgers, 2000)
- **If** (and only if!) the true state is part of the ensemble the climatology ($\mathbf{x}_a$, $\mathbf{S}_a$) is built from **then** $\mathbf{x}_{map}$ is the most probable solution (most probable atmospheric state)
- Since radiative transfer is often not linear enough in real live, both ($\mathbf{x}_{ml}$ and $\mathbf{x}_{map}$) solutions need iterative approaches

T. von Clarmann, 2015

Other constraints: Tikhonov smoothing

- If a priori knowledge is not available, or I do not want to use it for what reason so ever, another approach to constrain the solution is such that the derived profile becomes smooth.
- We replace $\mathbf{S_a}^{-1}$ by the term $\gamma\mathbf{L_1}^T\mathbf{L}_1$ ... and receive

$$\hat{\mathbf{x}} = \mathbf{x}_0 + \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} + \gamma\mathbf{L}_1^T\mathbf{L}_1\right)^{-1}\mathbf{K}^T\mathbf{S}_y^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{x}_0))$$

- Note that this solution is not expanded around $\mathbf{x_a}$ but around $\mathbf{x_0}$.
- Meaning of $\gamma\mathbf{L_1}^T\mathbf{L}_1$:

$$\begin{pmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix} \mathbf{x} = \mathbf{L}_1\mathbf{x}$$

Is the sum of the differences between adjacent profile grid points

… and we need this term squared:

$$\mathbf{x}^T\mathbf{L}_1^T\mathbf{L}_1\mathbf{x} = \mathbf{x}^T \begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ & & & & \ddots & & & \\ 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix} \mathbf{x}.$$

T. von Clarmann, 2015

Characterization of the retrieval results

- The averaging kernel provides information how the true atmospheric profile is represented in the retrieval (and to which degree it depends on *a priori*):
- We define: $A = (\partial x_{map}/\partial x_{true})$

  = ratio of the result coming from the observation

  then:

  $$I-A = (\partial x_{map}/\partial x_a)$$

  Using:

  $$x_{map} = x_a + (K^T S_y^{-1} K + S_a^{-1})^{-1} K^T S_y^{-1} (y - F(x_a))$$

  We obtain:

  $$A = (K^T S_y^{-1} K + S_a^{-1})^{-1} K^T S_y^{-1} K$$

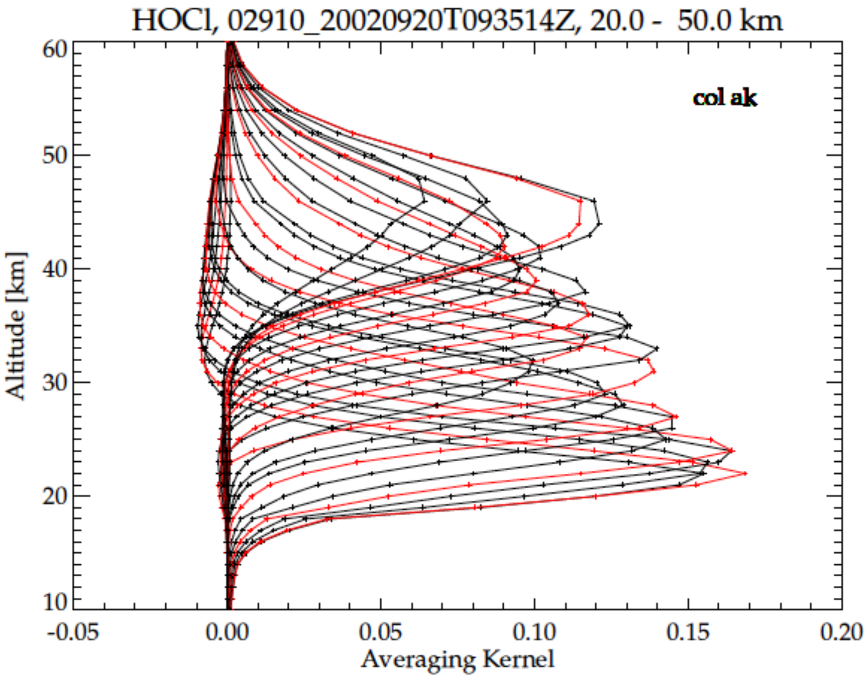
  $$x_{map} = Ax + (I-A)\, x_a$$

T. von Clarmann, 2015

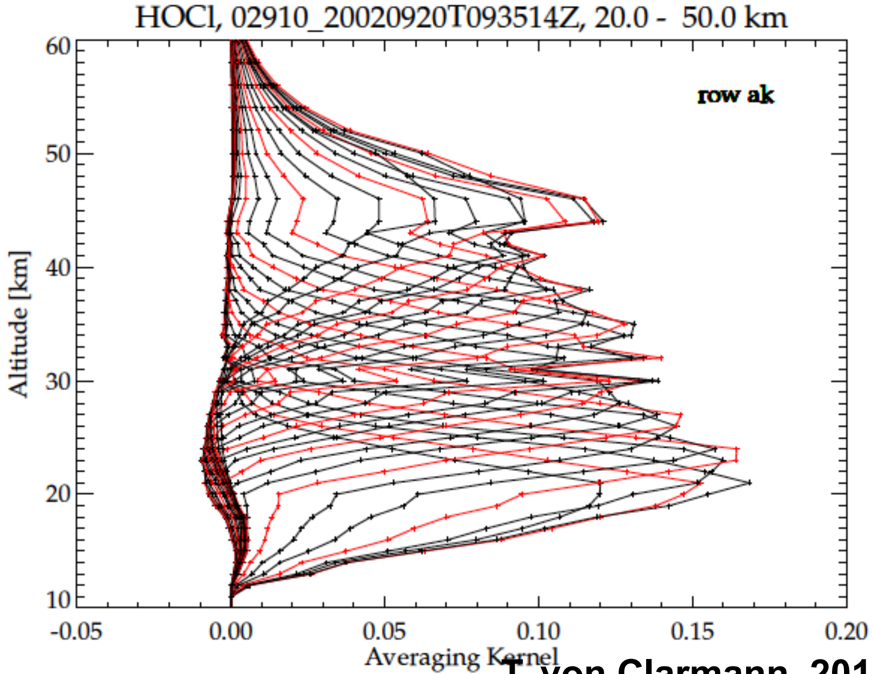
Meaning of the averaging kernel

- **A** is called averaging kernel, quadratic matrix
- Rows of **A**: provides the weight with which the true atmospheric profile values contribute to the retrieval result related to this row
- Columns of **A**: response of the retrieval to a delta perturbation in the atmospheric profile => understood as **vertical resolution**
- Careful: if log(vmr) is retrieved, the averaging kernels are for log(vmr)!

columns



rows



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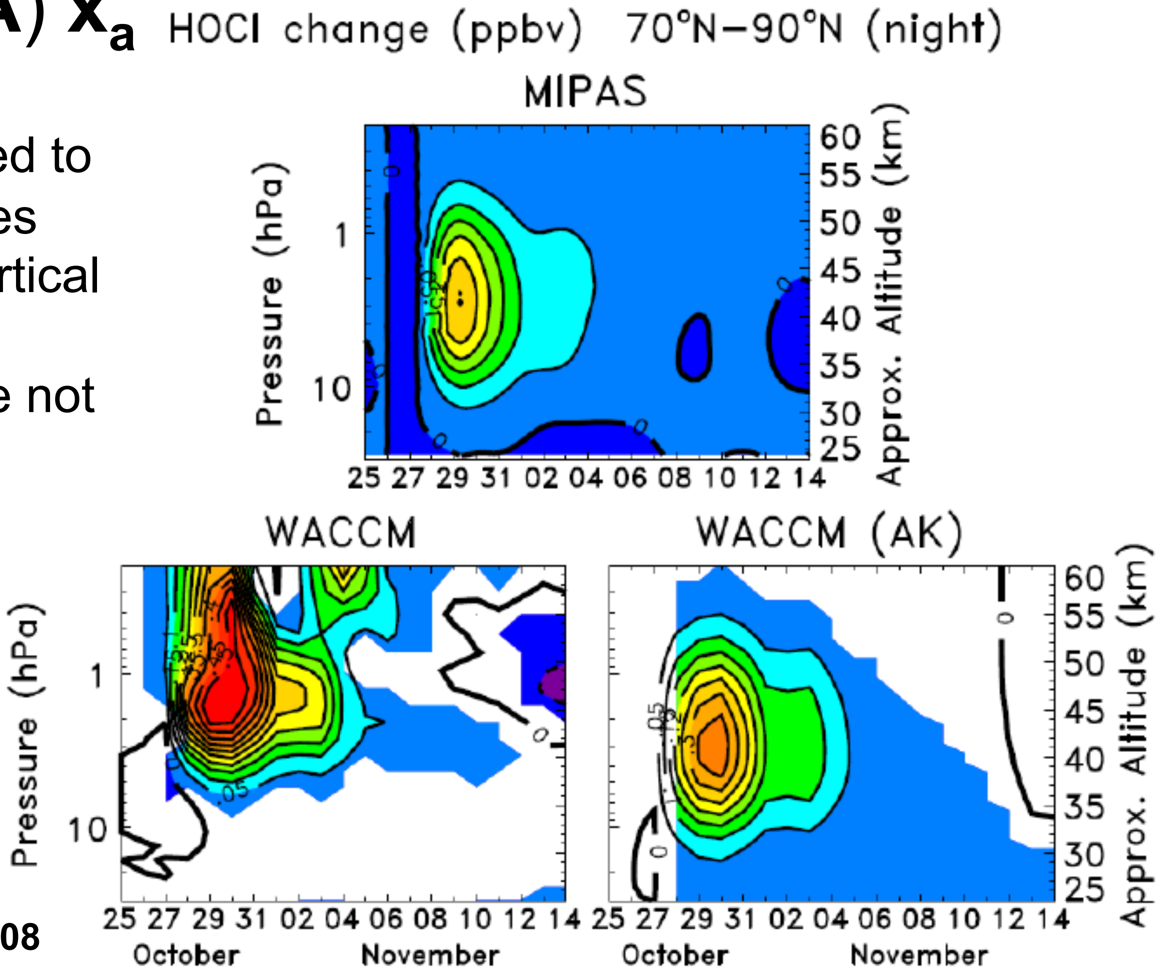
How to use the averaging kernel? Example 1: compare model results to observations

$$x_{comp} = A\,x_{mod} + (I-A)\,x_a$$

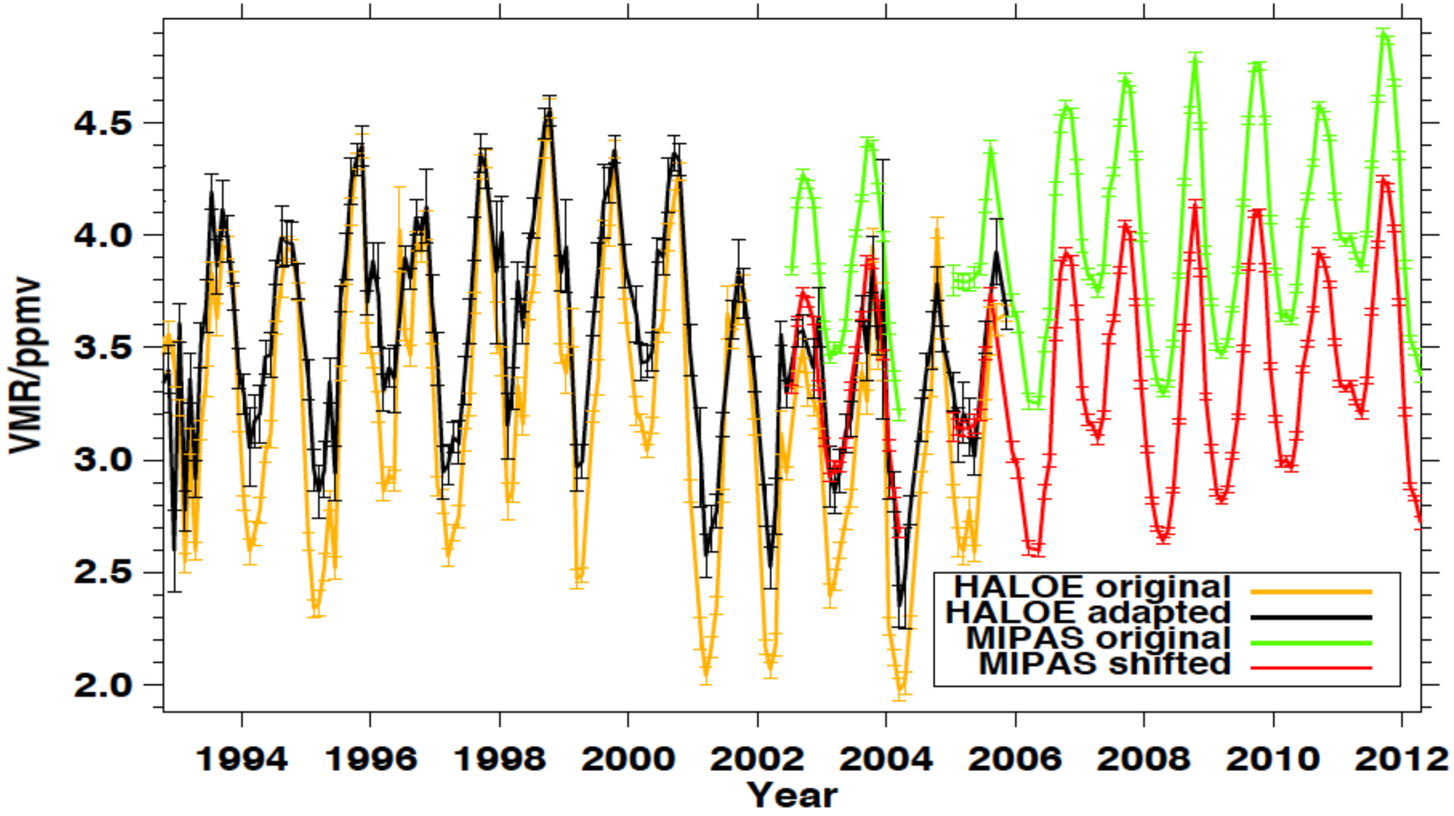
HOCl averaging kernels applied to WACCM model results changes both vertical resolution and vertical position of the maximum
Reason: averaging kernels are not symmetric



Jackman et al., 2008

How to use the averaging kernel? Example 2: Build a time series from 2 different instruments

$$x_{comp} = A\, x_{inst} + (I-A)\, x_a$$



Schieferdecker et al., 2015

Further retrieval diagnostics

- Gain function and retrieval covariance matrix:

$$\mathbf{G} = \mathbf{x}_a + (\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} + \gamma\mathbf{L}_1^T\mathbf{L}_1)^{-1}\mathbf{K}^T\mathbf{S}_y^{-1}$$

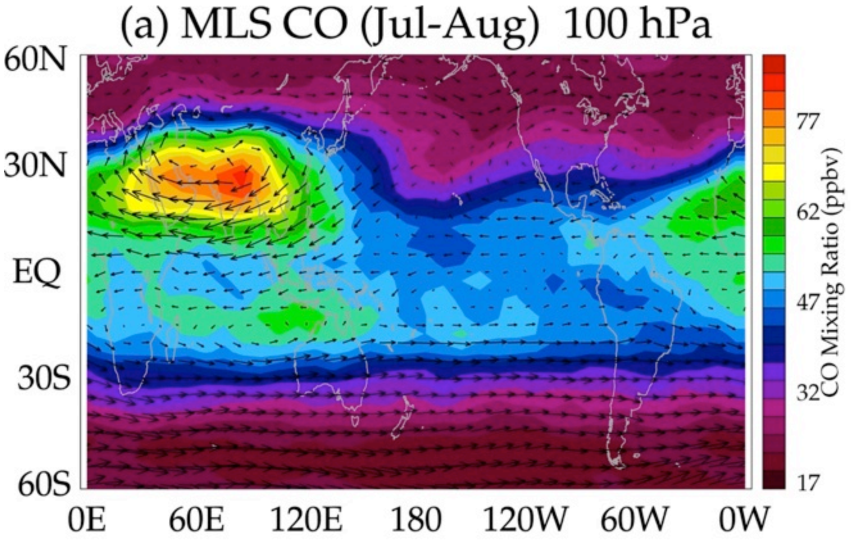
$$\mathbf{S}_x = \mathbf{G}\mathbf{S}_y\mathbf{G}^T.$$

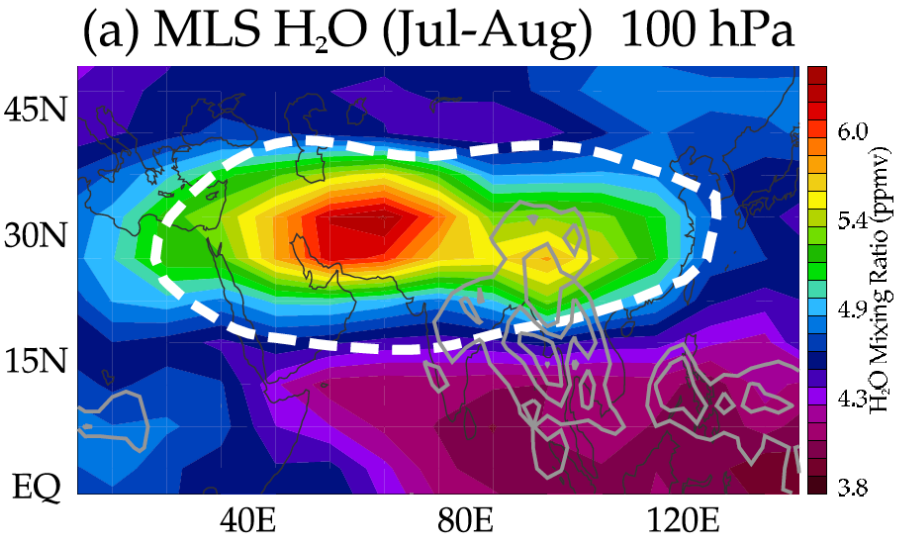
$$\mathbf{A} = \mathbf{G}\mathbf{K} = (\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} + \gamma\mathbf{L}_1^T\mathbf{L}_1)^{-1}\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}$$

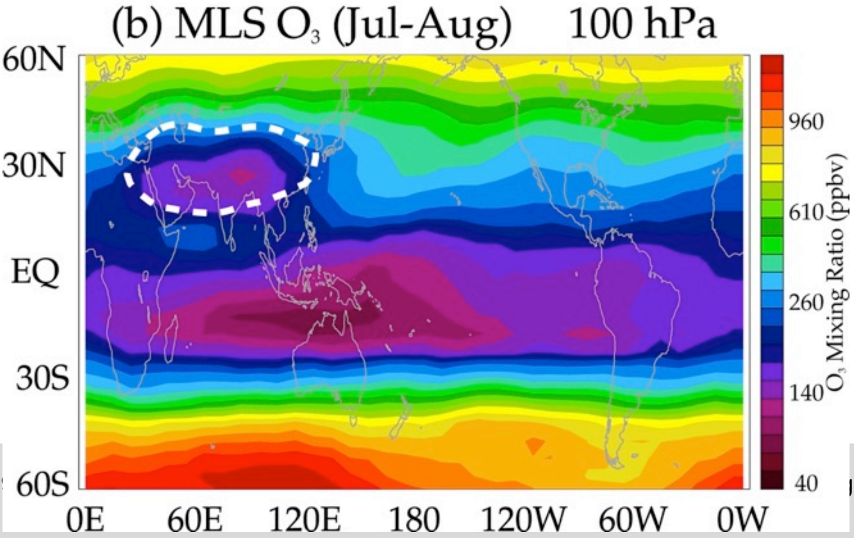
- $\mathbf{S}_\mathbf{x}$ is the mapping of the spectral error covariances on the retrieval result (often called “random” or “retrieval” error)
- There are further errors:
- errors due to further parameters in the radiative transfer calculations that are known with uncertainties only (temperature, line of sight, other species’ concentrations, …)
- So-called “systematic” errors are uncertainties that go always in the same direction and, thus, produce a bias (e.g. spectroscopic data)
- Careful: What is given as “error” of a retrieval result varies strongly from group to group!
- Also note: filter criteria apply! Check for filter criteria for each data set!

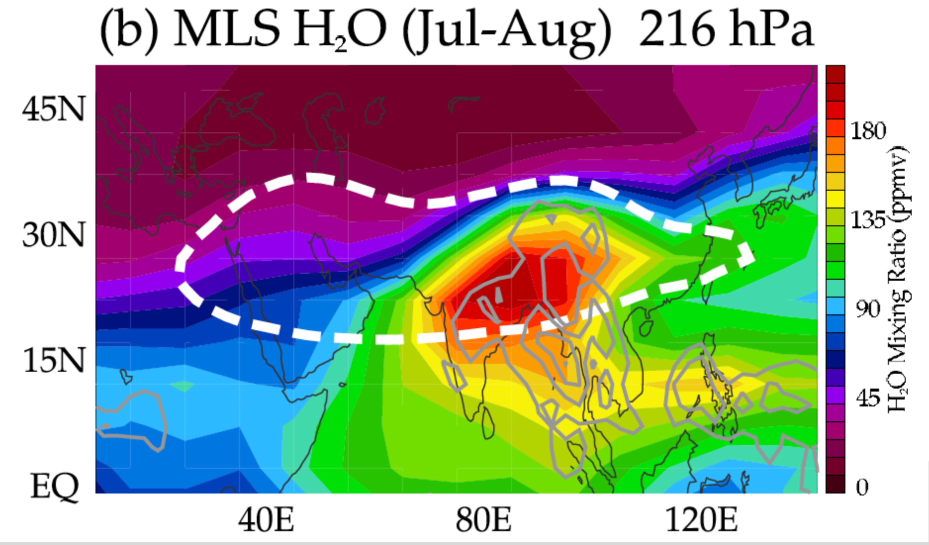
Examples: some satellite observations related to the Asian monsoon: MLS

MLS data used in Park et al., JGR, 2007

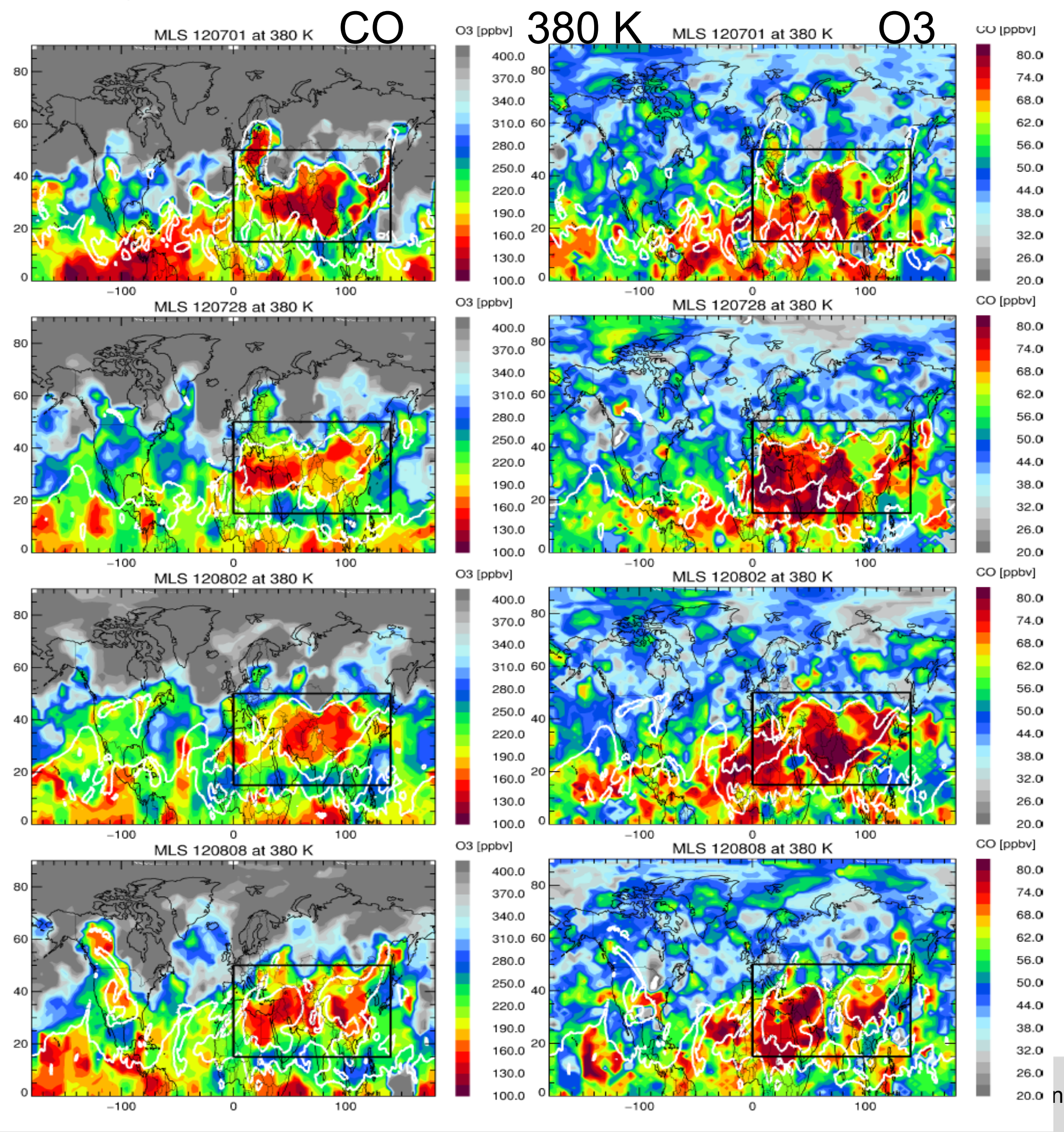

(a) MLS CO (Jul-Aug) 100 hPa


(a) MLS H_2O (Jul-Aug) 100 hPa


(b) MLS O_3 (Jul-Aug) 100 hPa

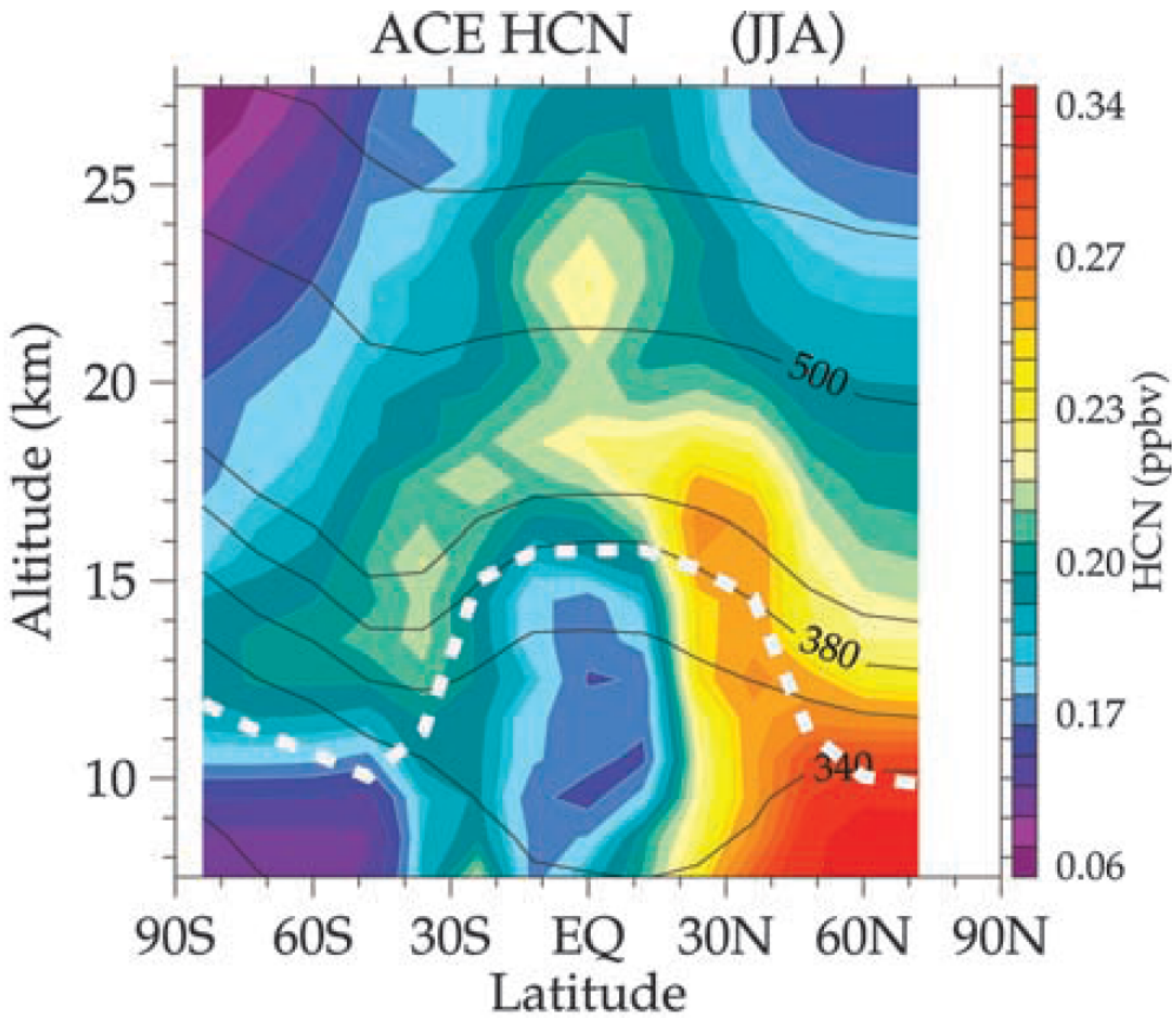

(b) MLS H_2O (Jul-Aug) 216 hPa

Single day observations from MLS to study variability



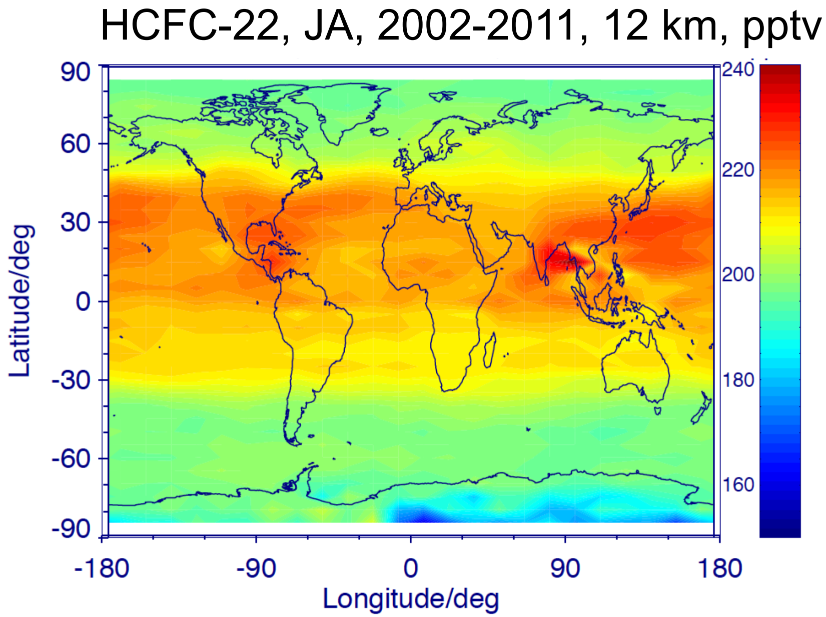
MLS data used in Vogel et al., ACPD, 2015

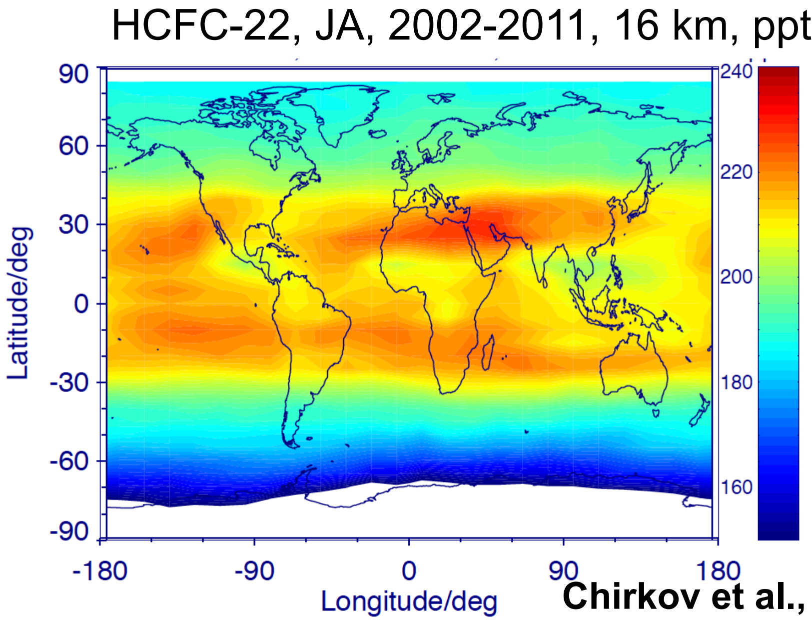
Vertical distribution of HCN from ACE-FTS



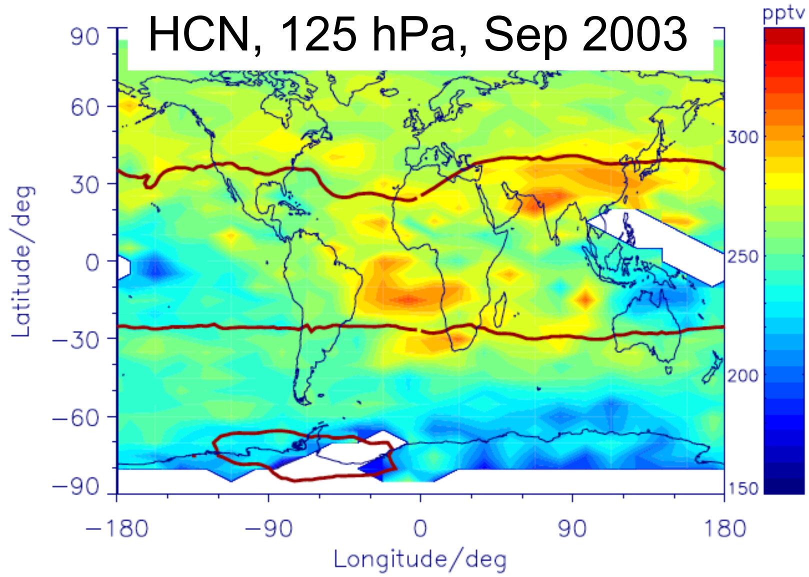
ACE-FTS data of HCN used in Randel et al., Science, 2010

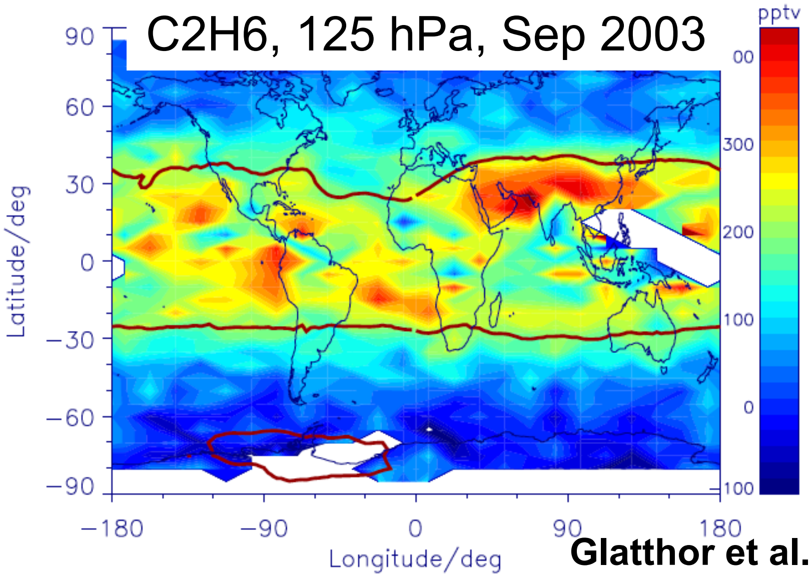
HCFC-22, HCN, and C2H6 from MIPAS


HCFC-22, JA, 2002-2011, 12 km, pptv


HCFC-22, JA, 2002-2011, 16 km, pptv

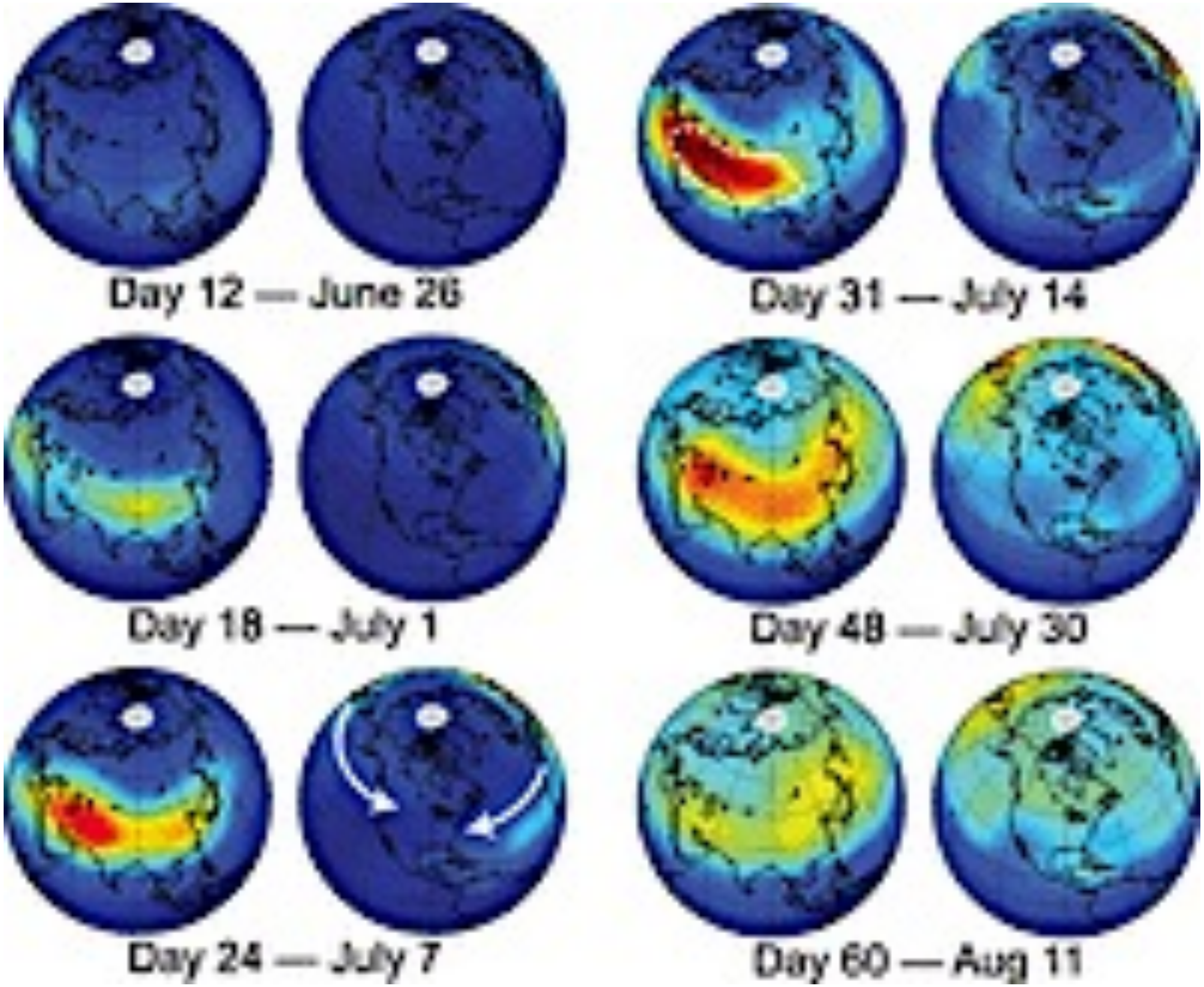
Chirkov et al., 2015


HCN, 125 hPa, Sep 2003


C2H6, 125 hPa, Sep 2003

Glatthor et al., 2009

Mean stratospheric aerosol optical depth in the monsoon anticyclone from OSIRIS: Nabro, 2011



Bourassa et al., Science, 2012

Data availability and download

- ACE-FTS data: http://www.ace.uwaterloo.ca/data.html
- GOMOS data: https://earth.esa.int/web/guest/data-access/browse-data-products/-/article/gomos-level-2-atmospheric-constituents-profiles-1506
- HIRDLS data: http://gdata1.sci.gsfc.nasa.gov/daac-bin/G3/gui.cgi?instance_id=hirdls
- MIPAS data: https://earth.esa.int/web/guest/data-access/browse-data-products/-/article/mipas-atmospheric-pressure-temperature-data-constituents-profiles-1547 (operational product, ESA) or

  http://www.imk-asf.kit.edu/english/308.php (research product, KIT)
- MLS data: http://mls.jpl.nasa.gov/index-eos-mls.php
- OSIRIS data: http://osirus.usask.ca
- SCIAMACHY data: http://www.iup.uni-bremen.de/sciamachy/dataproducts/index.html
- SMILES data: http://smiles.nict.go.jp/pub/data/index.html
- SMR data: http://odin.rss.chalmers.se

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