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Introduction to Infrared
Radiative Transfer

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JCSDA Summer Colloquium on Data Assimilation

Stevenson, Washington

National Environmental Satellite, Data, and Information Service

Radiative Transfer Theory Notes for the discussion today is on-line

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ftp site: ftp://ftp.orbit.nesdis.noaa.gov/pub/smcd/spb/cbarnet/

..or.. ftp ftp.orbit.nesdis.noaa.gov, cd pub/smcd/spb/cbarnet

Sounding NOTES, used in teaching UMBC PHYS-741: Remote Sounding and UMBC PHYS-640: Computational Physics (w/section on integration)

~/reference/rs_notes.pdf

~/reference/phys640_s04.pdf

These are *living* notes, or maybe a scrapbook – they are not textbooks.

Excellent text books on the topic of radiative transfer are:

1. Andrews, D.G., J.R. Holton and C.B. Leovy 1987. Middle Atmospheric Dynamics. Academic Press 489 pgs.
2. Goody, R.M. and Y.L. Yung 1989. Atmospheric radiation. Oxford Univ. Press 519 pgs.

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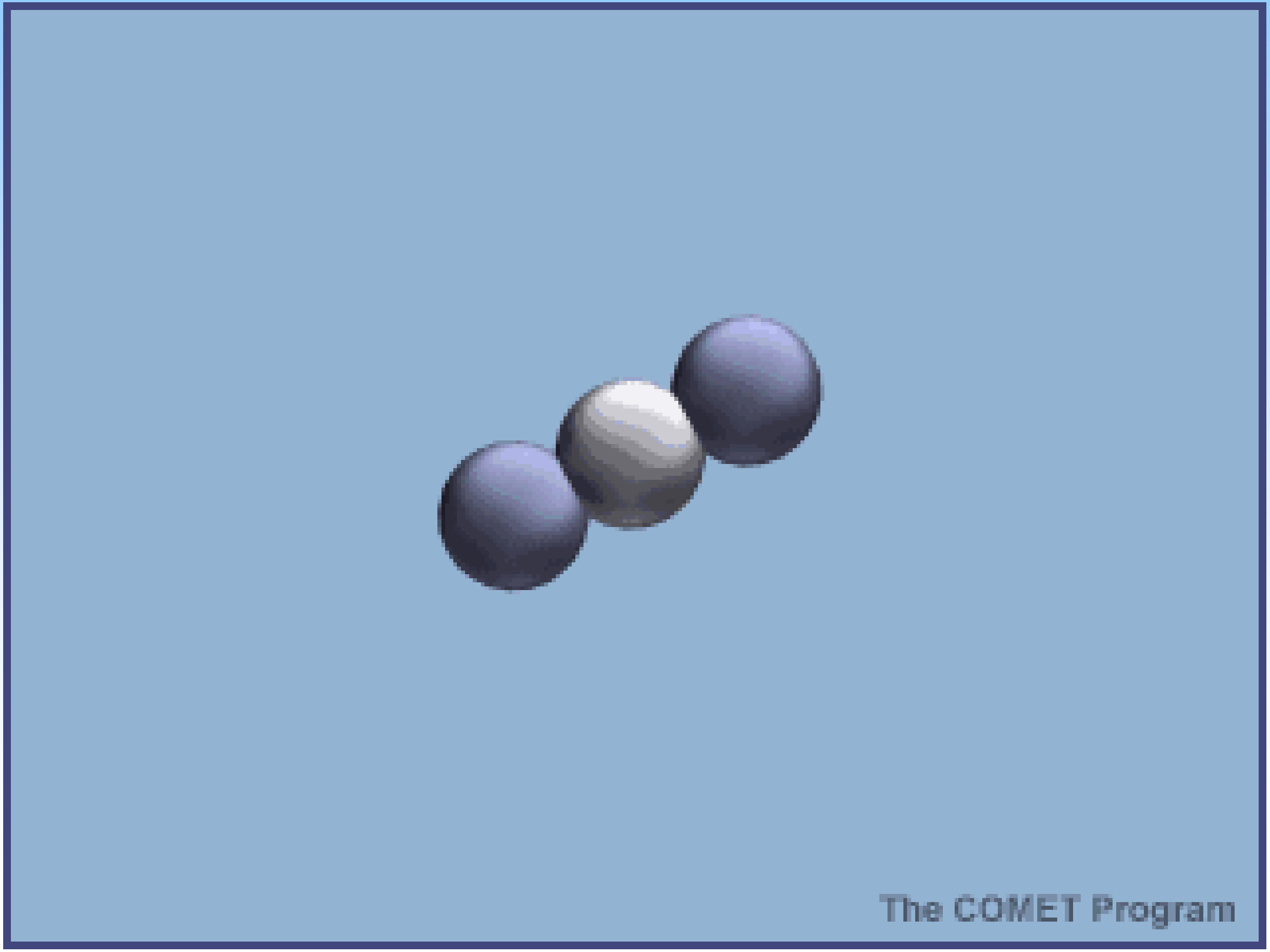
Topics for Radiative Transfer Lecture

- Introduction to spectroscopy
  - Molecular vibration and rotation
  - HITRAN database
  - Computation of Earth leaving radiance (for clear scenes)
- SideBar – what does 2xCO2 look like
- Estimating the geophysical state from radiances
  - A “poor mans” retrieval
- Some final thoughts on using hyper-spectral infrared radiances in data assimilation
  - Short-wave channels
  - Water channels
  - Emissivity
- How to handle clouds

Infrared Absorption

Molecules absorb in electronic, vibrational, and rotational modes.

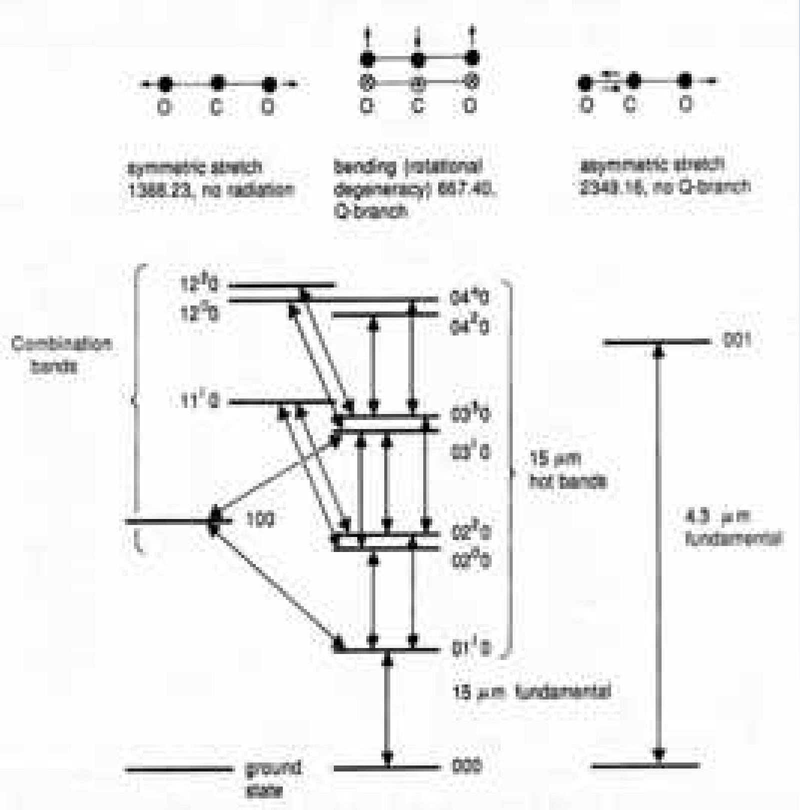


In thermal infrared we use wavenumbers to represent channels or frequencies

- Traditionally, in the infrared we specify the channels in units of wavenumbers, or cm^{-1}
  - $\nu \equiv f/c$
    - f = frequency in Hertz (or s^{-1})
    - c = speed of light = 29,979,245,800 cm/s
- Wavenumbers can be thought of as inverse wavelength, for example,
  - $\nu \equiv 10000/\lambda$
    - λ = wavelength in μm (microns)

Molecular Vibrational Modes (Example: CO_2)

- CO_2 has 4 modes of vibration. Each is quantized.
  - ν_1 is symmetric stretch (not active in infrared due to lack of dipole moment)
  - ν_2 is a bending that is doubly degenerate
  - ν_3 is a asymmetric stretch
- Energy of vibrational mode is given by
  - $E_{vib} = \Sigma\, hc \cdot \nu_k \cdot (i_k + ½)$ for $i_k = 0, 1, 2, \ldots$



Isotope	transition	band	S	d
$^{12}C^{16}O^{16}O$	$00^00 \rightarrow 01^10$	667.38	194	1.56
	$01^10 \rightarrow 02^20$	667.75	15	0.78
	$01^10 \rightarrow 10^00$	720.81	5	1.56
	$01^10 \rightarrow 00^00$	618.03	4	1.56
	$02^20 \rightarrow 03^30$	688.11	0.85	0.78
	$10^00 \rightarrow 11^10$	647.06	0.7	1.56
$^{13}C^{16}O^{16}O$	$00^00 \rightarrow 01^10$	648.48	2.01	1.56
$^{12}C^{18}O^{16}O$	$00^00 \rightarrow 01^10$	662.37	0.77	1.56

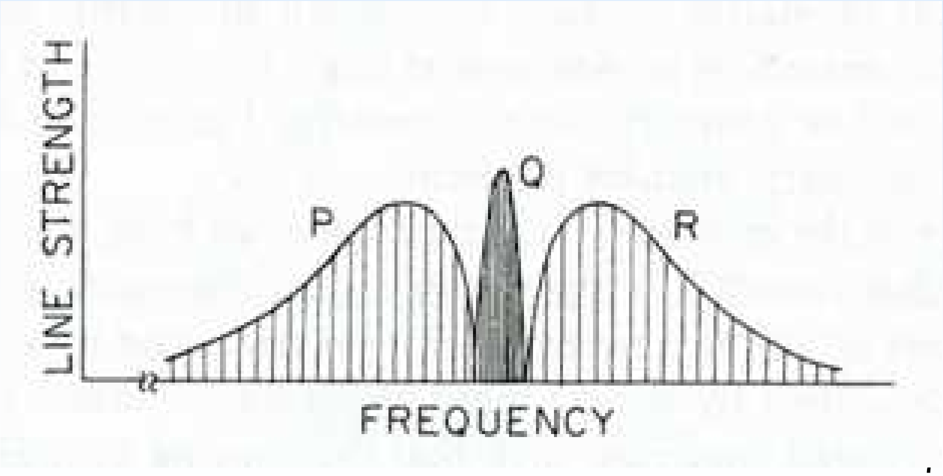
Rotational Modes

- The energy of rotation is quantized and given by
  - $E_{rot} = hc \cdot B \cdot j \cdot (j+1)$, $j = 0, 1, 2, 3, \ldots$
- But as the molecule rotates it also has centrifugal forces
  - $E_{rot} = hc \cdot (B \cdot j \cdot (j+1) - D \cdot j^2 \cdot (j+1)^2$

P-branch lines form when $\Delta j = +1$

Q-branch lines form when $\Delta j = 0$

R-branch lines form when $\Delta j = -1$



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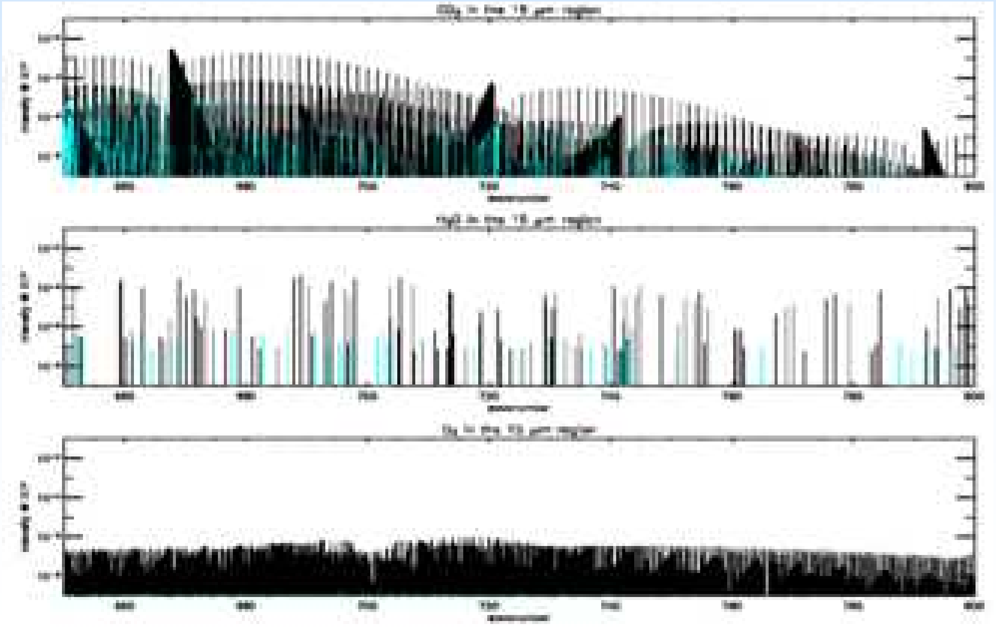
All the Physics is Contained in a quantity called the Absorption Coefficient

- The absorption coefficient is a complicated and highly non-linear function of molecule *i* and line *j*
- Line Strengths, S_{ij}, result from many molecular vibrational-rotational transitions of different molecular species and isotopes of those species(blue).

$$\kappa_i(\nu, p, T, \theta) \simeq \sum_{j=1}^{J} \frac{N_i \cdot S_{ij}}{\pi} \frac{\gamma_{ij}}{(\nu - \nu_{ij})^2 + (\gamma_{ij})^2} \cdot \sec(\theta)$$

Where width of line, γ_{ij}, is a function of the molecule structure (natural broadening), temperature (doppler broadening) and pressure (collisional broadening)

$$\gamma_{ij} \simeq \gamma_{ij}^0 \cdot \frac{p}{P_0} \cdot \sqrt{\frac{T}{T_0}}$$



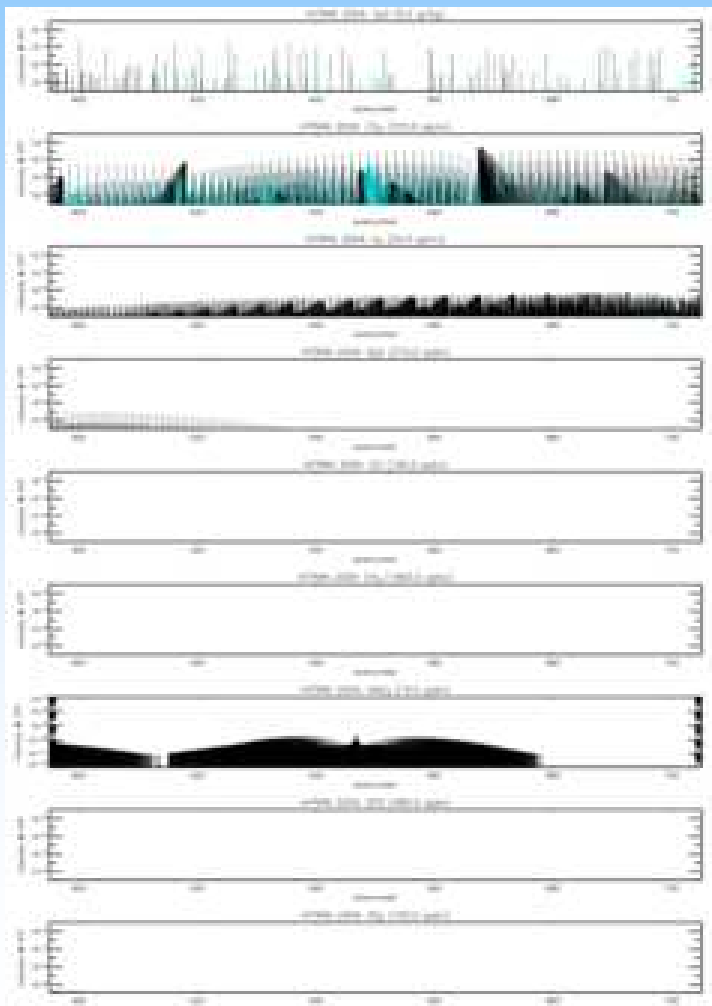
Line strength (at T=300K) of CO2, H2O, and O3 in the 15 μm band.

Line strength, S, is also a function of temperature

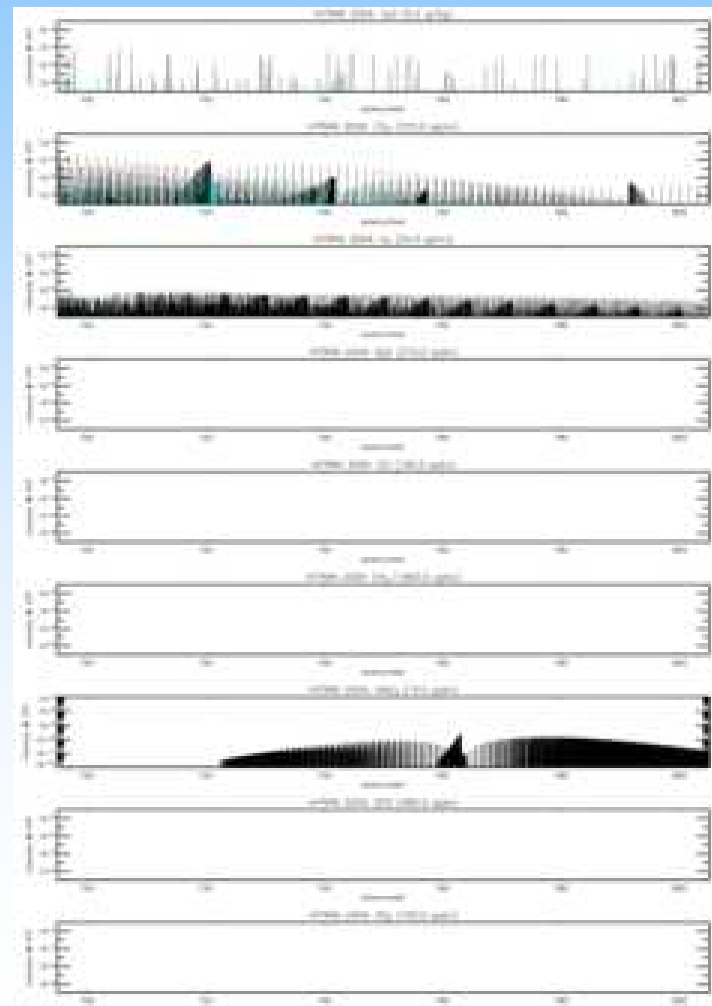
$$S(T) = S(T_0)\cdot(T/T_0)\cdot\frac{(1-\mathrm{EXP}(1-1.439\nu/T))^3}{(1-\mathrm{EXP}(1-1.439\nu/T_0))^3}$$

Example of vibration rotational line strengths in 15 μm band region

600 to 700 cm^{-1}



700 to 800 cm^{-1}



H_2O

CO_2

O_3

N_2O

CO

CH_4

HNO_3

OCS

SO_2

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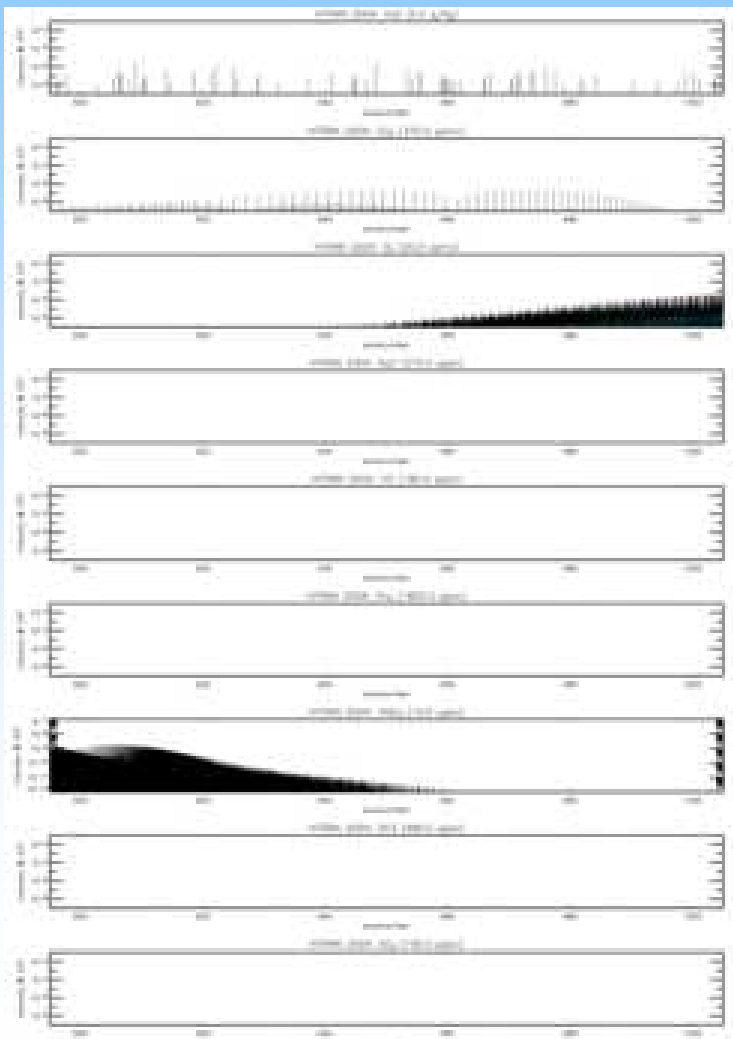
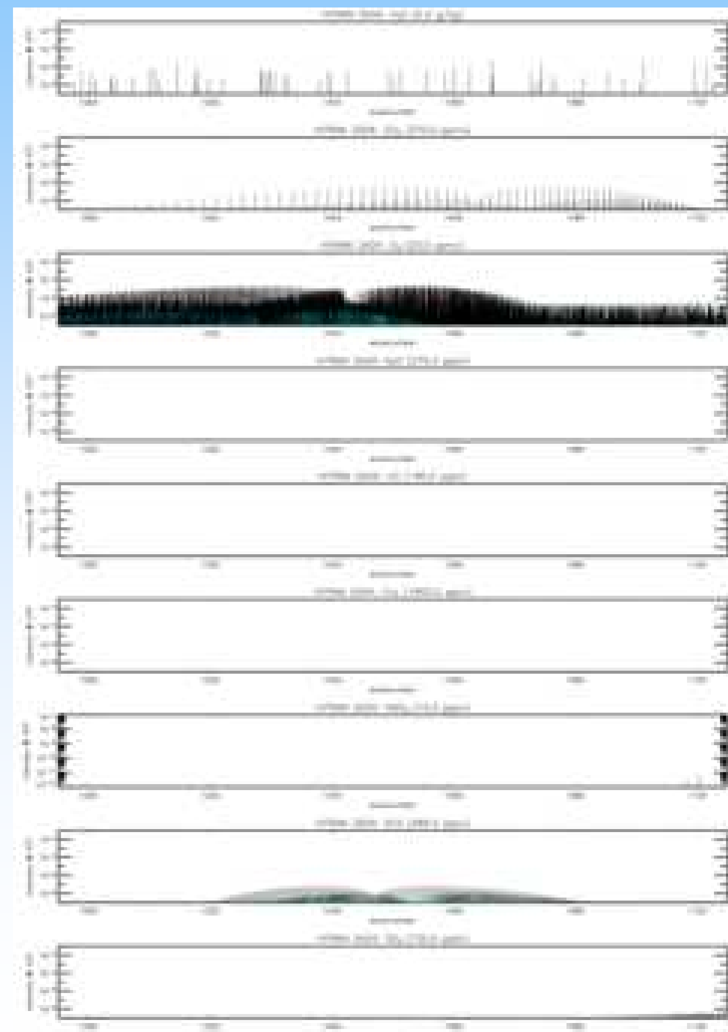
Example of vibration rotational line strengths in 10 μm band region

900 to 1000 cm^{-1}



1000 to 1100 cm^{-1}



H_2O

CO_2

O_3

N_2O

CO

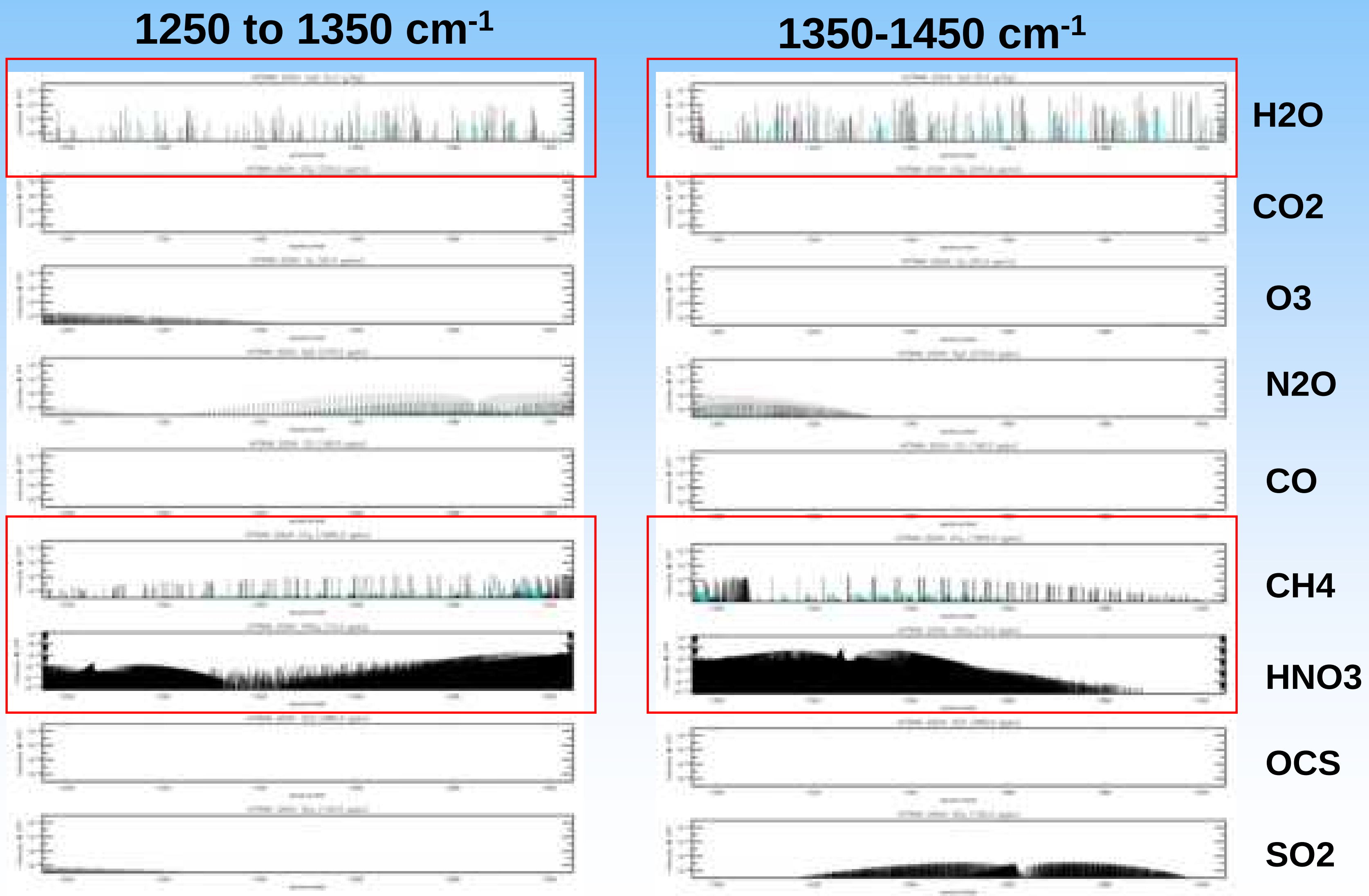
CH_4

HNO_3

OCS

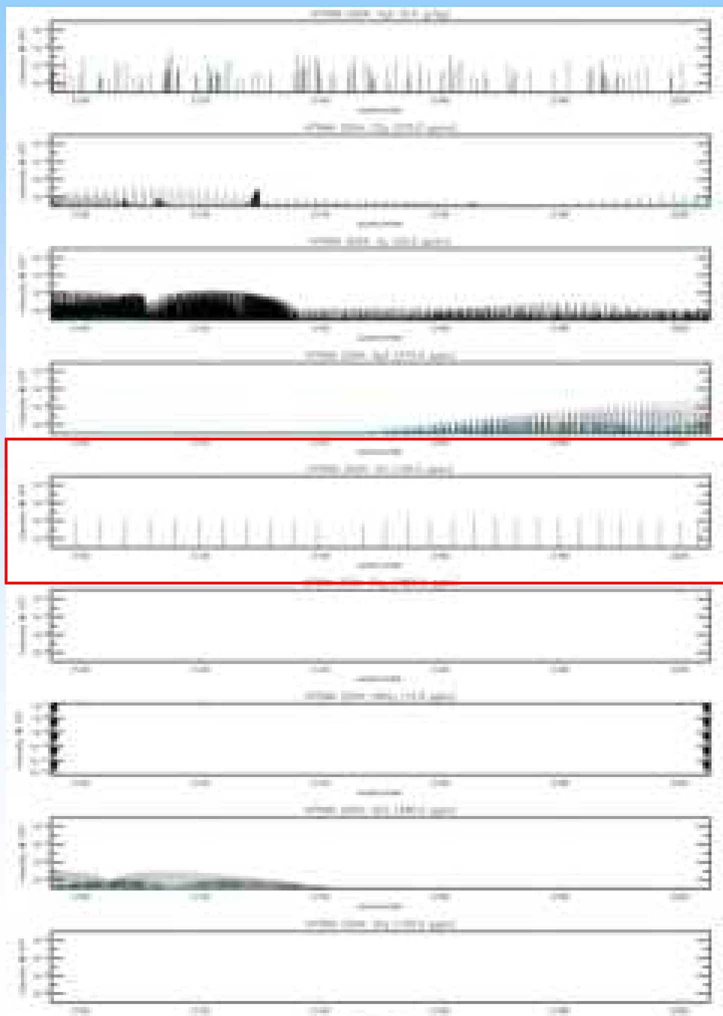
SO_2

Example of vibration rotational line strengths in 6 μm band region

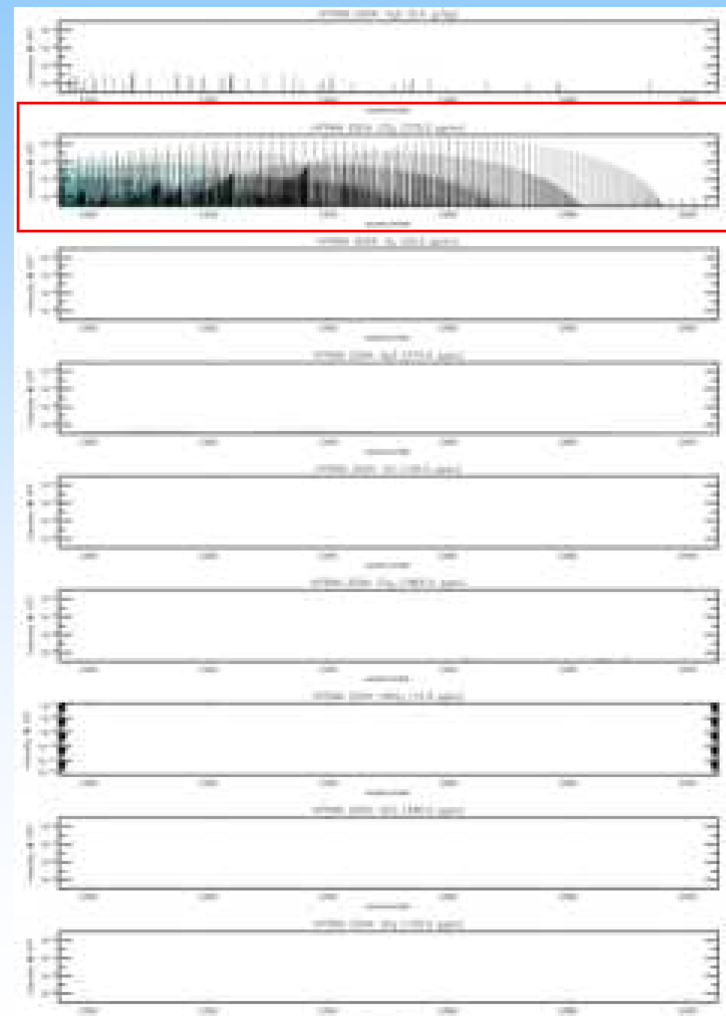


Example of vibration rotational line strengths in 4 μm band region

2100 to 2200 cm^{-1}



2300 to 2400 cm^{-1}



H2O

CO2

O3

N2O

CO

CH4

HNO3

OCS

SO2

Atmosphere Transmittance

- The Optical Depth is the sum of absorption coefficients for all isotopes and species multiplied by the path-length, usually written in terms of pressure levels p_i and p_j and view angle θ

Optical Depth = $\Delta z(|p_i - p_j|) \cdot \sec(\theta) \cdot \left[\sum_{i=1}^{I} k_n^i\right]$

- The transmittance of a layer is given by the exponential of the optical depth

$$\tau_\nu(p_i \rightarrow p_j, \theta) = \exp\left(-\Delta z(|p_i - p_j|) \cdot \sec(\theta) \cdot \left[\sum_{i=1}^{I} k_n^i\right]\right)$$

- The view angle can be included in the absorption coefficient and transmittance from a level in the atmosphere (at height z) to the top of the atmosphere can be written as

$$\tau_\nu^{\uparrow}(p, X, \theta) = \exp\left(-\int_{z'=z(p,X)}^{\infty} \sum_i \kappa_i(\nu, p(z'), X, \theta) \cdot dz'\right)$$

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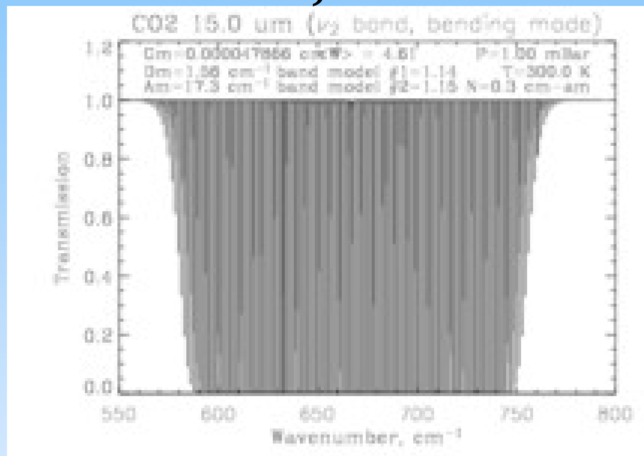
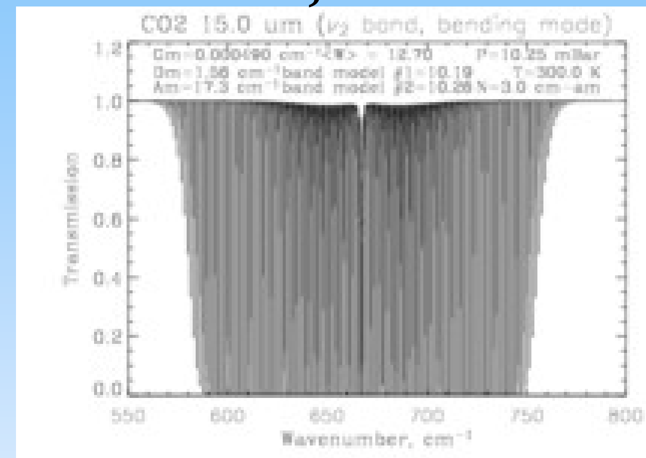
CO_2 transmittance at different pressures (simple model, pure $^{12}C^{16}O_2$ as rigid rotator)

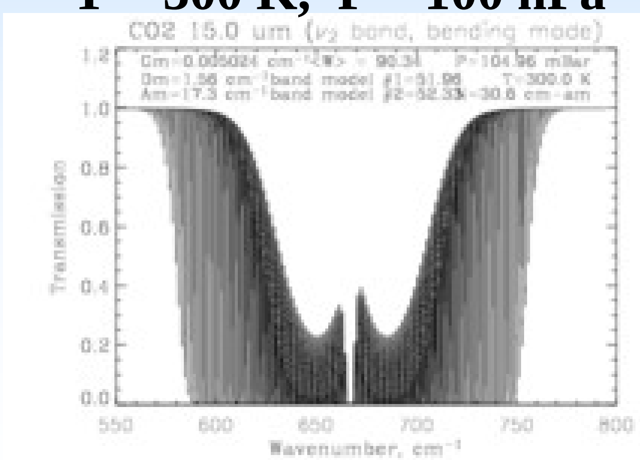
T = 300 K, P = 1 hPa



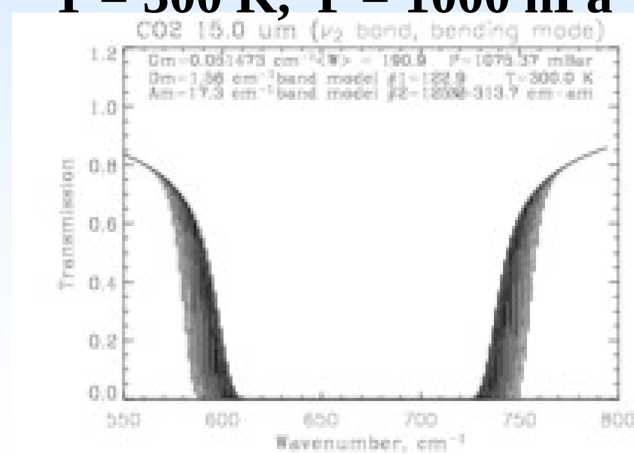
T = 300 K, P = 10 hPa



T = 300 K, P = 100 hPa

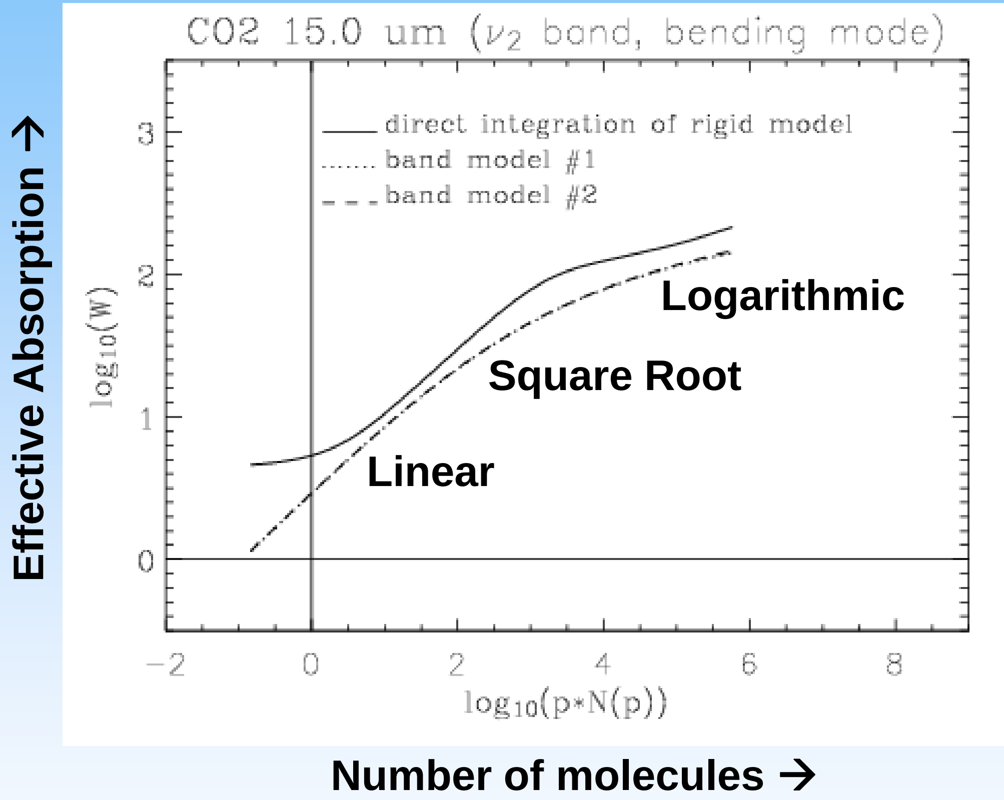


T = 300 K, P = 1000 hPa



"Curve of Growth" of a Molecule Band Model

- The growth of the effective absorption (area within the transmittance curves on previous page) of a molecular band has three distinct regions
  - Linear region - where lines grow in strength
  - Square root region - where lines are saturated at cores but continue to broaden
  - Logarithmic – where lines merge



Planck Function

- The Planck function represents the radiance as a function of frequency from an object or gas at a given temperature, T, in thermodynamic equilibrium
- It can be written in terms of wavenumber or wavelength as

$$B_\nu(T) = \frac{2 \cdot h \cdot c^2 \cdot \nu^3}{e^{\frac{h \cdot c \cdot \nu}{k \cdot T}} - 1}$$

$$B_\lambda(T) = \frac{2 \cdot h \cdot c^2}{\lambda^5 \cdot \left(e^{(hc/\lambda kT)} - 1\right)}$$

The radiance through an inhomogeneous slab is given by

- The radiance emitted from a slab is given by

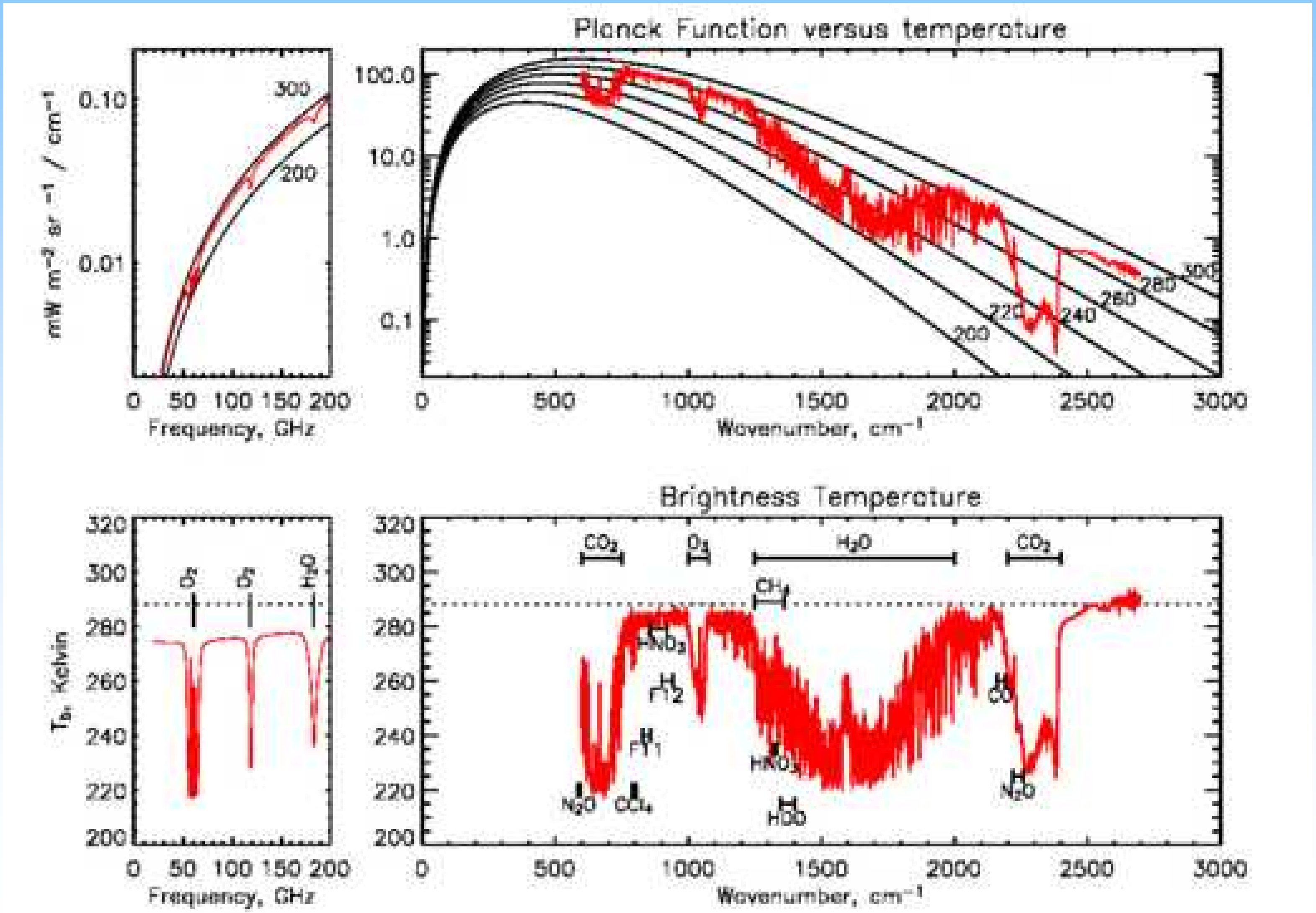
$$R_\nu = \int_{\tau=\tau_1}^{\tau_2} B_\nu(T(\tau)) \cdot \partial\tau_\nu$$

- Usually, atmospheric constituents and state is given as a function of height or pressure, so the radiative transfer equation becomes

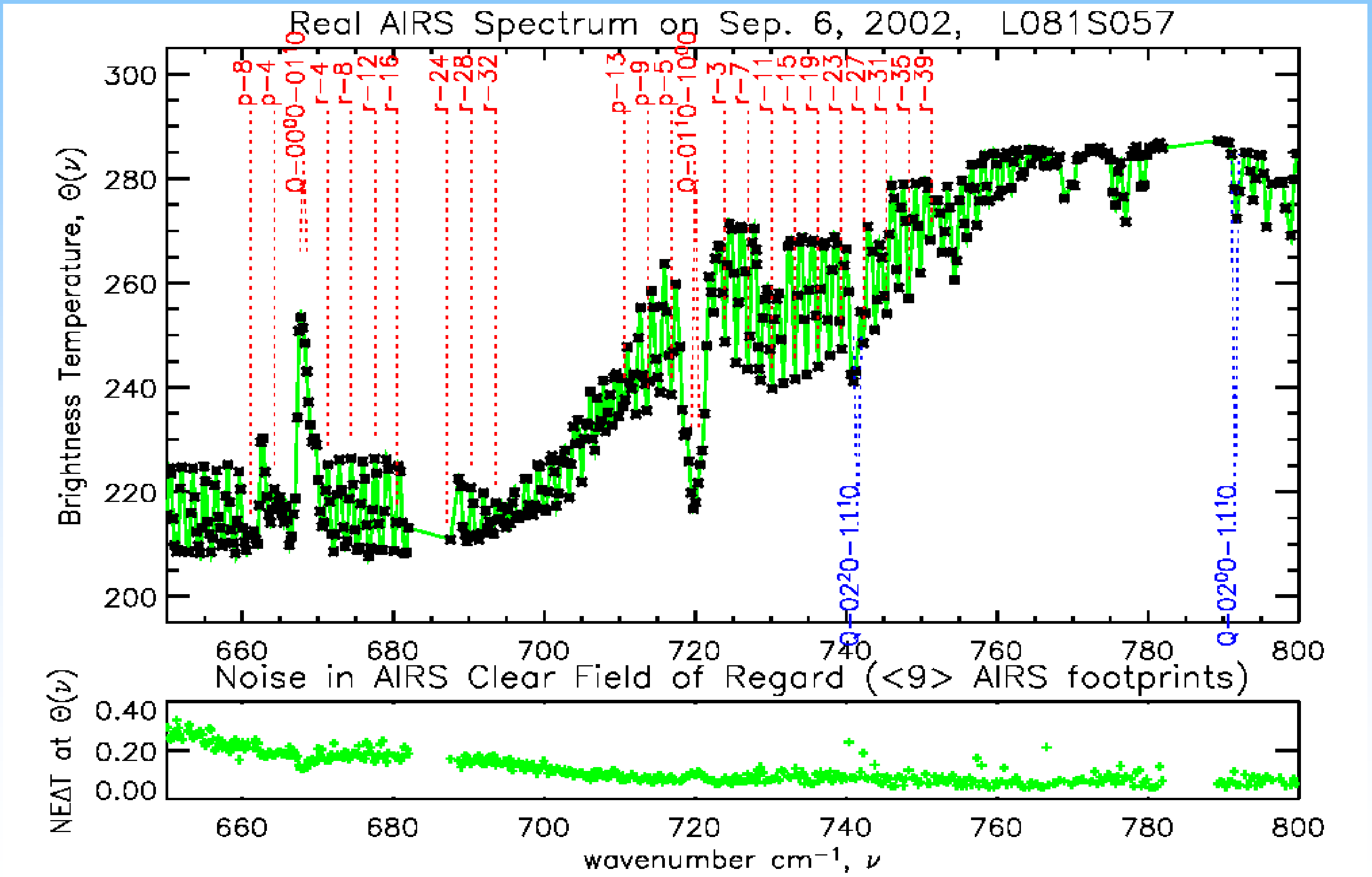
$$R_\nu = \int_{z=0}^{\infty} B_\nu(T(z)) \cdot \frac{\partial\tau_\nu^{\uparrow}(p(z), X(z), \theta)}{\partial z} \cdot \partial z$$

$$R_a(\nu, \theta) = \int_{p=P_s}^{0} B_\nu(T(p)) \cdot \frac{d\tau_\nu^{\uparrow}(p, X(p), \theta)}{dp} \cdot dp$$

Planck function w/ Earth Spectrum

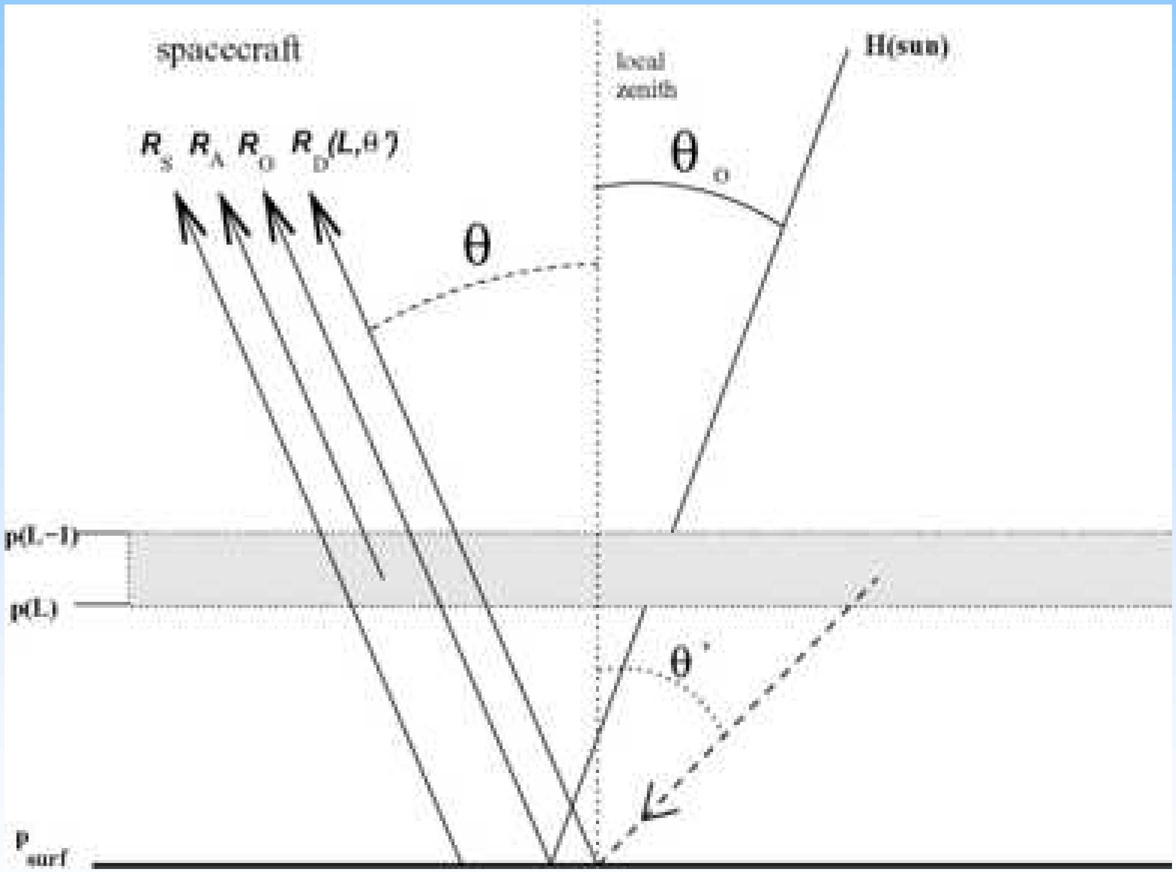


Example of 15 μm band radiance measurement from AIRS on Sep. 6, 2002



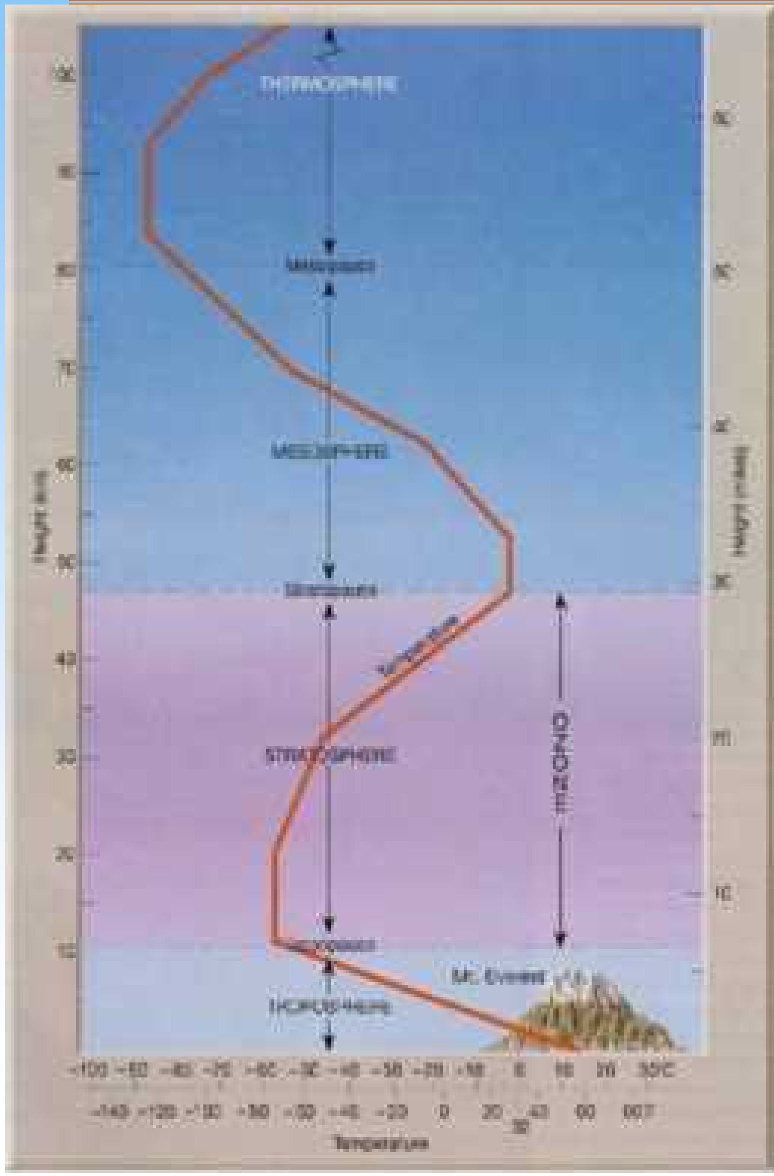
Radiance at the Satellite is Composed of Many Terms

- Surface Radiance, R_S
- Up-welling Radiance, R_A
- Direct Solar radiance, R_O
- Down-welling Reflected Radiance, R_D
- Scattering (not shown) is composed of reflections radiance from particles within the atmosphere.
- Multiple scattering (not shown) is reflections between particles.



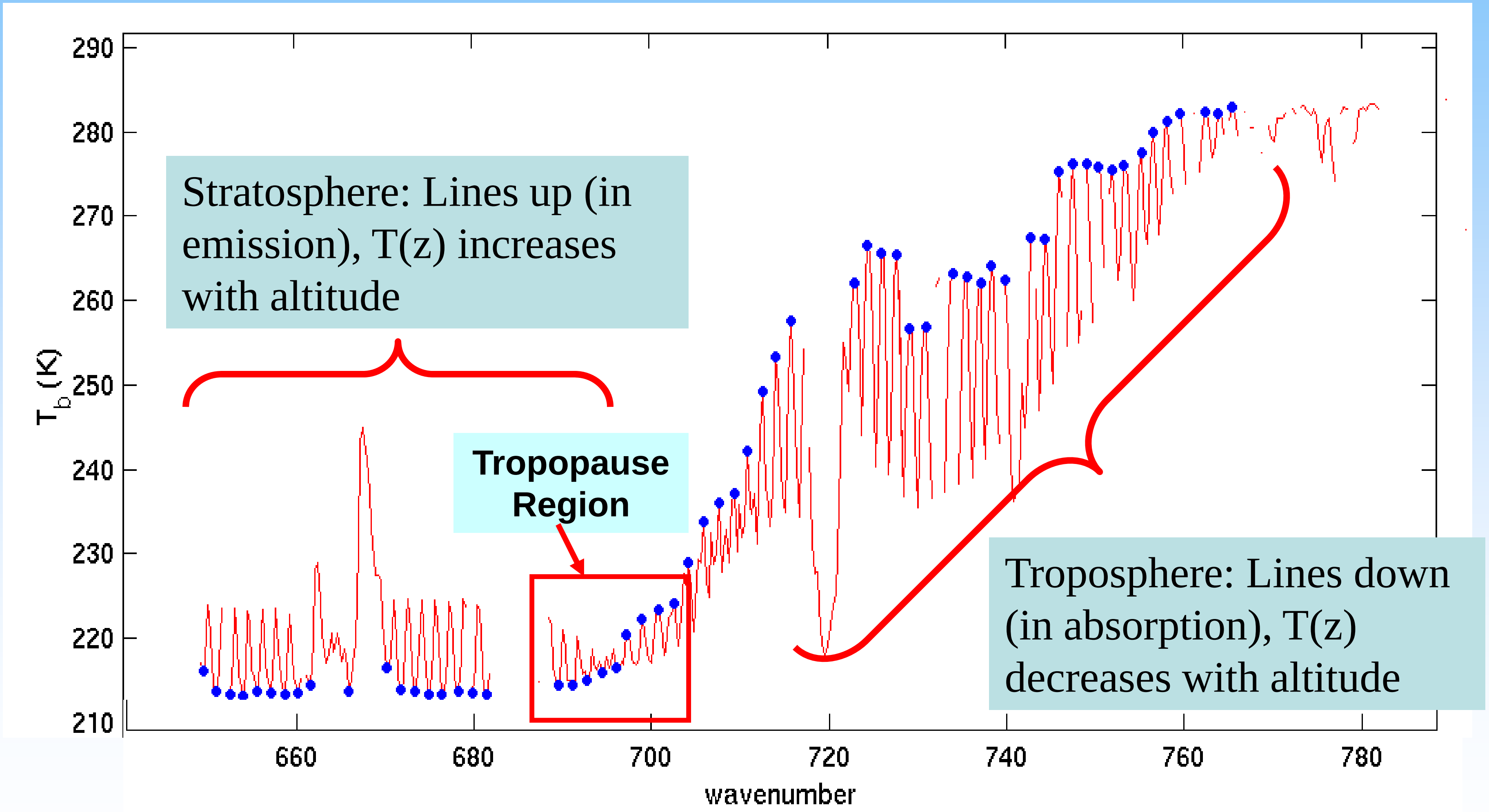
In microwave and clear (or cloud cleared) infrared scenes scattering is negligible.

A thermal sounder requires vertical temperature gradients



- High lapse rate in troposphere allows “seeing” molecular lines in absorption (against warm surface radiance).
- Stratospheric lines are seen in emission because stratosphere warms with height.
- Tropopause is difficult, because channels sensitive in that region “see” an isothermal temperature profile and, therefore, thermal imager loses sensitivity.
  - Plus it is cold, therefore, high noise in thermal infrared.

Example of 15 μm Spectrum with "in-between" the Lines Marked with Blue Dots



Thermal Sounder Forward Model Example: Upwelling Radiance Term

Each channel samples a finite spectral region

Absorption coefficients, κ, for a any spectrally active molecular species, *i*, (*e.g.*, water, ozone, CO, etc.) must be computed.

κ is also a strong function of pressure, temperature, and interactions between species.

$$R_n(\vec{X}) \simeq \int_{\nu} \Phi_n(\nu) \int_{p} B_\nu(T(p)) \cdot \frac{\partial \exp\left(-\int_{z'=\infty}^{z(p)} \sum_i \kappa_i(\vec{X}, p, \ldots) dz'\right)}{\partial p} \cdot dp \cdot d\nu$$

Inversion of this equation is highly non-linear and under-determined.

Vertical temperature gradient is critical for thermal sounding.

Full radiative transfer equation includes surface, down-welling, and solar reflection terms.

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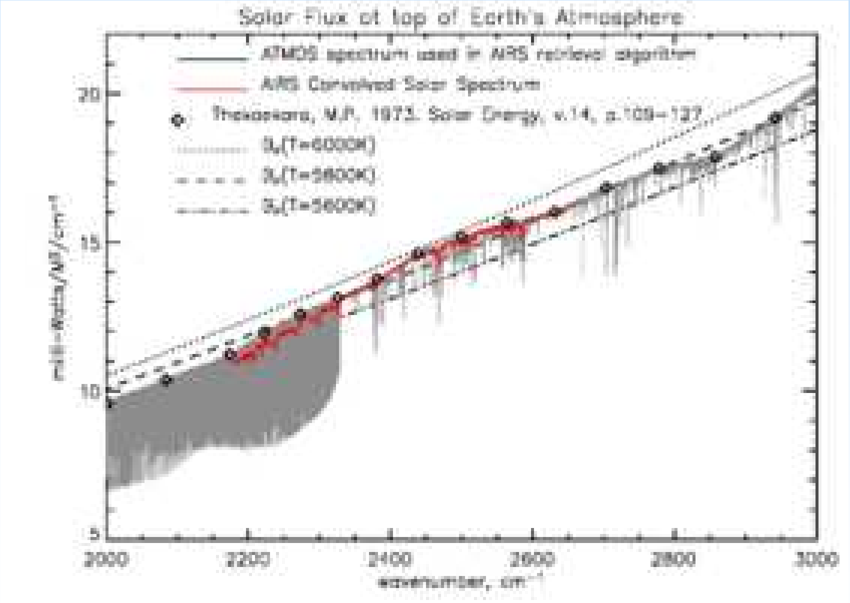
The Solar (or Direct) term, ***without scattering***, is given by

$$R_{\odot} = \rho_{\odot}(\nu, \theta, \theta_{\odot}) \cdot \tau_{\nu}^{\downarrow\uparrow}(p_s, X, \theta, \theta_{\odot}) \cdot \Omega(t) \cdot H_{\odot}(\nu) \cdot \cos(\theta)$$

$$\Omega(t) = \pi \cdot \left(\frac{0.6951 \cdot 10^{9}}{D_{\odot}(t)} \right)^{2}$$

$$\simeq 6.79 \cdot 10^{-5} - 0.23 \cdot 10^{-5} \cdot \cos(2\pi(t - t_0)/t_y)$$

- Source Function, H, is the Solar radiance at 1AU
- Ω(t) is the ratio of solid angle of the sun as a function of the Earth's orbital distance to reference distance (1 AU).
- Bi-directional transmittance contains all the atmospheric absorption along the solar ray.
- Surface reflectivity is a strong function of geometry and surface type.



Down-welling thermal term

$$R_d(\nu,\theta) = \tau_\nu^{\uparrow}(P_s,X,\theta)\cdot\int_{\alpha=0}^{2\pi}\int_{\theta'=0}^{\frac{\pi}{2}}\rho_\nu(\theta,\theta',\alpha)\cdot\sin(\theta')\cdot\cos(\theta')\cdot d\theta'\cdot d\alpha \cdot\int_{p=P_s}^{0}B_\nu(T(p))\cdot\frac{d\tau_\nu^{\downarrow}(p,X,\theta')}{dp}\cdot dp$$

In the microwave we assume the down-welling transmittance is monochromatic and compute a diffuse angle that is a function of surface type. Over ocean the microwave diffusive angle is a function of wind speed and can be retrieved.

$$\Theta_d(n,\theta) = \tau_\nu^{\uparrow}(P_s,\theta)\cdot(1-\epsilon_\nu)\sum_{L=1}^{N_L}\left[\overline{T(L)}\cdot\Delta\tau_\nu^{\downarrow}(L,\theta)\right]$$

$$\Delta\tau_\nu^{\downarrow}(L,\theta) \simeq \left(\frac{\tau_\nu^{\uparrow}(P_{surf},\theta)}{\tau_\nu^{\uparrow}(p(L),\theta)}\right)^f - \left(\frac{\tau_\nu^{\uparrow}(P_{surf},\theta)}{\tau_\nu^{\uparrow}(p(L-1),\theta'_\nu)}\right)^f$$

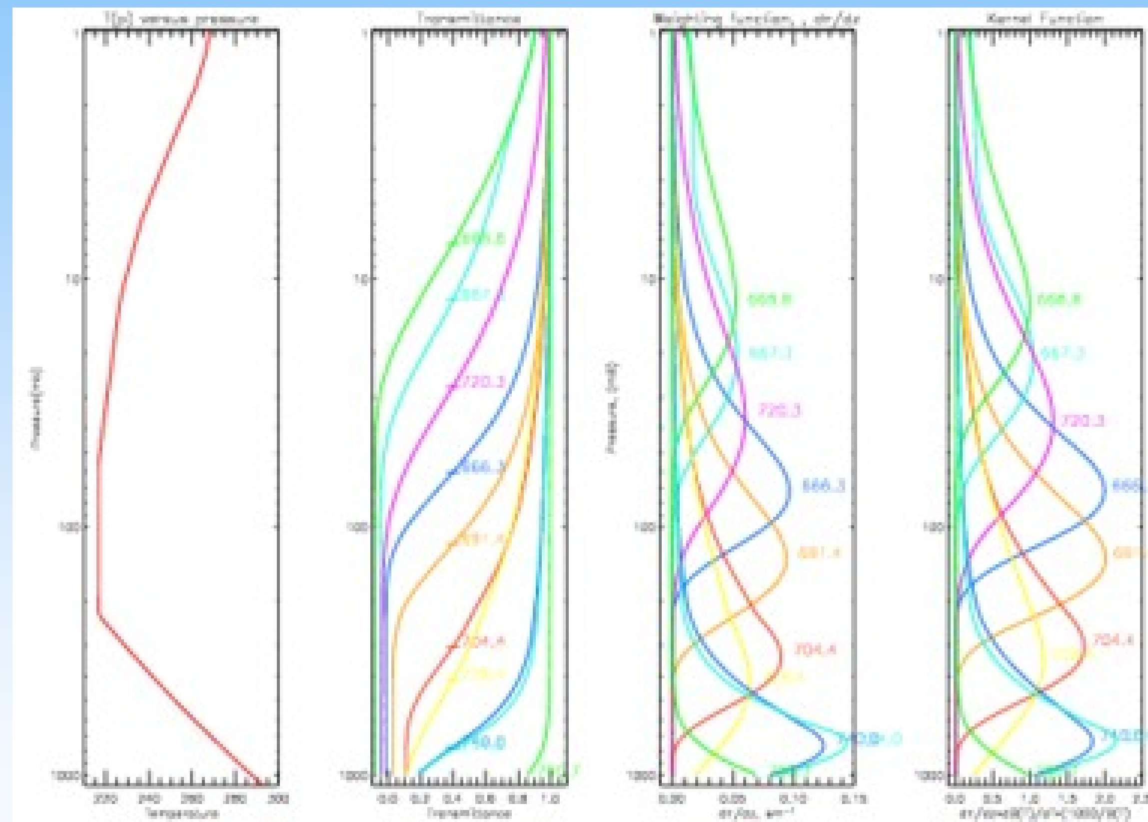
$$f = \text{ratio of secant angles}$$

A “poor mans” retrieval

- Knowledge of the radiative transfer enables one to perform a retrieval of geophysical products from the radiances.
- The next few slides describe a “poor man’s” retrieval to illustrate the underlying concepts of a physical retrieval

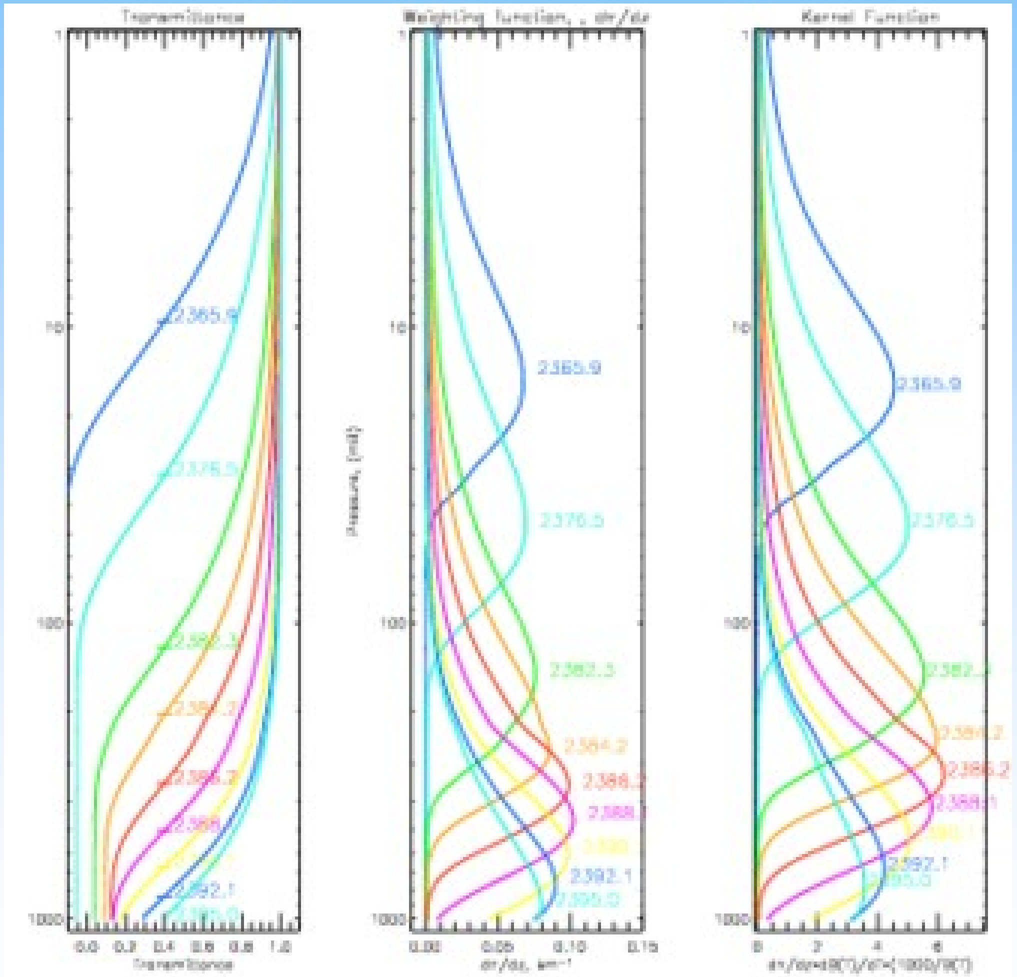
Given a temperature profile we can compute transmittance-to-space for individual channels

- Transmittance changes rapidly from one to zero in a vertical region.
- The derivative of transmittance is vertically localized.
- The Planck weighted derivative (called Kernel function) is shown at right
  - this is the vertical “sensitivity” of a channel



Same as previous slide, but some of the short-wave channels

- Short-wave (SW) infrared (4.3 μm or 2400 cm^{-1}) has sharper kernel functions.
- Also, SW is a relatively "pure" band of CO2 and is unaffected by water and ozone absorption.
- Also, the Planck function is non-linear in the SW region and sharpens the vertical sensitivity.
- This is why the retrieval community likes using the SW and encourages DA to use them.



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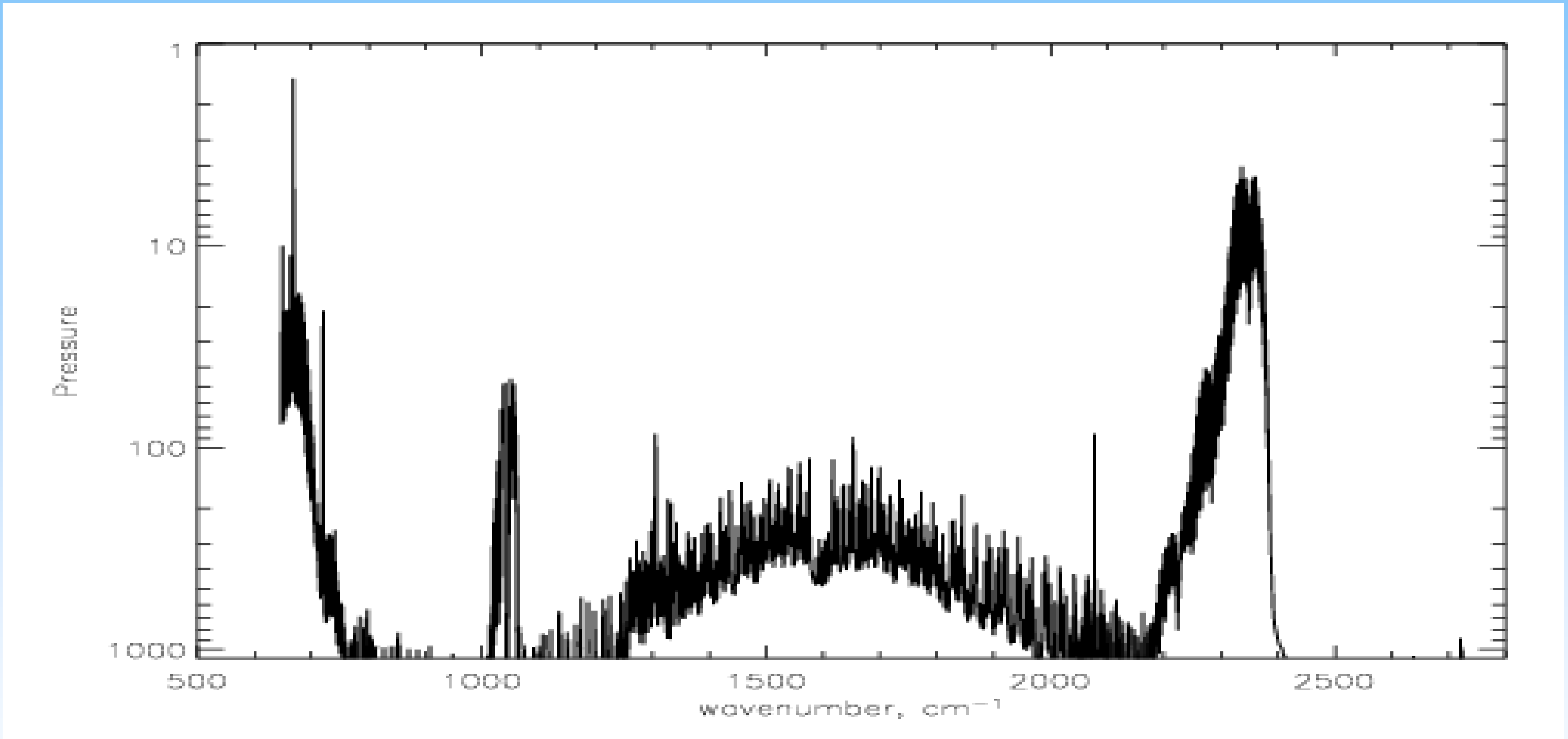
The pressure level of sensitivity, *p(ν)*, is highly channel (and scene) dependent



- The altitude of maximum sensitivity for a given geophysical state as a function of channel (wavenumber) is shown.
- One can take a measured radiance and knowing the altitude of sensitivity can estimate the underlying geophysical state.
- This is the underlying basis of a physical retrieval.

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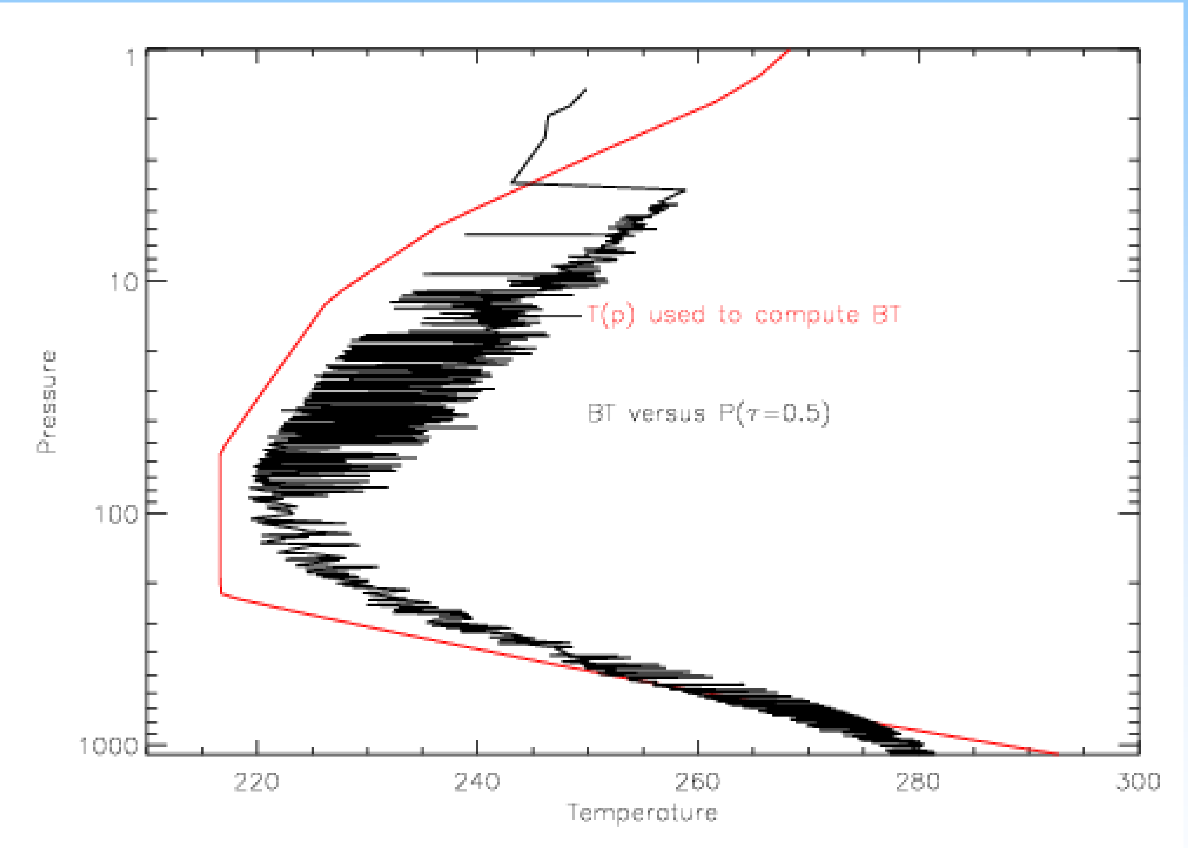
A "poor mans" retrieval can be done by simple inspection of the brightness temperatures

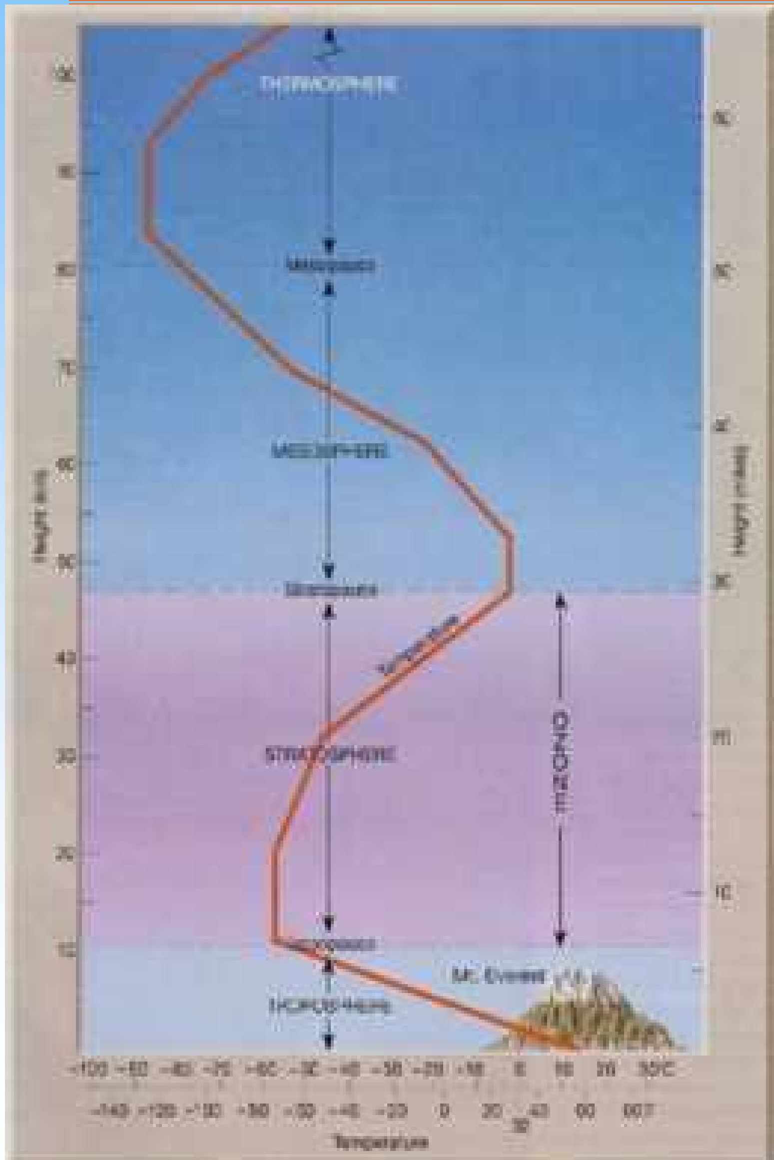
- At right is the temperature profile used to generate the spectrum (red)
- In black is shown the brightness temperature as a function of where the channels are sensitive, T = BT(z(ν))



Sidebar: what does 2xCO_2 look like

- Does increase in carbon dioxide cause global warming?
- Need to understand radiative transfer and curve of growth to understand global warming

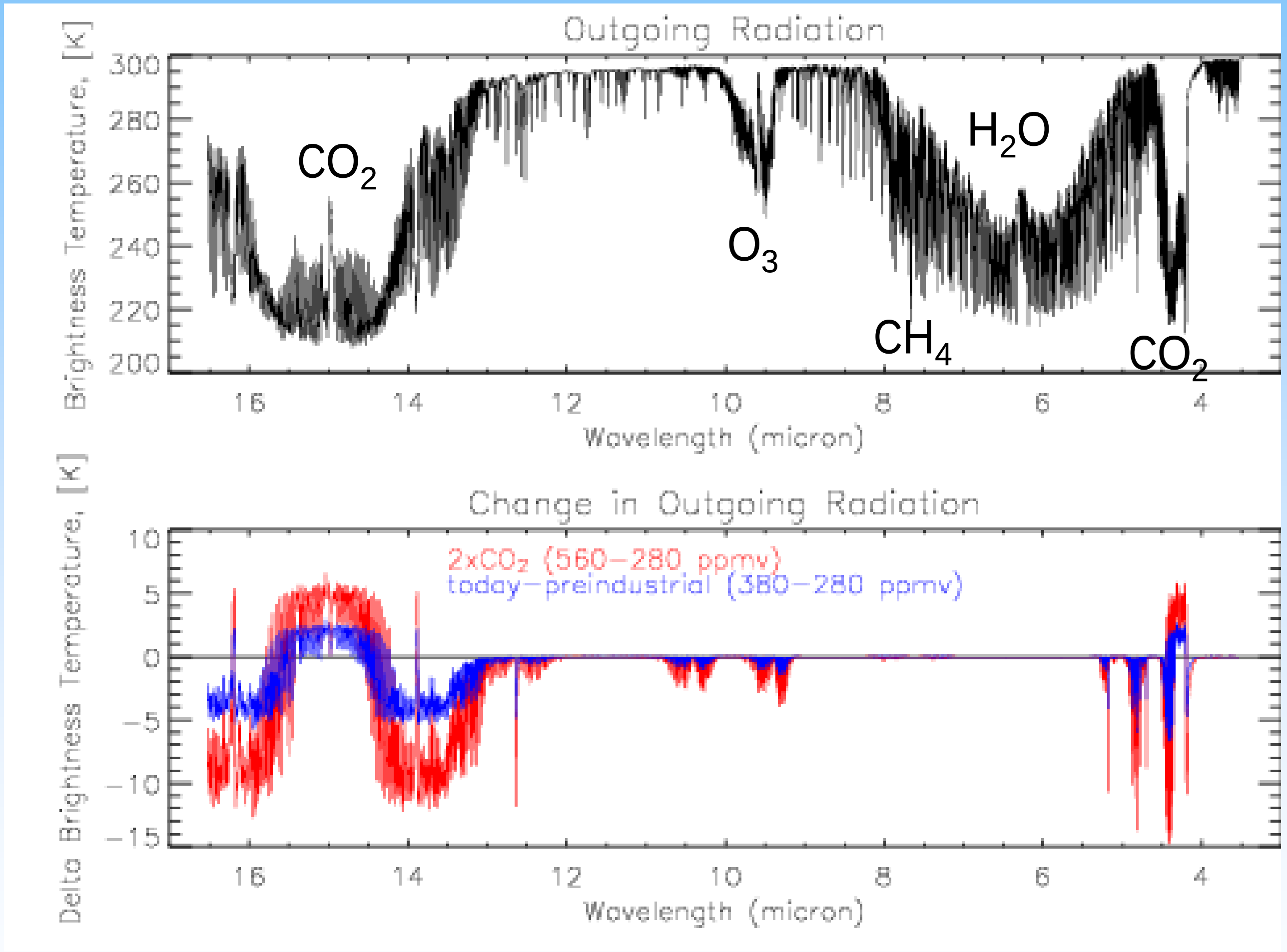
The atmospheric “greenhouse gases” determine the altitude energy is radiated to space.



- As more absorbing gas is added the atmosphere becomes more opaque and the effective level of radiation to space is higher.
- If the gas is most effective in stratosphere then it becomes a more efficient radiator and atmosphere cools.
  - Because stratosphere warms with height.
- If the gas is most effective in troposphere then it is a less efficient radiator and atmosphere warms.
  - Because troposphere cools with height.

Molecules radiate efficiently in the infrared: The view from space with infrared "eyes"

- CO_2, water, methane, and ozone absorb efficiently at thermal (infrared) wavelengths.
  - Molecules vibrate and rotate efficiently at these frequencies.
- Figure at right is change in outgoing radiation since pre-industrial (blue) and for doubling of CO_2 (red, maybe 2075)



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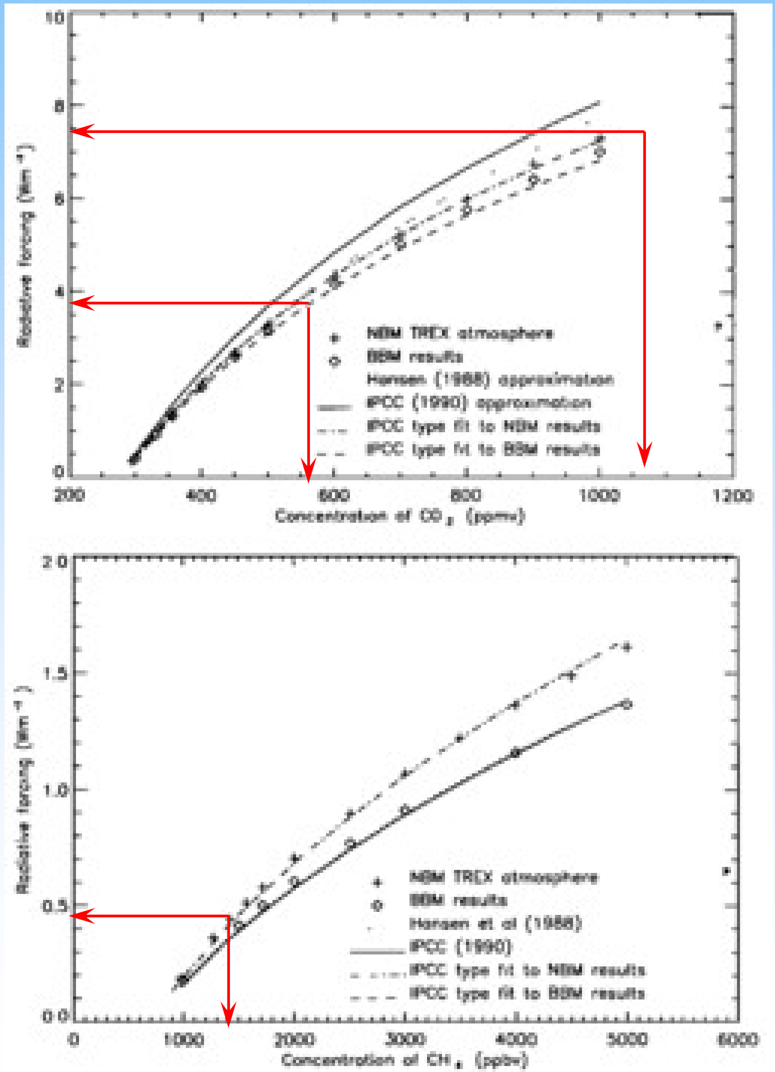
Radiative Forcing by GHG’s

- At right is shown the direct radiative forcing due to increasing CO2 or CH4 in the atmosphere (Myhre 1998)
- It is non-linear and can be best expressed in terms of doubling of CO2 from pre-industrial (280 ppm) values. (560 ppm and 1120 ppm are shown as red lines in the fig.)
- Radiative forcing due to CO2 adds 3.7 W/m^2 per doubling of CO2.
- In equilibrium, this will be balanced by the Planck feedback (σT^4), and will result in 1.2 C of warming in equilibrium
- Doubling of methane from pre-industrial (700 ppb) results in about 0.45 W/m^2 or about 50 times more forcing per molecule than CO2.

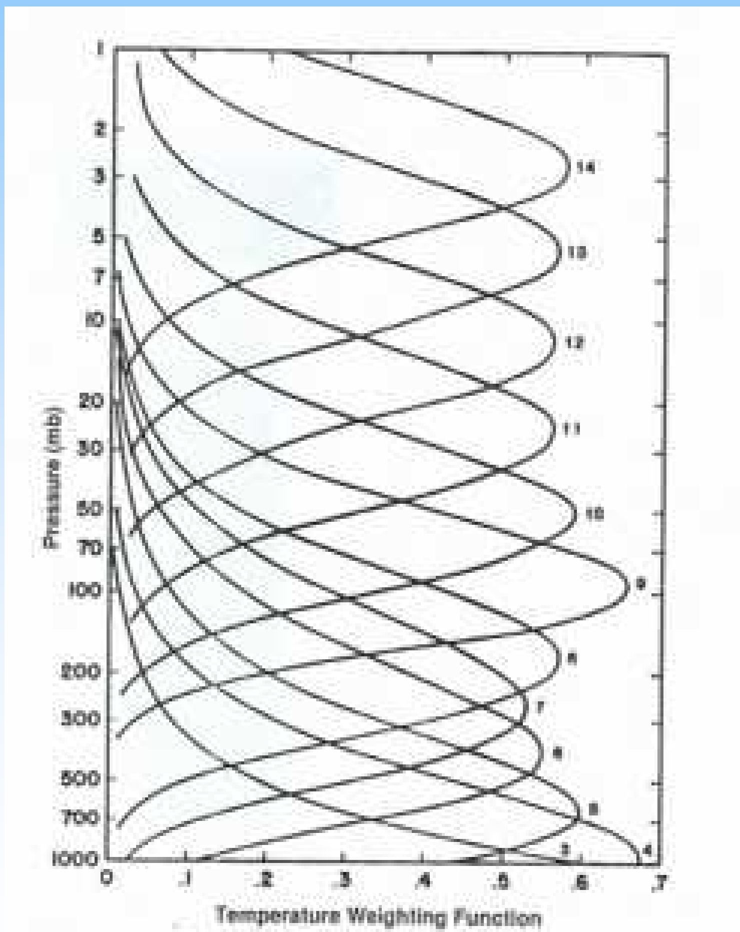


Thoughts on use of hyperspectral measurements in Data Assimilation

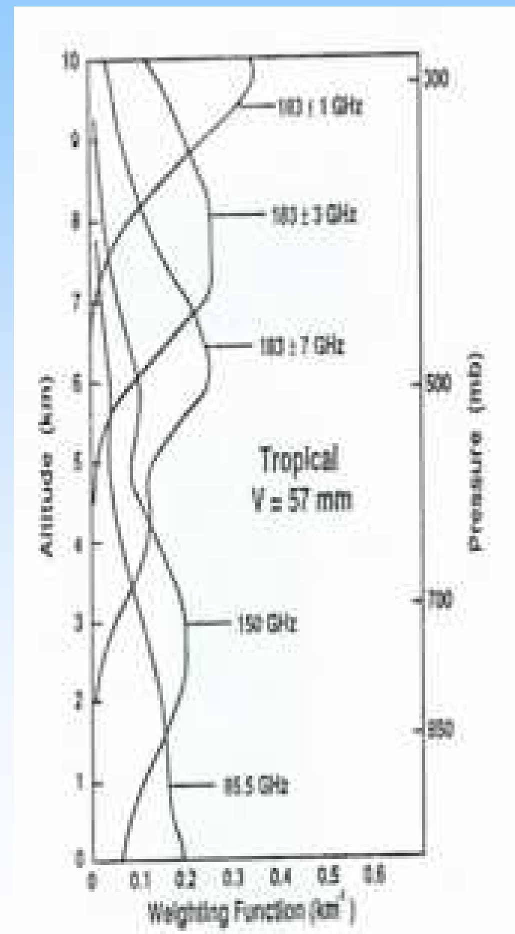
- The advantage of the hyper-spectral infrared is the high vertical sensitivity and high sampling.
- To date, these advantages have not been exploited in operational data assimilation.
  - SW channels are not used
  - Water channels have little impact in DA
    - They are more non-linear than the microwave
      - Infrared water channels are also strongly sensitive to temperature.
    - Therefore, they require accurate background covariance matrices
    - Retrieval systems mitigate this issue by separating temperature and moisture into separate spectral regions.
  - Infrared emissivity can be retrieved (versus modeled) from hyper-spectral measurements.

AMSU Temperature & Moisture Channel Weighting Functions

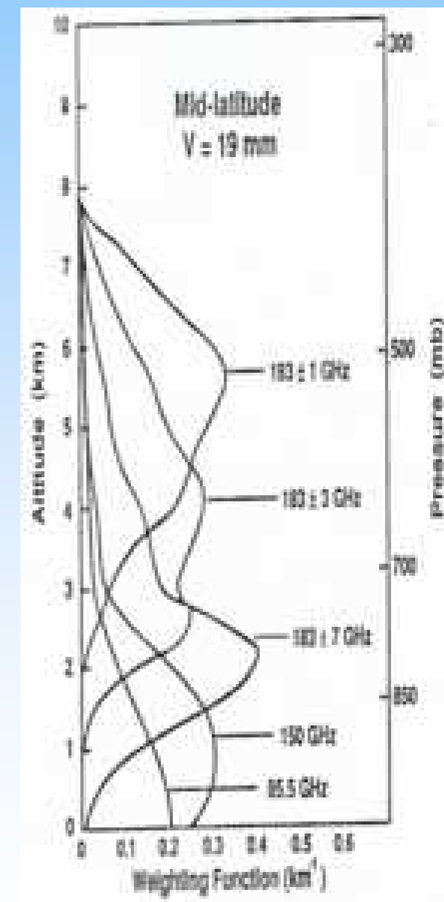
W = dτ/dz



W = dτ/dq tropical



W = dτ/dq mid-lat



K = $dB_{\upsilon}(t)/dT * d\tau/dz$, Figures from M.A. Janssen 1993 John Wiley & Sons

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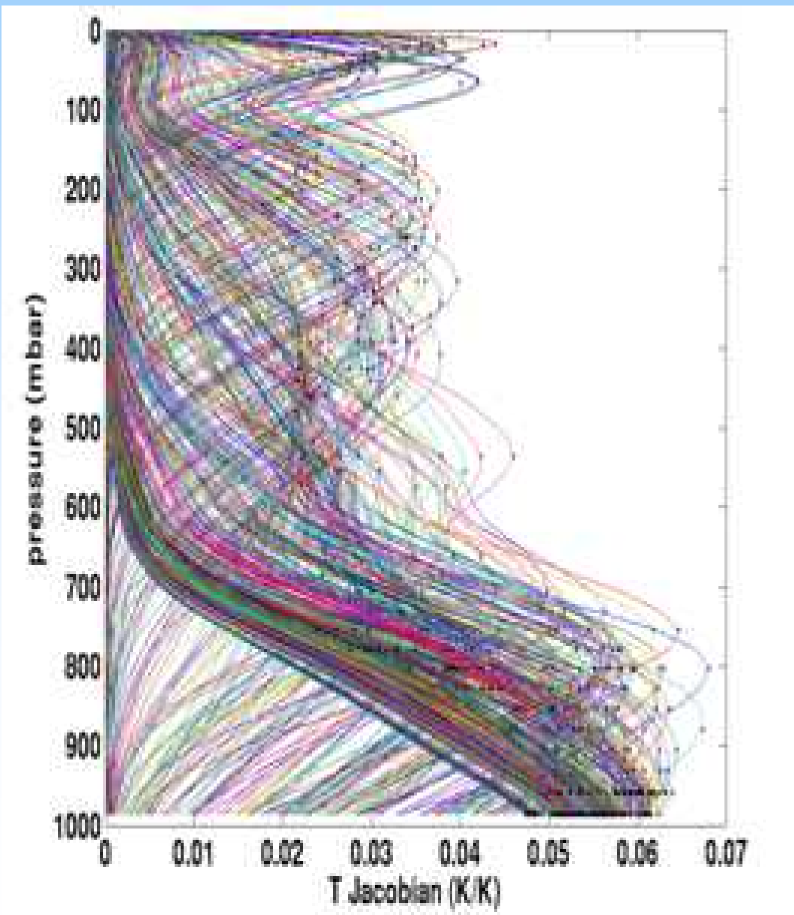
Example Infrared Channel Kernel Functions, $K_{n,j}$ for Temperature and Moisture

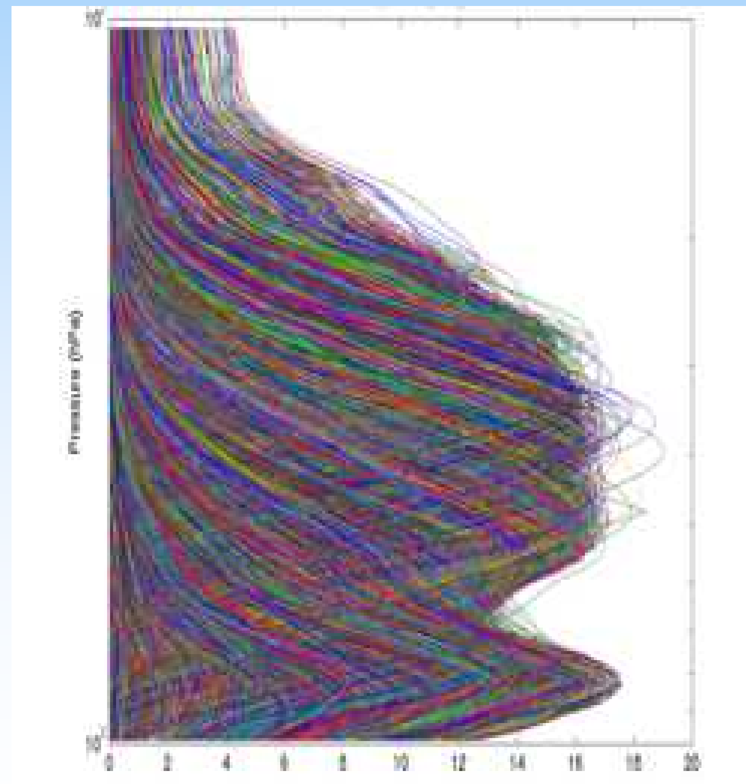
AIRS 15 µm (650-800 cm-1) band

K = dR/dT

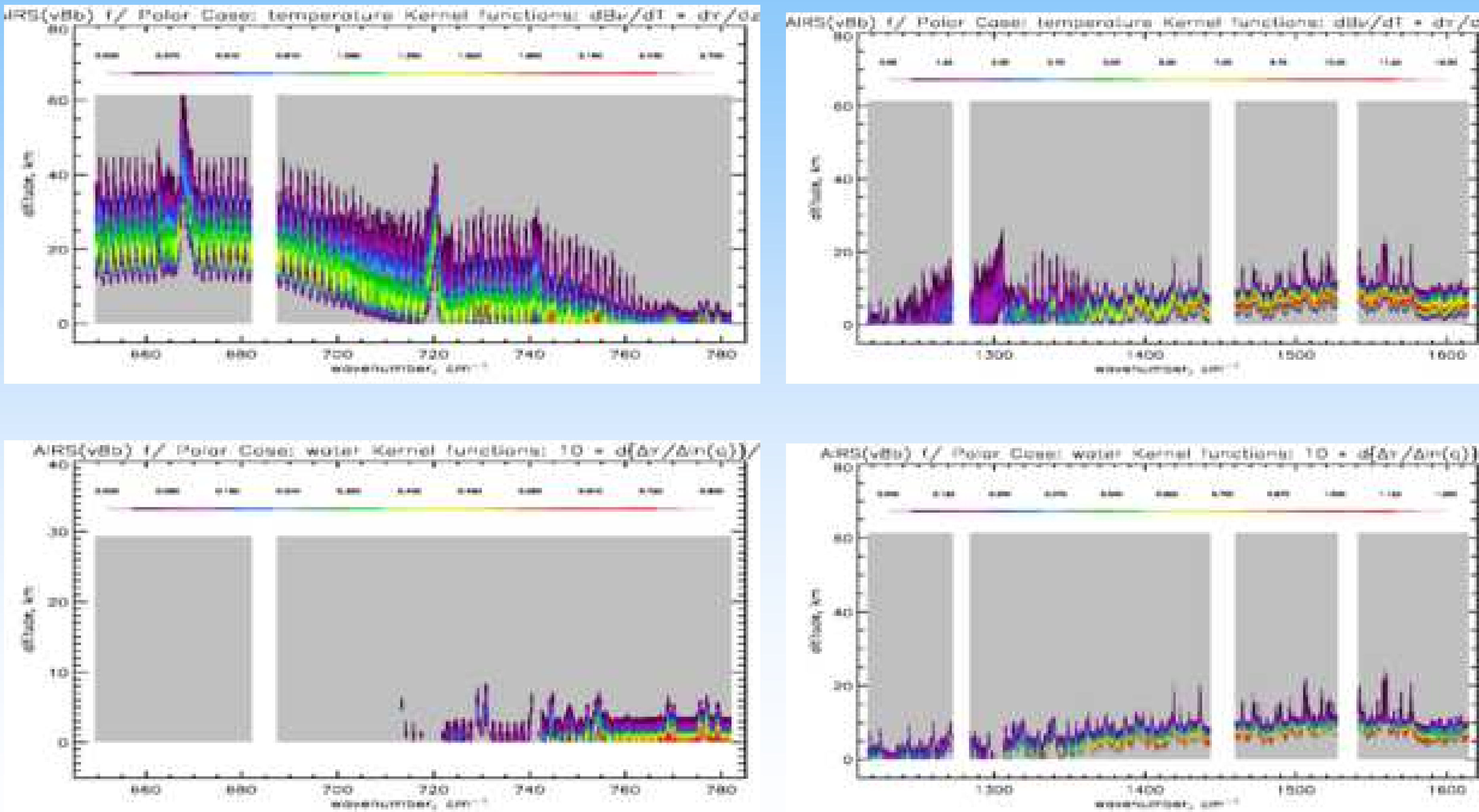


AIRS 6.7 µm (1200-1600 cm^{-1}) band

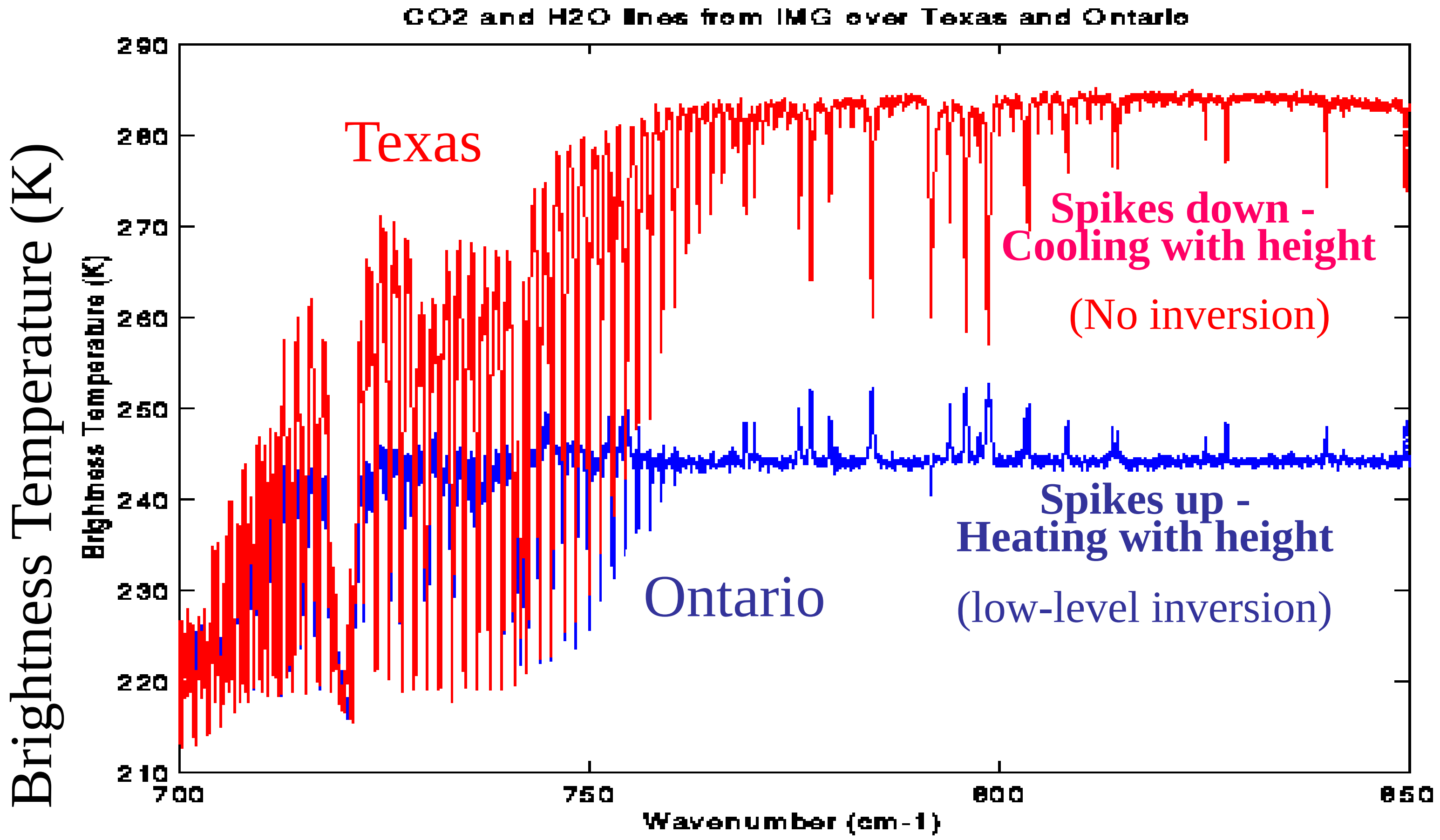
K = dR/dq



AIRS 15 μm & 6.7 μm Temperature (top) and Moisture Channel Kernels Functions

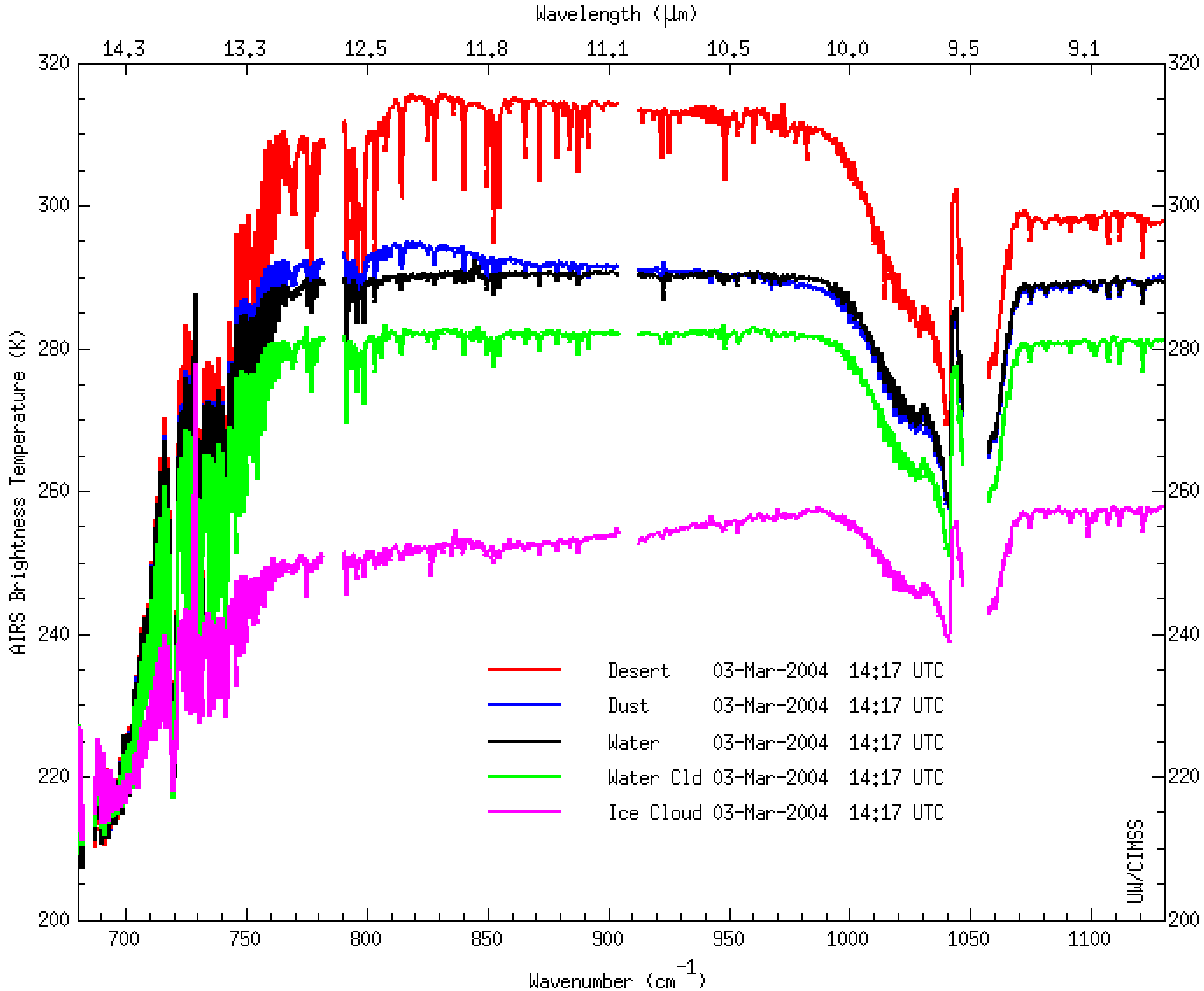


Weak Lines (Water & CO2) in Window Region Sound Boundary Layer Inversions



How to handle clouds

- One can simultaneously retrieve clouds
  - This requires adding scattering to the forward radiative transfer code written in terms of
    - a single-scattering albedo
    - a phase-function (efficiency of scattering as a function of particle characteristics (shape and absorption characteristics)
    - Requires multiple streams (downwelling, upwelling, and diffusive terms).
  - Scattering also increases the effective path-length of atmospheric (molecular) absorption.
  - Effects of clouds is large, but poorly constrained by the infrared.
    - Best approach would include visible, infrared, and microwave
    - Data assimilation might have a unique capability in this context.
- AIRS science team chose cloud clearing approach because
  - Number of free parameters in a cloud retrieval is very high and would degrade ability to retrieve other parts of the geophysical state.
- Of course, this is a active area of debate within the community.


Wavelength (µm)
14.3
13.3
12.5
11.8
11.1
10.5
10.0
9.5
9.1
AIRS Brightness Temperature (K)
320
300
280
260
240
220
200
Desert 03-Mar-2004 14:17 UTC
Dust 03-Mar-2004 14:17 UTC
Water 03-Mar-2004 14:17 UTC
Water Cld 03-Mar-2004 14:17 UTC
Ice Cloud 03-Mar-2004 14:17 UTC
UW/CIMSS
700
750
800
850
900
950
1000
1050
1100
Wavenumber (cm-1)

National Environmental Satellite, Data, and Information Service

References for the AIRS fast radiative transfer methodology

- Strow, L.L., S.E. Hannon, S. DeSouza-Machado, H.E. Motteler and D.C. Tobin 2006. Validation of the atmospheric infrared sounder radiative transfer algorithm. J. Geophys. Res. v.111 D09S06 doi:10.1029/2005JD006146, 24 pgs.
- Strow, L.L., S.E. Hannon, S. DeSouza-Machado, H.E. Motteler and D.C. Tobin 2003. An overview of the AIRS radiative transfer model. IEEE Trans. Geosci. Remote Sens. v.41 p.303-313.
- Hannon, S.E., L.L. Strow and W.W. McMillan 1996. Atmospheric infrared fast transmittance models: a comparison of two approaches. SPIE v.2830 p.94-105.