Atmospheric Composition Sounding

ESA Summer School

ESRIN

13th August 2010

Lecture 2 by B.Kerridge

IR Spectrometry

Outline

1. Principles
   – Radiative transfer & basic retrieval diagnostics
2. Instrument attributes
3. IASI & TES
4. Summary and future advances

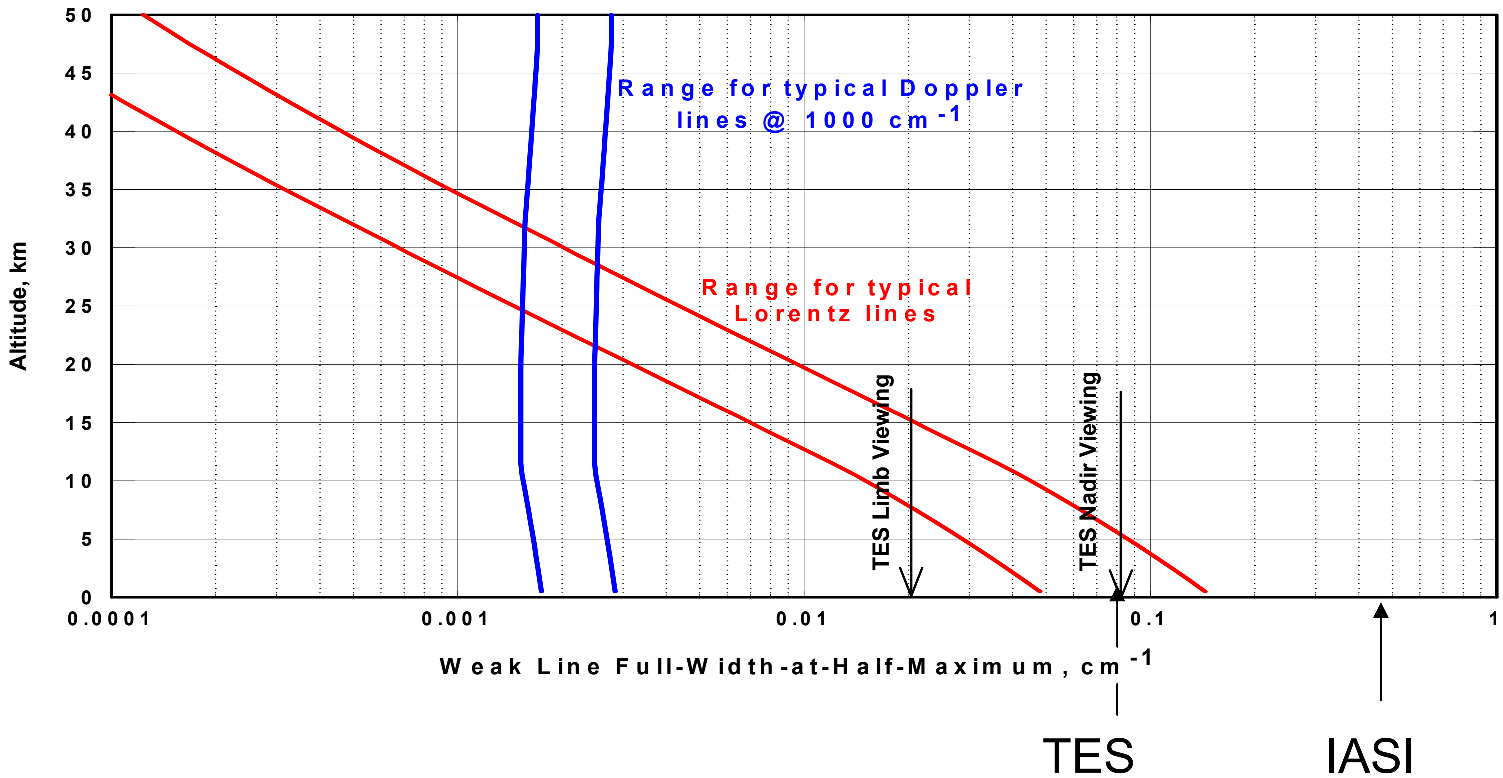
Nadir IR Spectrometry

- Sounding free troposphere
  - *where pollutants are transported*

Principles of ir nadir sounding

1. In mid IR region $3.3\mu m$ ($3{,}000 cm^{-1}$) < λ < $20\mu m$ ($500 cm^{-1}$) most molecular transitions are *vibration-rotation bands*
   - Transitions between vibrational levels ($\Delta\nu_v$ ~$1{,}000\ cm^{-1}$) and simultaneously between rotational levels
   - – $\Delta\nu_r \ \alpha\ 1 / M_r$
   - → $\Delta\nu_r \sim$ several cm^{-1} for H_2O, CO ↔ << $1 cm^{-1}$ for eg HNO_3
   - → For heavy molecules, rotational structure of vib-rot bands unresolved
2. $\lambda > 5\mu m$ ($2000 cm^{-1}$) thermal emission predominantly
3. $\lambda < 5\mu m$ ($2000 cm^{-1}$) backscattered solar radiation increasingly significant with decreasing λ
4. Radiative and photochemical processes can affect populations of *vibrational* levels in stratosphere and above
   - have to be modelled in some cases, even if targeting low atmosphere

Variation with altitude of typical Doppler- and pressure-broadened (Lorentz) line widths



— Pressure-broadened widths decrease exponentially with height
— Line shape carries height information (if resolved).

Principles of Nadir-IR Composition Sounding

- Constituents detected through ***spectral contrast*** with surface emission (BB)
- Interferometers can yield hundreds of spectral elements
- Retrieval of *height-resolved* information requires:
  1. Variation in atmospheric opacity with wavelength
     $\Rightarrow$ H_2O a very suitable candidate
  2. Vertical temperature gradient
     $\Rightarrow$ Limited info at tropopause and near surface
  3. T profile to be known to high accuracy, along with surface T and ε

$$R(v) = B(v,0)\tau(v,0) + \int_{o}^{oo} B(v,z)\frac{d\tau}{dz}(v,z)dz$$

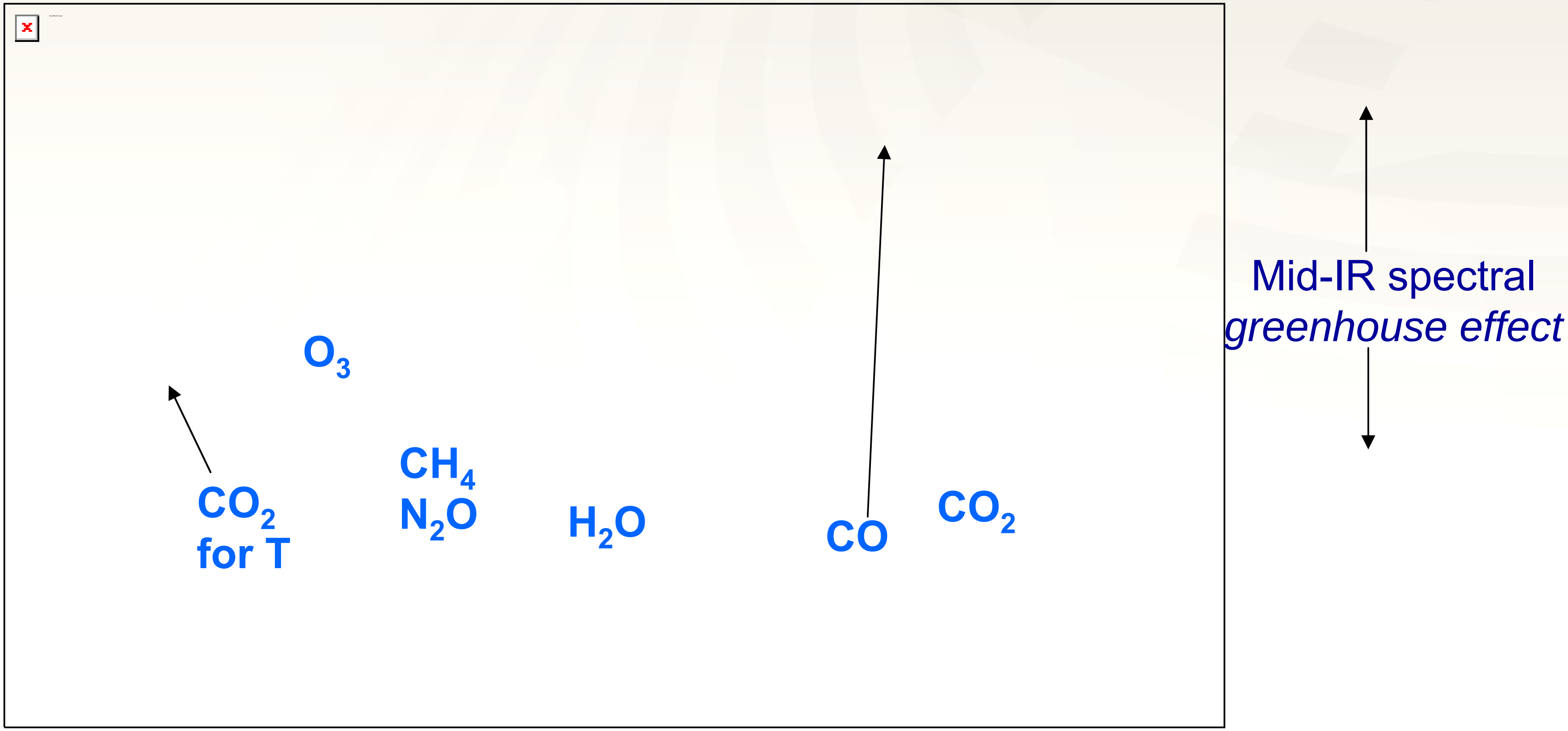
- Hypothetical case of isothermal Atmosphere:

$$R(v) = B(v,0)\tau(v,0) + B(v,T_A)[1 - \tau(v,0)]$$

$$= B(v,T_A) + [B(v,0) - B(v,T_A)]\tau(v,0)$$

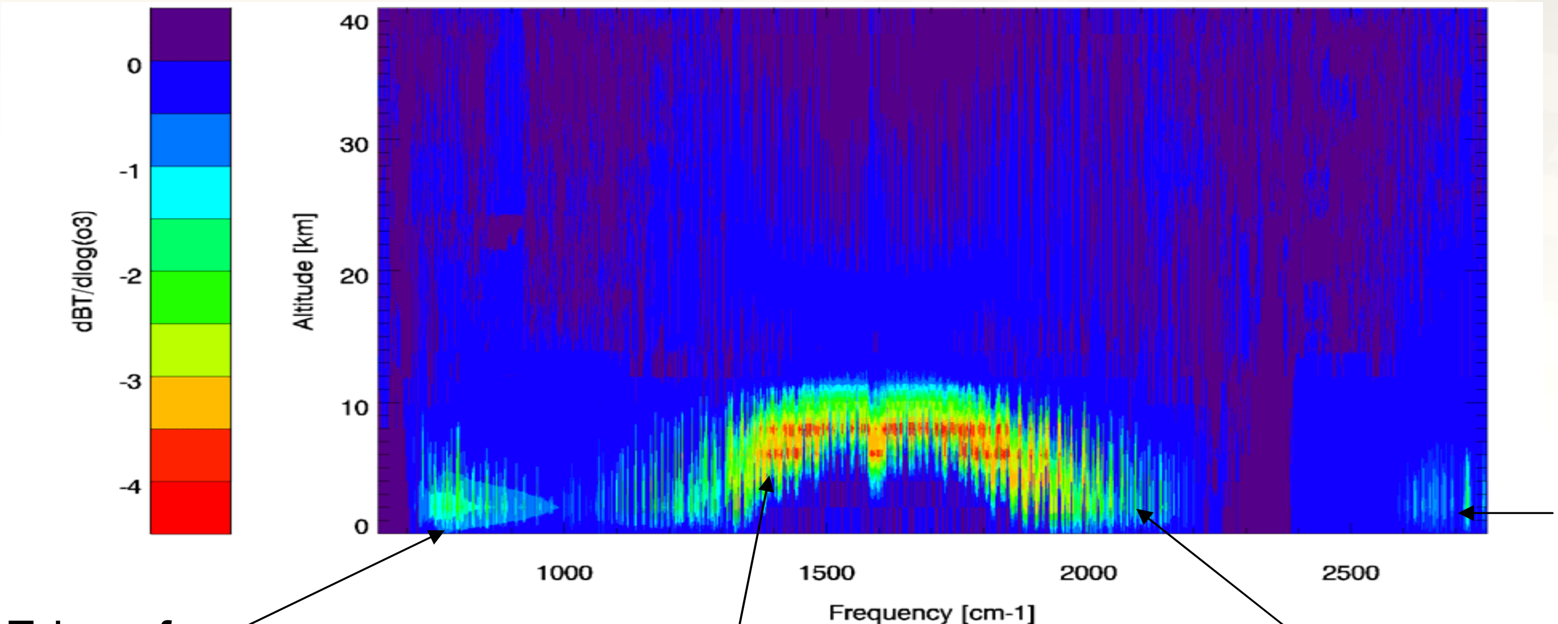
Column information only

Nadir-IR spectrum



- Simulation at IASI resolution ($0.5cm^{-1}$)
- H_2O & other *continua* underly vibration-rotation bands

H_2O spectral weighting functions (2km retrieval grid)



Edge of ν_3 band (2.7μm)

Edge of Rotation band

ν_2 band (6.3μm)

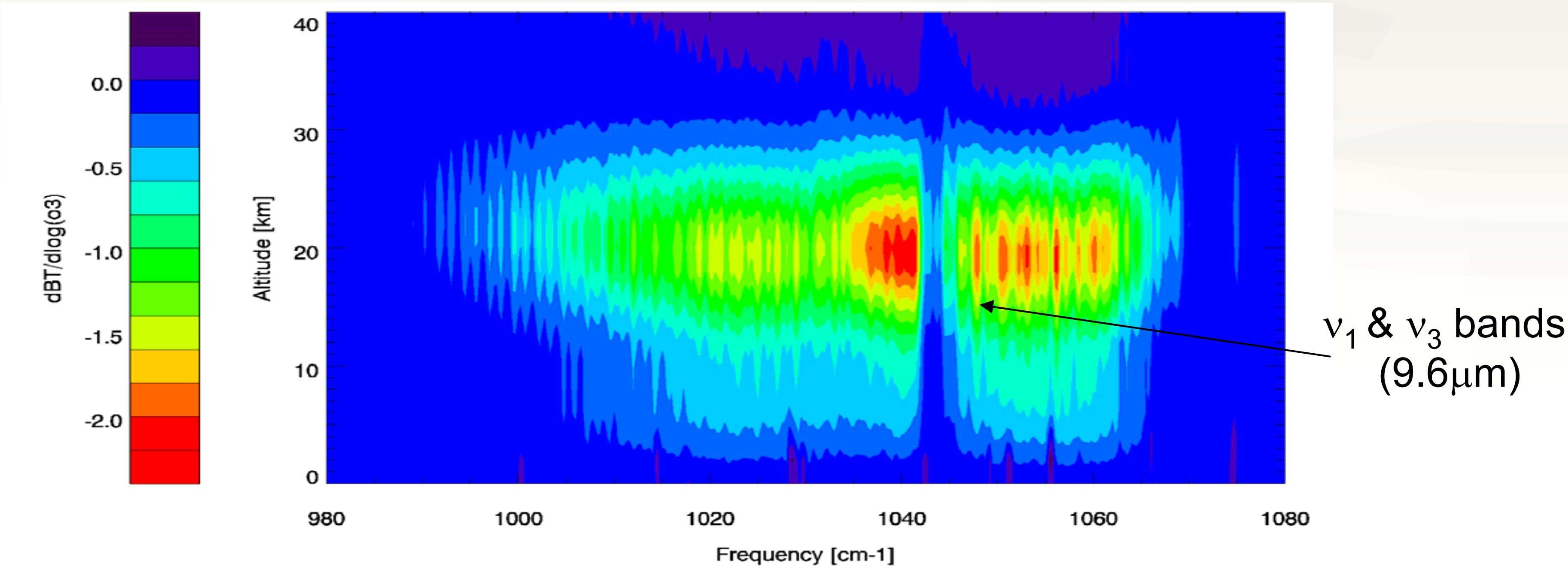
– Wide spectral variation in opacity
– K's peak over wide ht.range

→ *Vertical resolution high up to ~10km*

–K's non-negligible near surface, even though T(z) → T(ground)

– H_2O v.high in near-surface layer & decreases exponentially with height

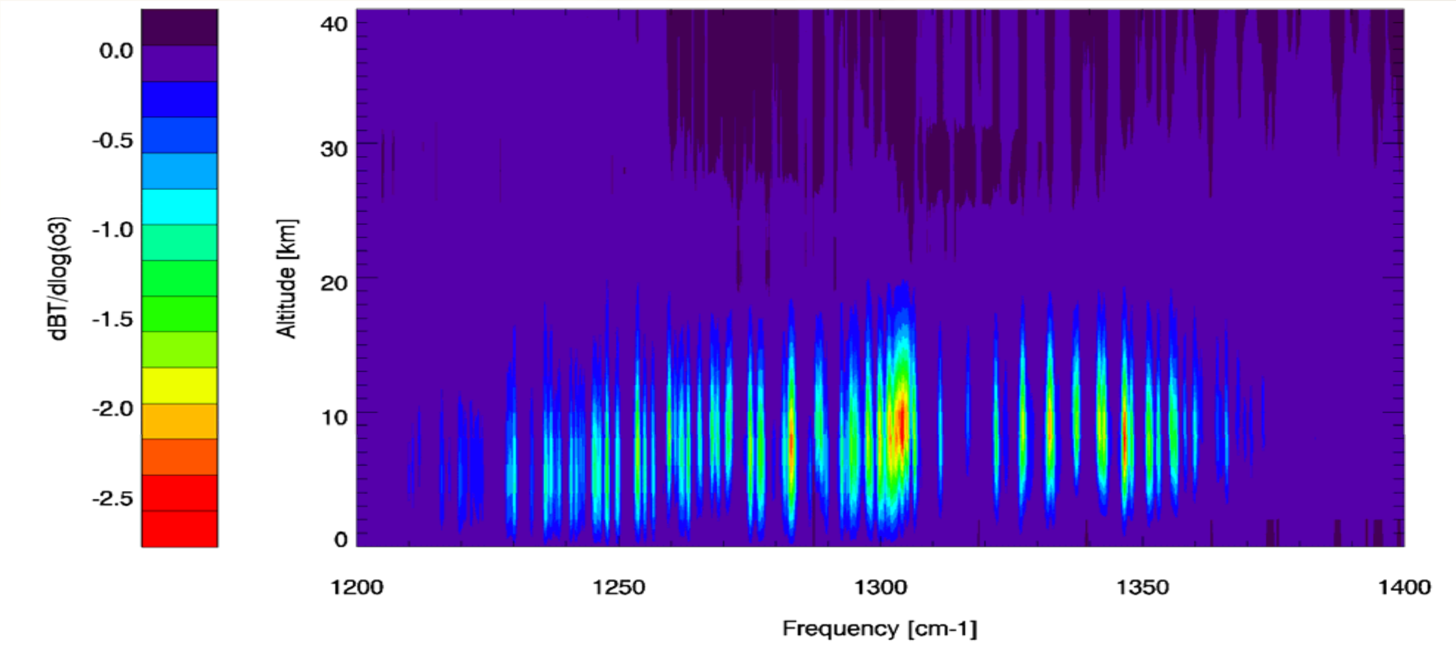
O_3 spectral weighting functions



— Spectral variation in opacity, though much less than for H_2O
— K's all peak ~20km ← *centre of stratospheric O_3 layer*
— K's extend up through strat. and down through trop.
— Spectral variation in K's from T-dependence of opacity

→ *Some height-resolution in mid-upper trop. & lower strat.*

CH_4 spectral weighting functions



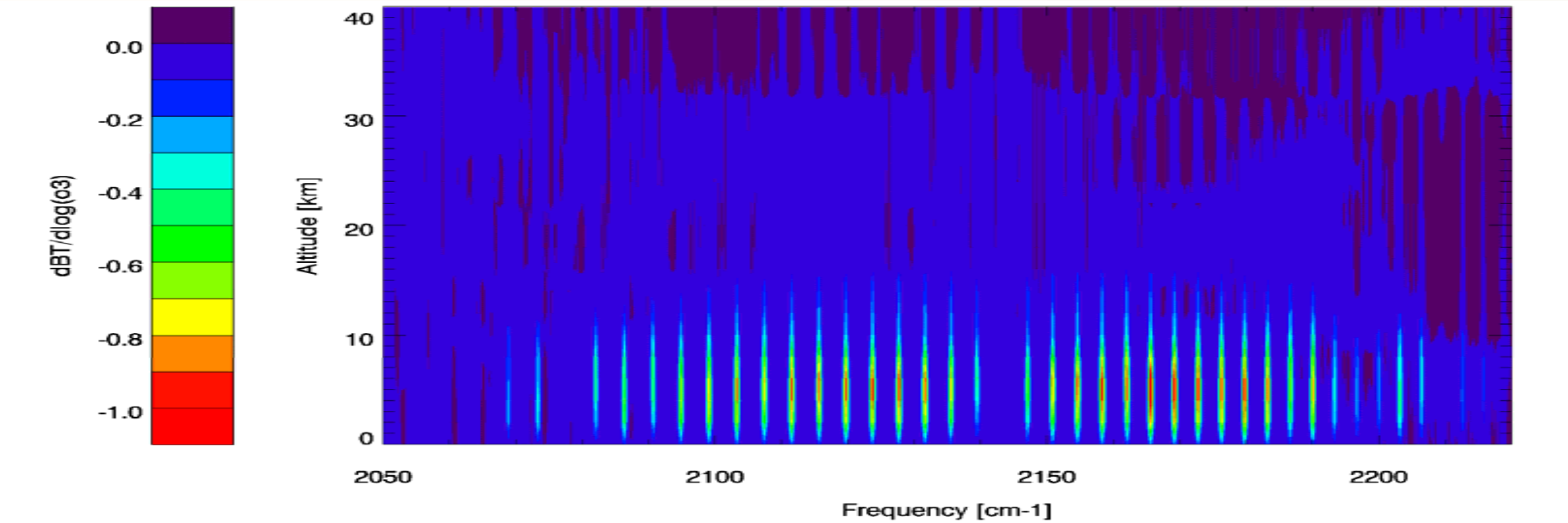
ν_4 & ν_2 bands (7.4μm)

– Spectral variation in opacity similar to O_3 (and > than 1.6, 2.35 & 3.5μm CH_4 bands)

– K's peak at different heights between ~4 – 8km

→ *Some height-resolution in troposphere*

CO spectral weighting functions



CO (0-1) band (4.7μm)

— Regular, widely-spaced lines (diatomic)

— Spectral variation in opacity less than O_3 (though greater than CO (0-2) band at 2.35μm)
— K's all peak at similar height ~4-6km
— K's extend up and down through trop.
— Spectral variation in K shapes from T-dependence of opacity

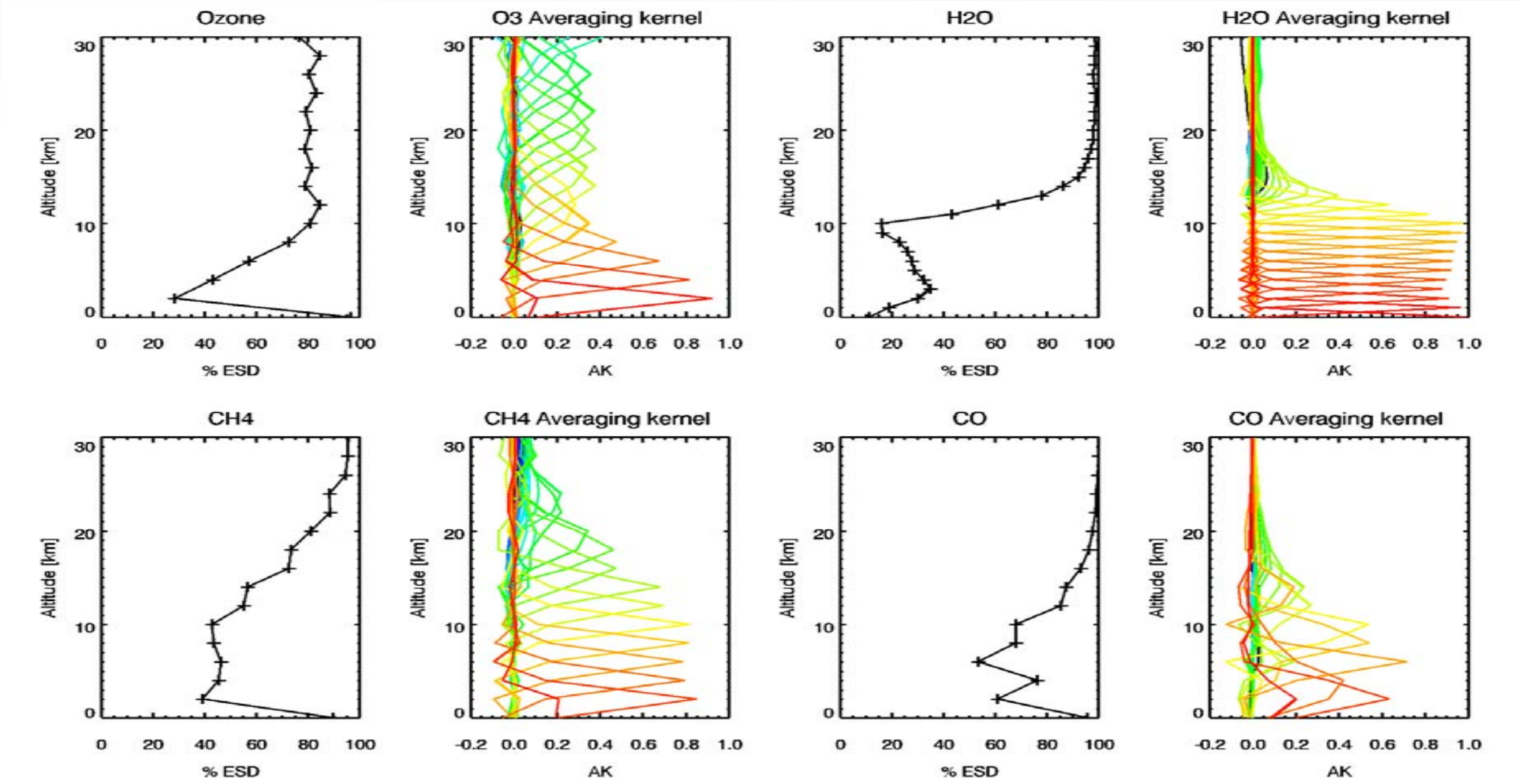
→ *Some height-resolution in mid-troposphere*

Linear diagnostics from Optimal Estimation retrieval simulation

- **x**: H_2O (Δz =1km); O_3, CH_4 & CO (Δz= 2km); surface T
  - Atmospheric T(z) assumed known
- $\mathbf{S_o}$: 100% error; diagonals only
- **y**: Complete IASI spectrum synthesized at nominal $\Delta\nu_{Inst}$
- $\mathbf{S_y}$: IASI NEBT; diagonals only

- $\sqrt{\mathbf{S_x(i,i)}}$: Estimated standard deviation (retrieval precision)
- **Averaging kernels**: a measure of how much observations improve on *prior* knowledge and vertical resolution of retrieval

Estimated Standard Deviations & Averaging Kernels for O_3, H_2O, CH_4 & CO



- ESDs & AKs generally reflect K's (T(z)), Δz & S_o
- For useful precision, Δz > 2km, except H_2O 0 - 10km
- Except for H_2O, sensitivity low in surface layer (where T(z) $\rightarrow$T(o))

Some further radiative transfer issues

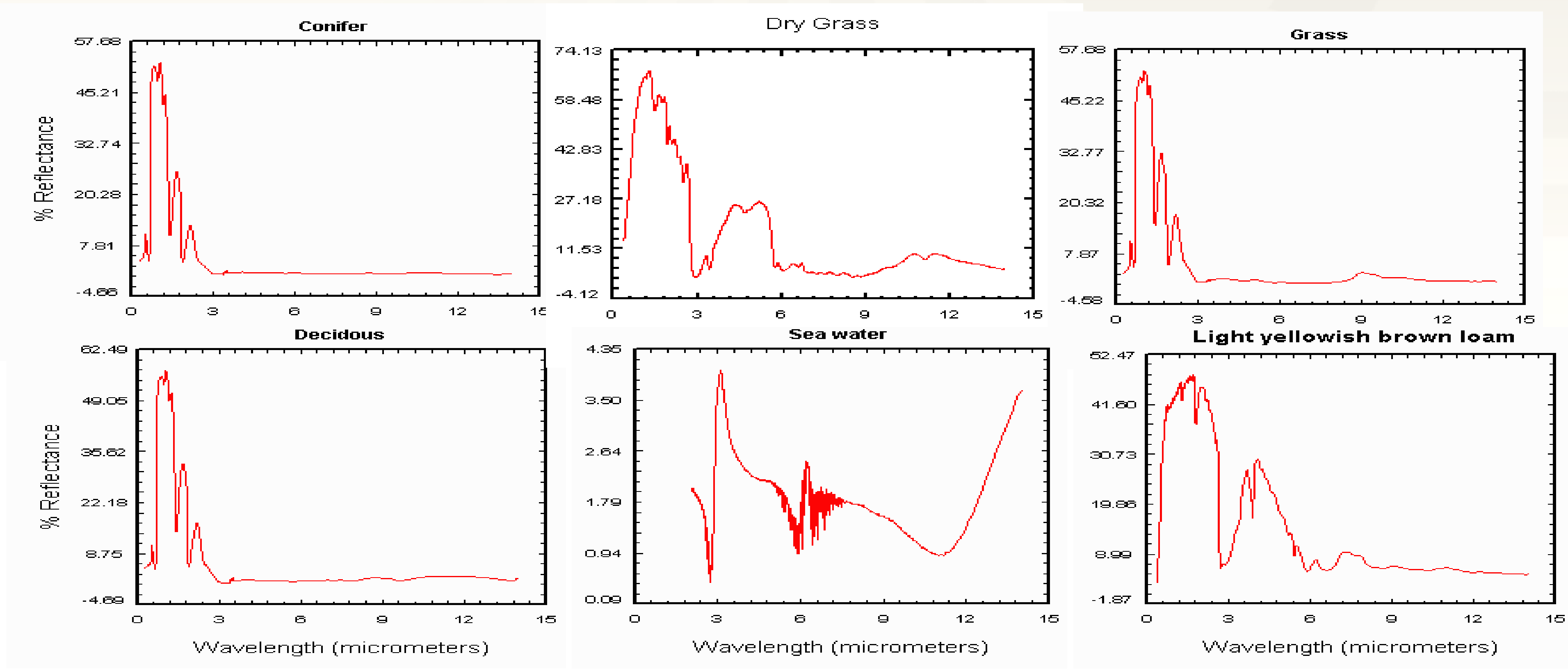
What if:

- $T(z) > T(0) \leftarrow$ *inversion*
- $T_{air}(0) \neq T_{surface}$
- Earth's surface not a perfect black-body
  - Surface emissivity < 1; surface reflectivity > 0
  - Surface emissivity & reflectivity exhibit variations
    - Spatio/temporal
    - Spectral
    - Angular & polarisation (cf shortwave bi-directional reflectance distribution function)

and what about:

- H_2O and other gaseous *continua*
- Aerosol (sea spray, dust/sand, smoke, sulphate, industrial pollution…)
- Fog, sea mist etc
- **Cloud**
- Sunlight
- Non-thermal atmospheric emissions (fluorescence, chemiluminescence)

Surface spectral emissivities



- **ASTER spectral library (http://speclib.jpl.nasa.gov)**

Surface spectral emissivities

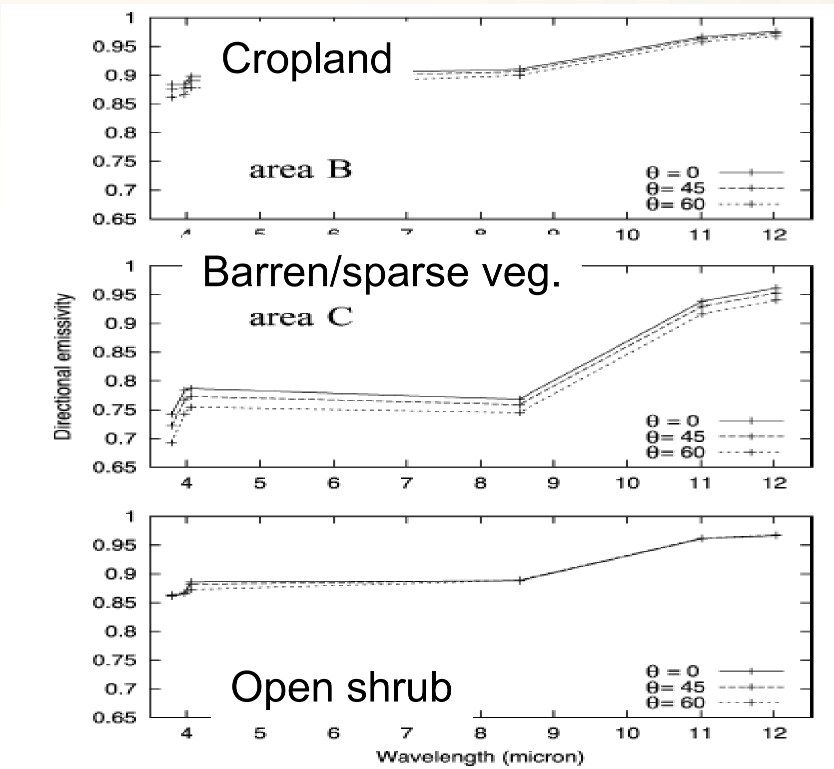


Fig. 13. Infrared spectral signature of the three land test areas defined in Table 5. Directional emissivity $\varepsilon_i(\theta)$ in MODIS bands 20, 22, 23, 29, 31 and 32 is derived for three sensor zenith angles (0°, 45° and 60°).

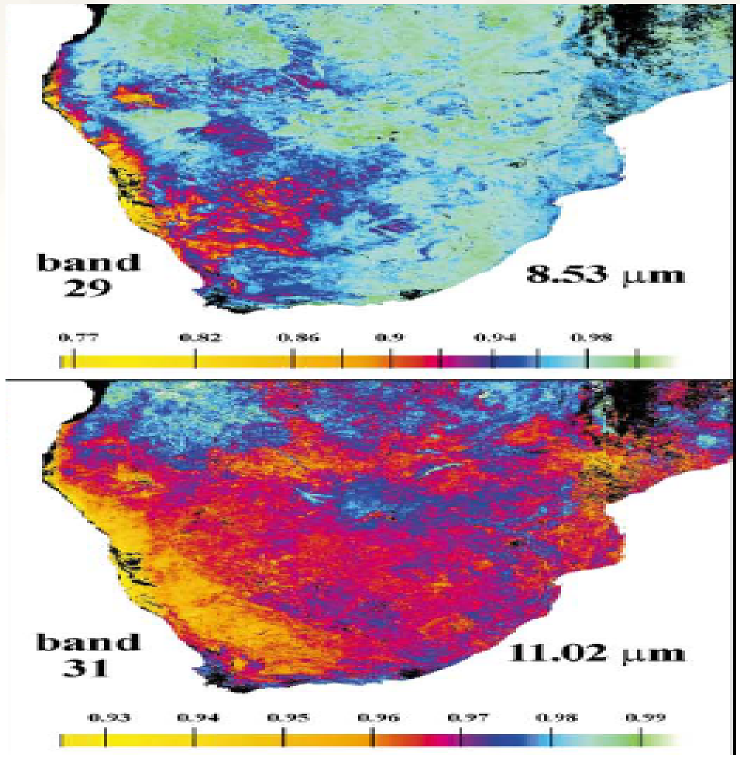
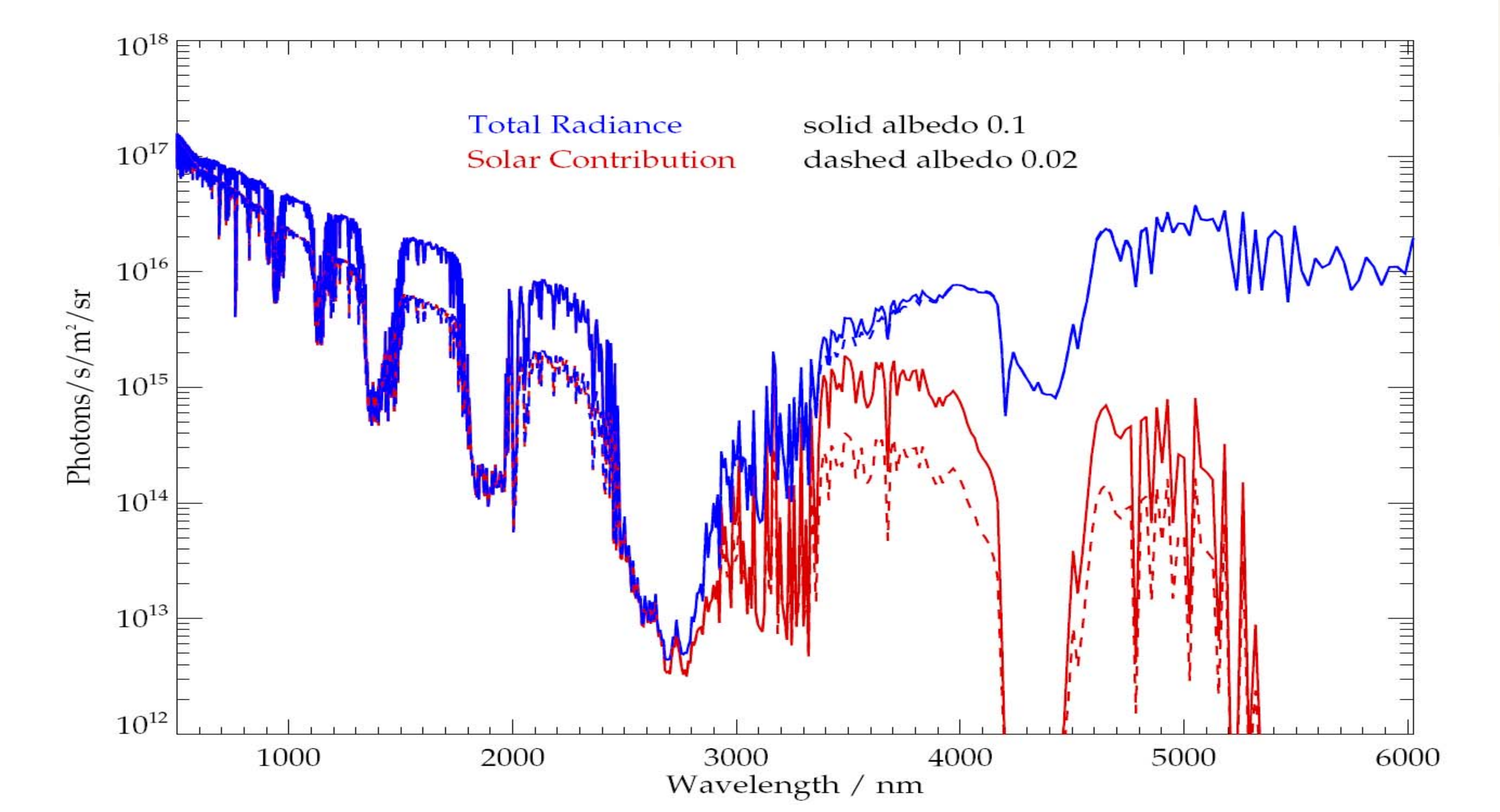


Fig. 14. Map of spectral emissivity at nadir in MODIS bands 20, 22, 23, 29, 31 and 32 over Southern Africa (south of the 10° South parallel) for the 16-day period starting August 20th, 2000.

F. Petitcolin, E. Vermote / Remote Sensing of Environment 83 (2002) 112–134

Contribution from reflected sunlight to nadir-IR radiance spectrum

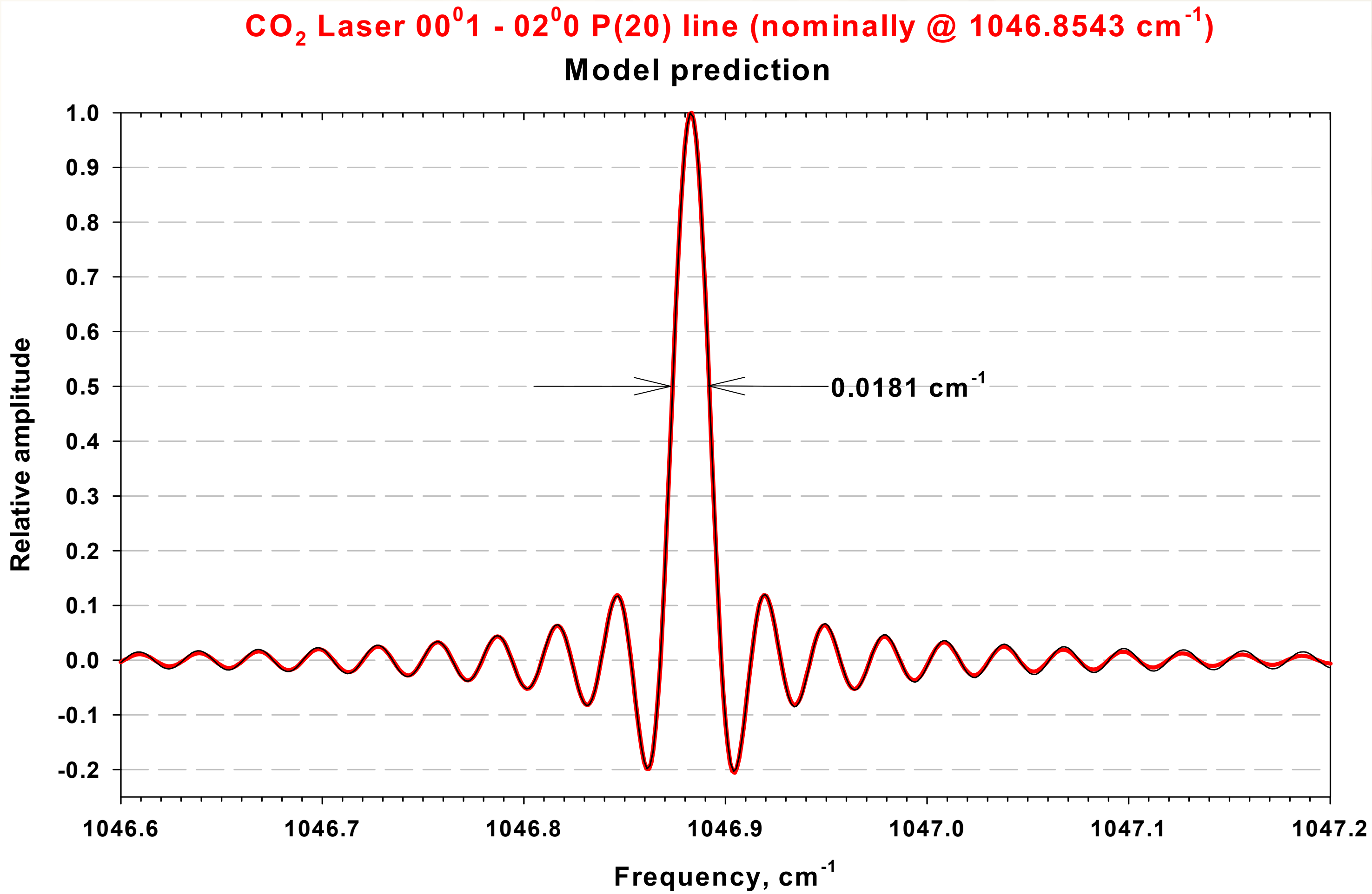


Instrument Attributes

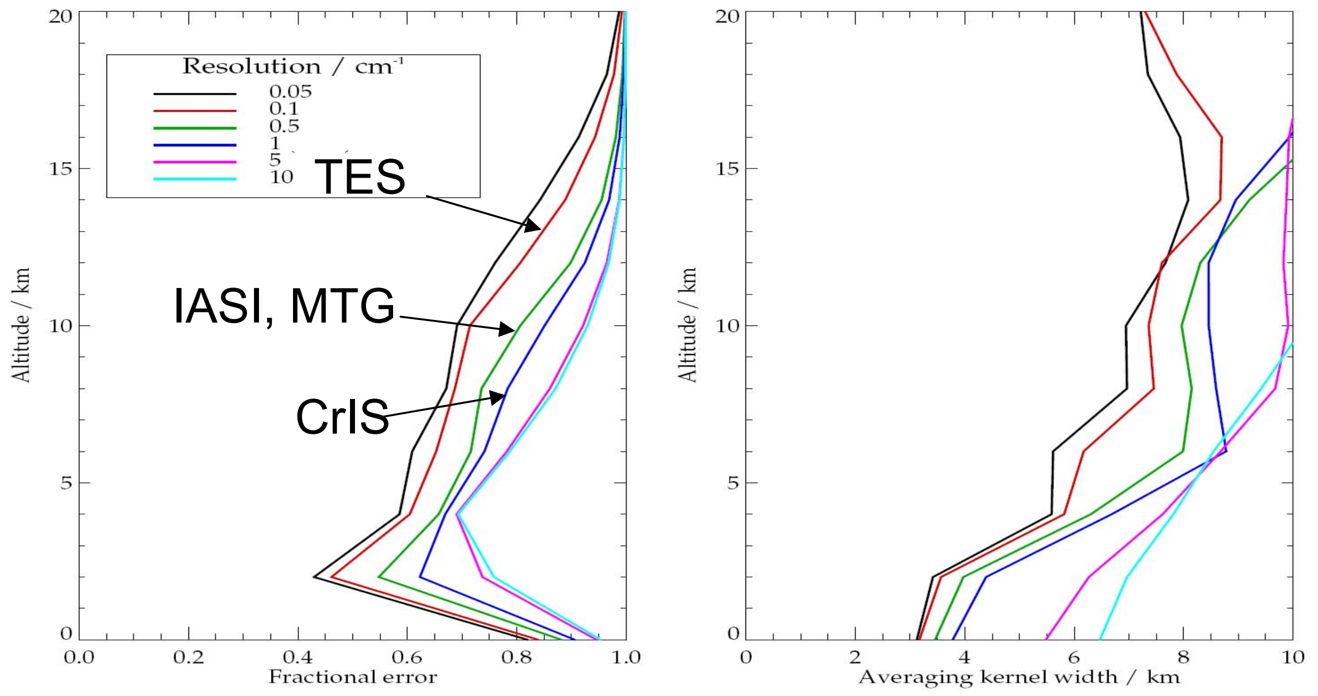
- Fourier Transform Spectrometry:
  1. Mechanical modulation of path-length (Michelson Interferometer)
     - $\Delta\nu_{Inst}$ (cm^{-1}) α 1/ [max optical path difference (cm)]
     - Higher resolving power:
       - improves discrimination between target and interfering gases
       - increases height-resolution
       - *but* requires larger interferometer
  2. NESR/NEBT depends on:
     - Type of (quantum) detector (wavelength region)
     - Optical throughput (AΩ)
       - IFOV → spatial resolution
       - Telescope → instrument size
     - Spectral bandwidth – defined by optical filter
     - Temperature (ie cooling of) detectors, band-pass filters, front-end optics
       → Either *detector-noise* or *photon-noise* limited
     - No. of points in interferogram; acquisition time
       → spatial sampling across- & along-track

→ Trade-off between spectral resolution, spatial resolution & instrument size

TES Instrumental Line Shape (ILS)



Spectral resolution for CO 4.7μm



Spectral resolution critical for CO: lines are few and well-separated

Idealized simulation:

– All instrument parameters held constant except: $\Delta\nu_{Inst}$ and NEBT α $1/\sqrt{\Delta\nu_{Inst}}$

– S_o: 100% errors on 2km grid; diagonal only.

IASI and TES

- Infrared Atmospheric Sounding Interferometer (IASI)
- Tropospheric Emission Spectrometer (TES)

IASI & TES characteristics

– TES launched in 2003 on NASA's Aura → *research satellite*
– IASI launched in 2006 on Eumetsat's EPS-MetOp → *operational satellite*

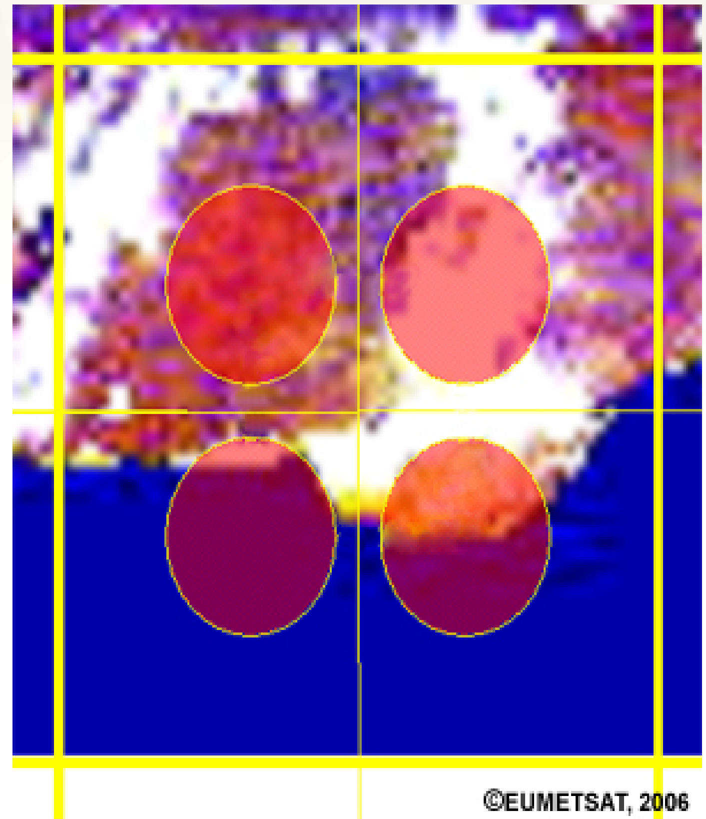
Instrument Parameter	**IASI**	**TES**
Spectral range :	3.62 to 15.5μm 645-2760cm-1	3.2-15.4 μm 650-3050 cm-1
Spectral resolution	0.35 to 0.5 cm-1	0.10cm-1 nadir 0.025cm-1 limb
Spectral sampling	0.25cm-1	0.0592 cm-1 nadir 0.0148 cm-1 limb
Radiometric resolution	0.1 to 0.5 K	
Fields of view at nadir	*4x* 12km diameter in 50km x 50km	(5km x 0.5km) *x16* (linear array)
Spatial coverage	Across-track swath: +/- 47.85^o about nadir	5.3 X 8.5 km nadir; 37 X 23 km limb
Measurement seq.	30 views across-track in 8s	Up to 208s dwell time on scene

IASI spatial sampling

Across track

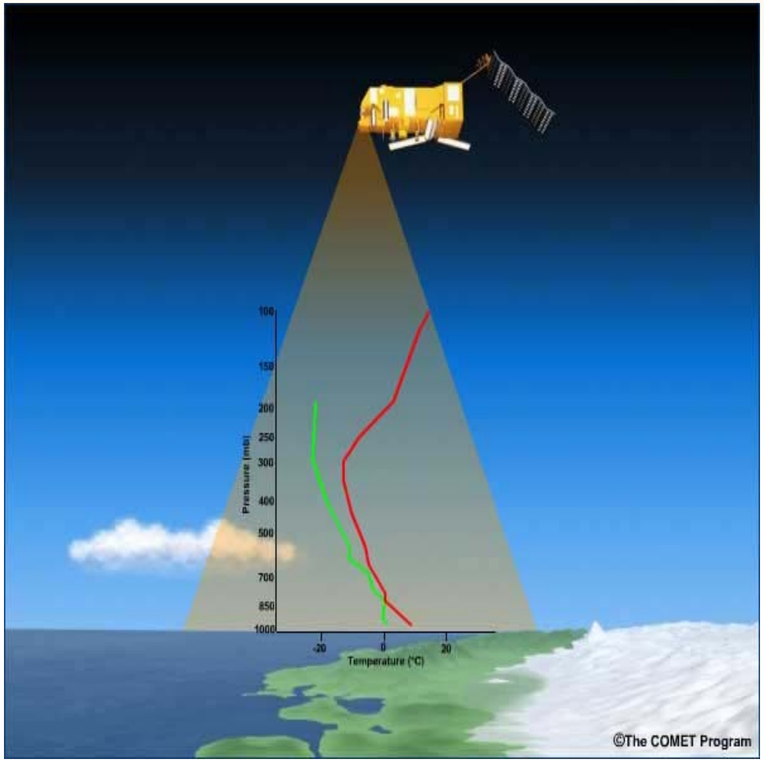
Along track

50km



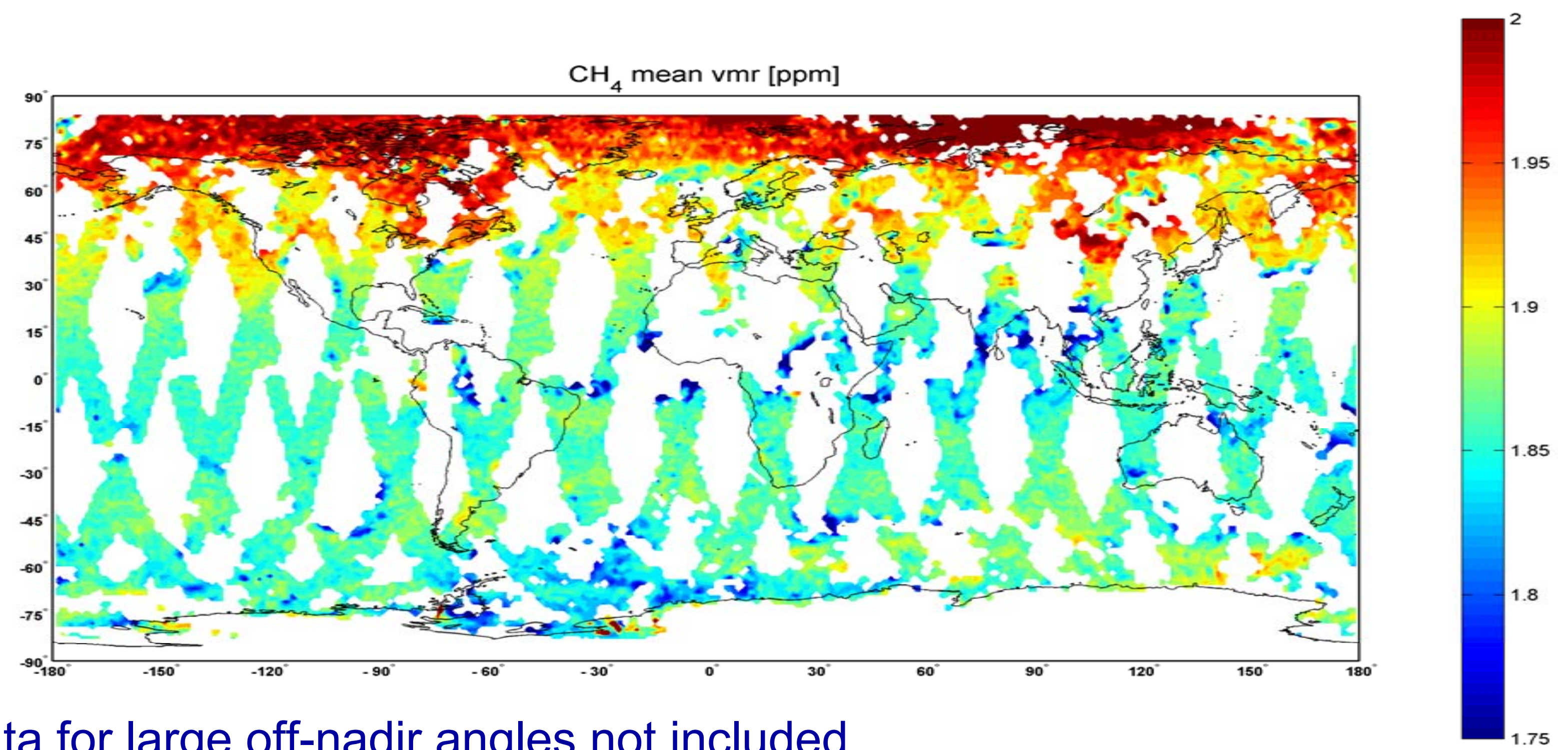
IASI has integrated imager

IASI strategy for cloud



Where should the line be drawn between cloud / no cloud?

CH_4 pressure-weighted mean mixing ratio retrieved from IASI 7.4μm - *1 day*

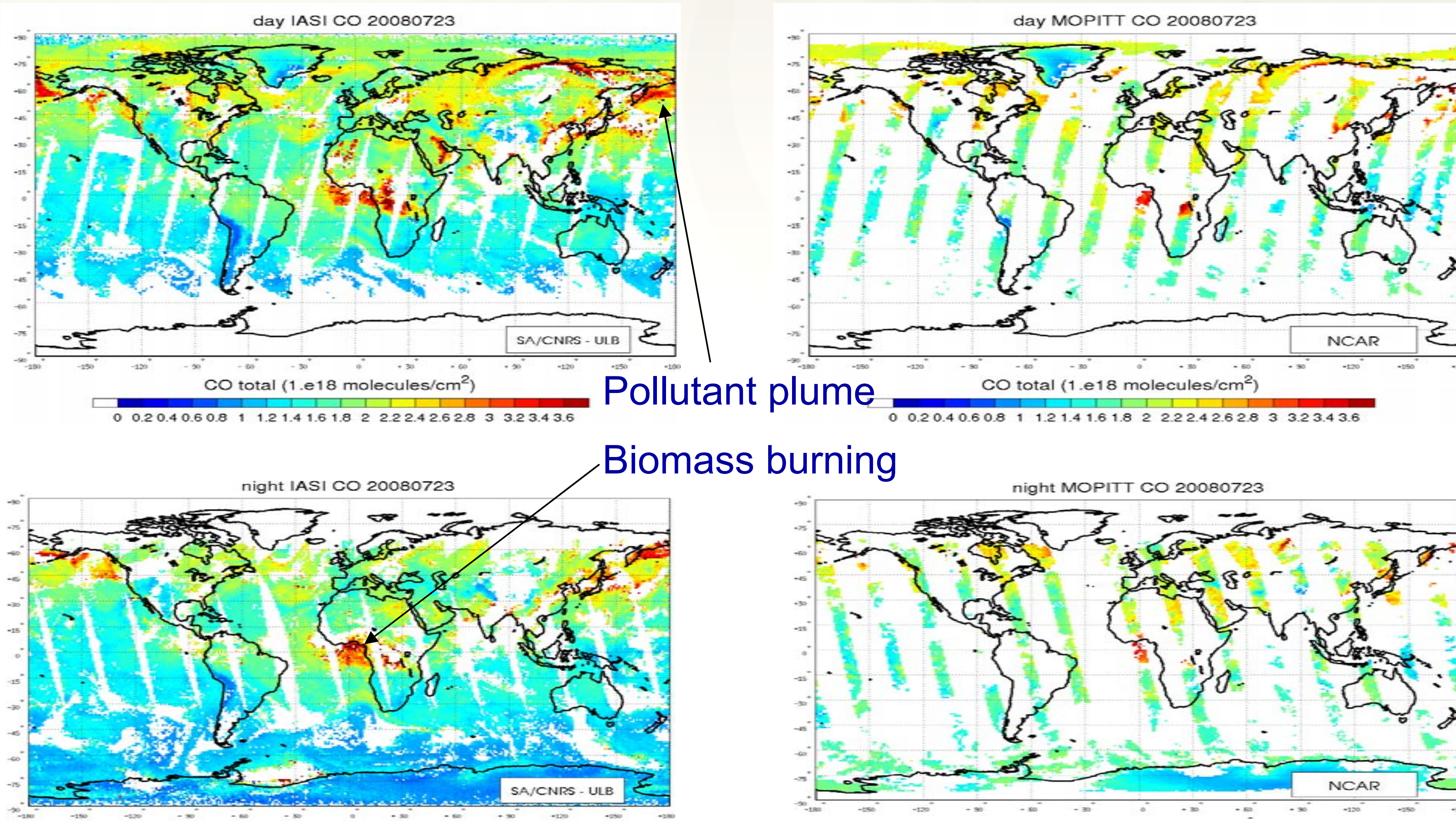


ppmv

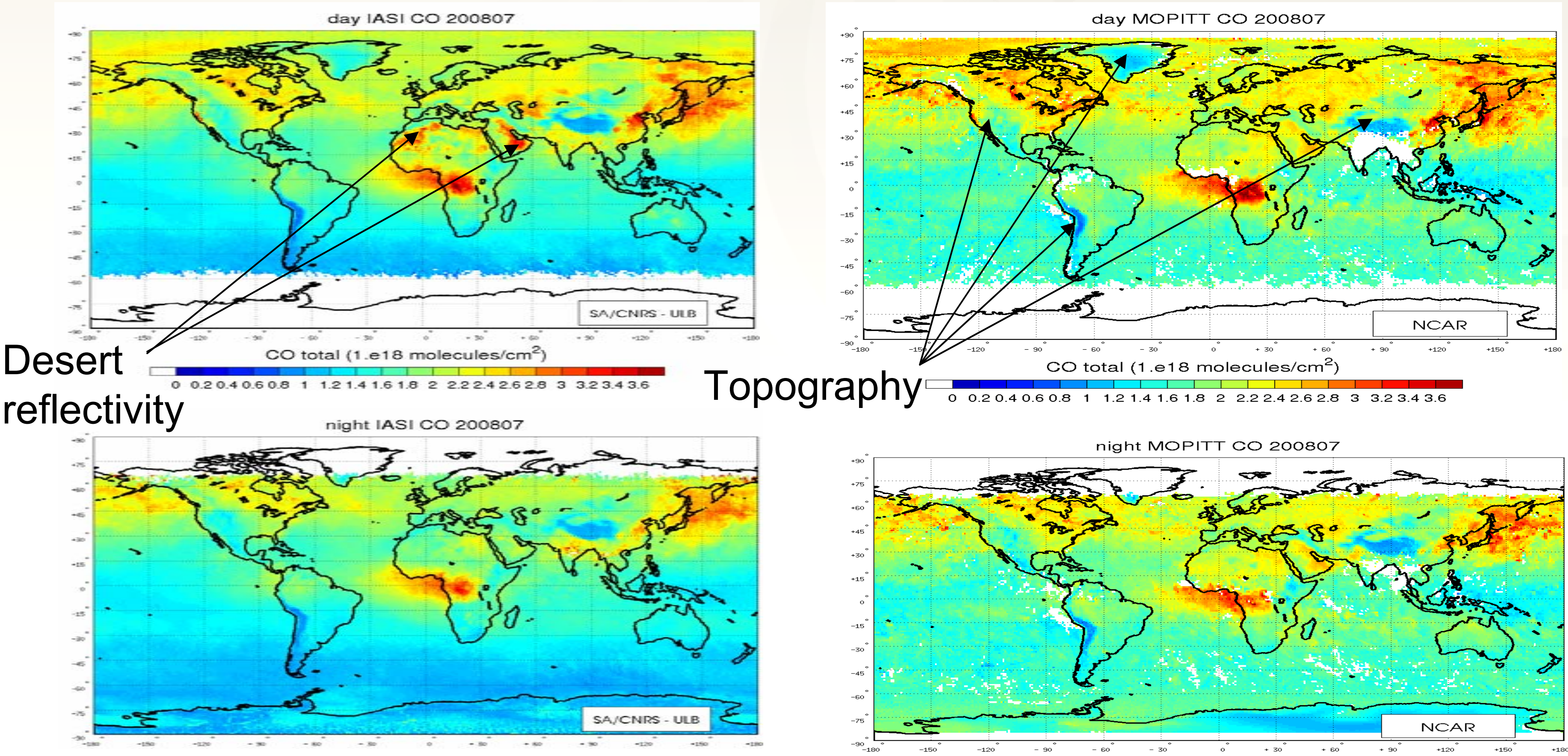
- Data for large off-nadir angles not included
- Improvements to spectral emissivity (eg desert, ice) & cloud ongoing.
- Deviations from uniform mixing of ~few % detected
- Inter-hemispheric asymmetry clear

Credit A. Razavi, ULB

Height-integrated CO retrieved from IASI 4.7μm and MOPITT: 23rd July'08

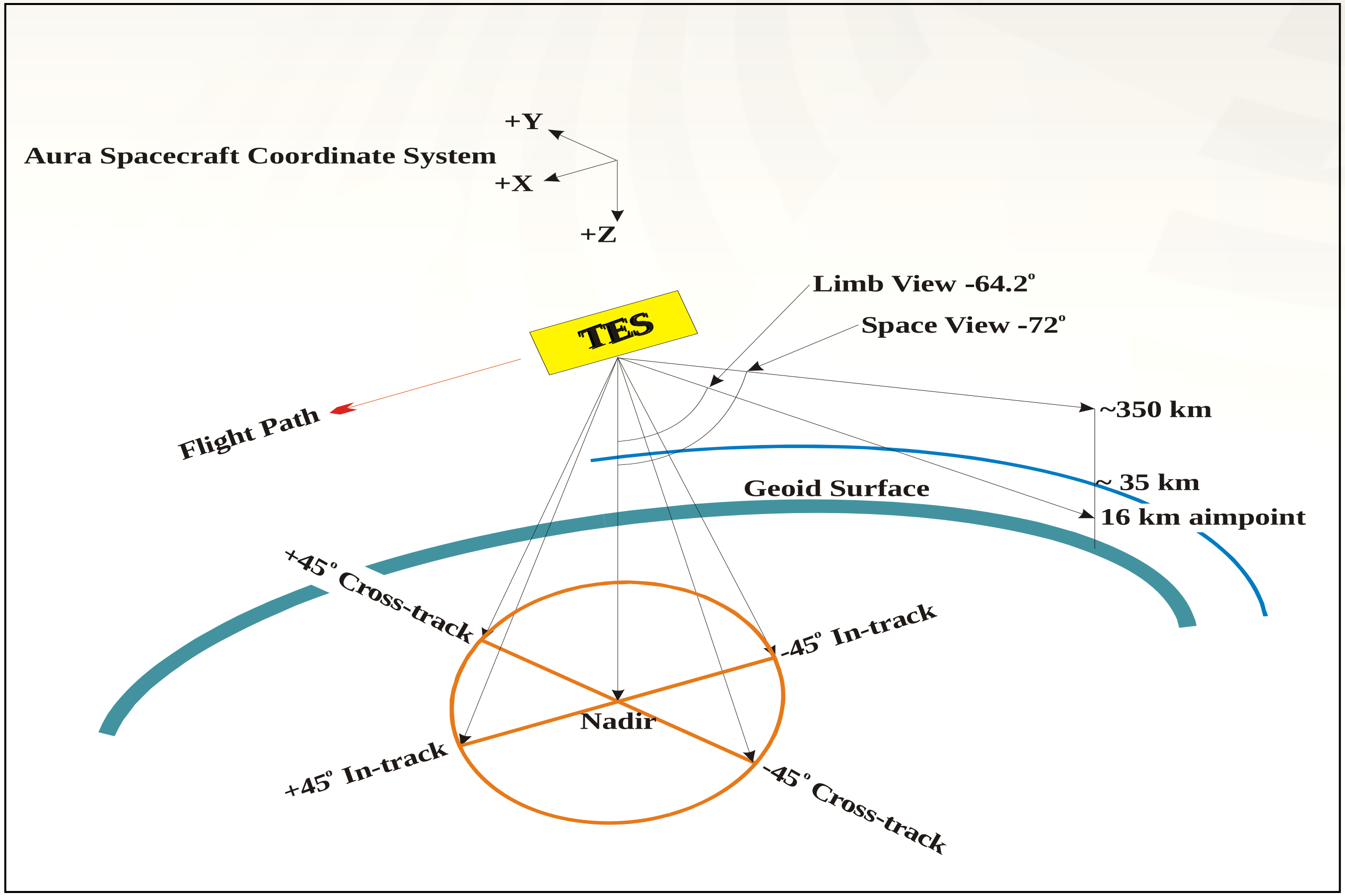


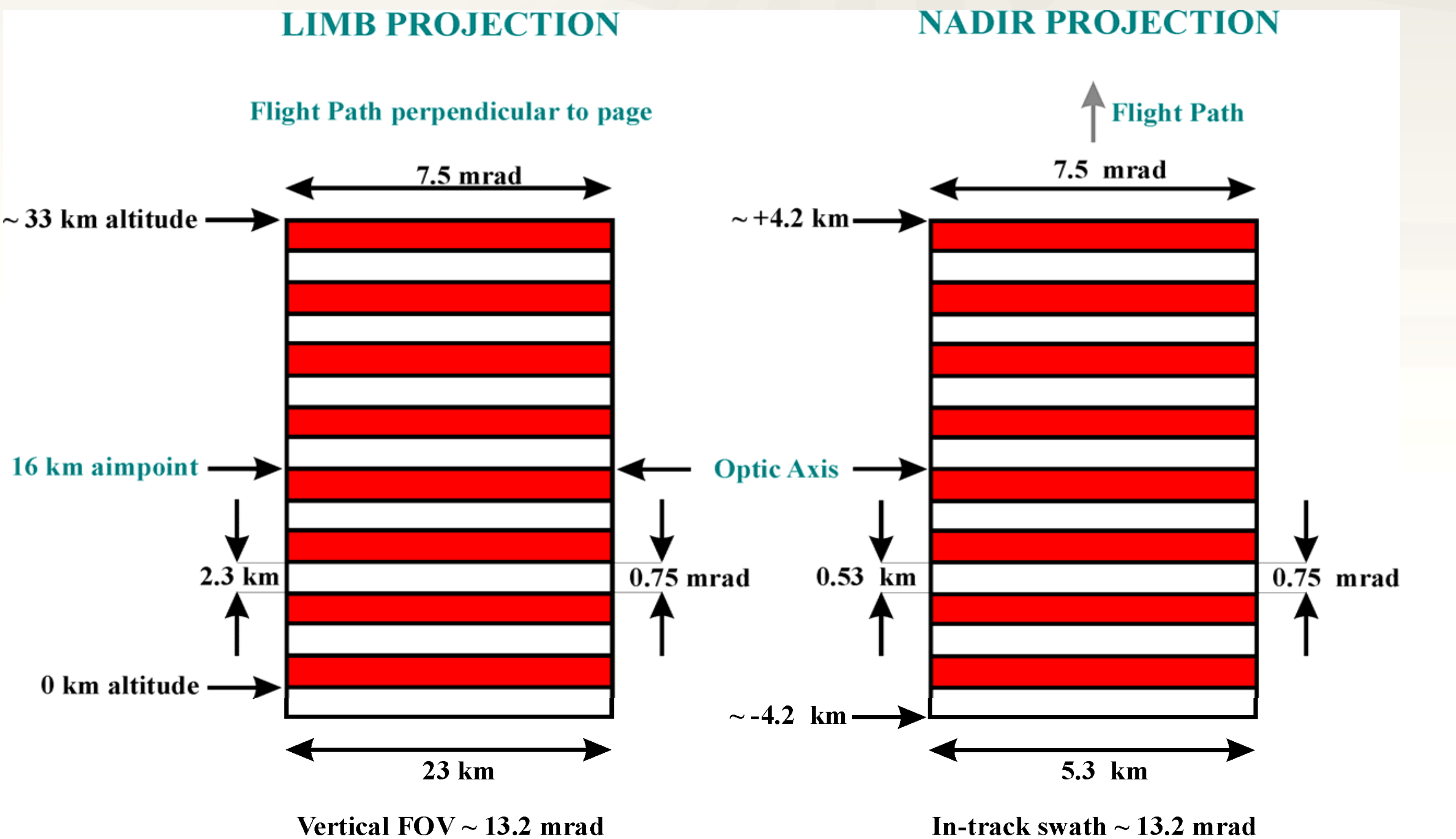
Height-integrated CO retrieved from IASI 4.7μm and MOPITT: July'08 mean



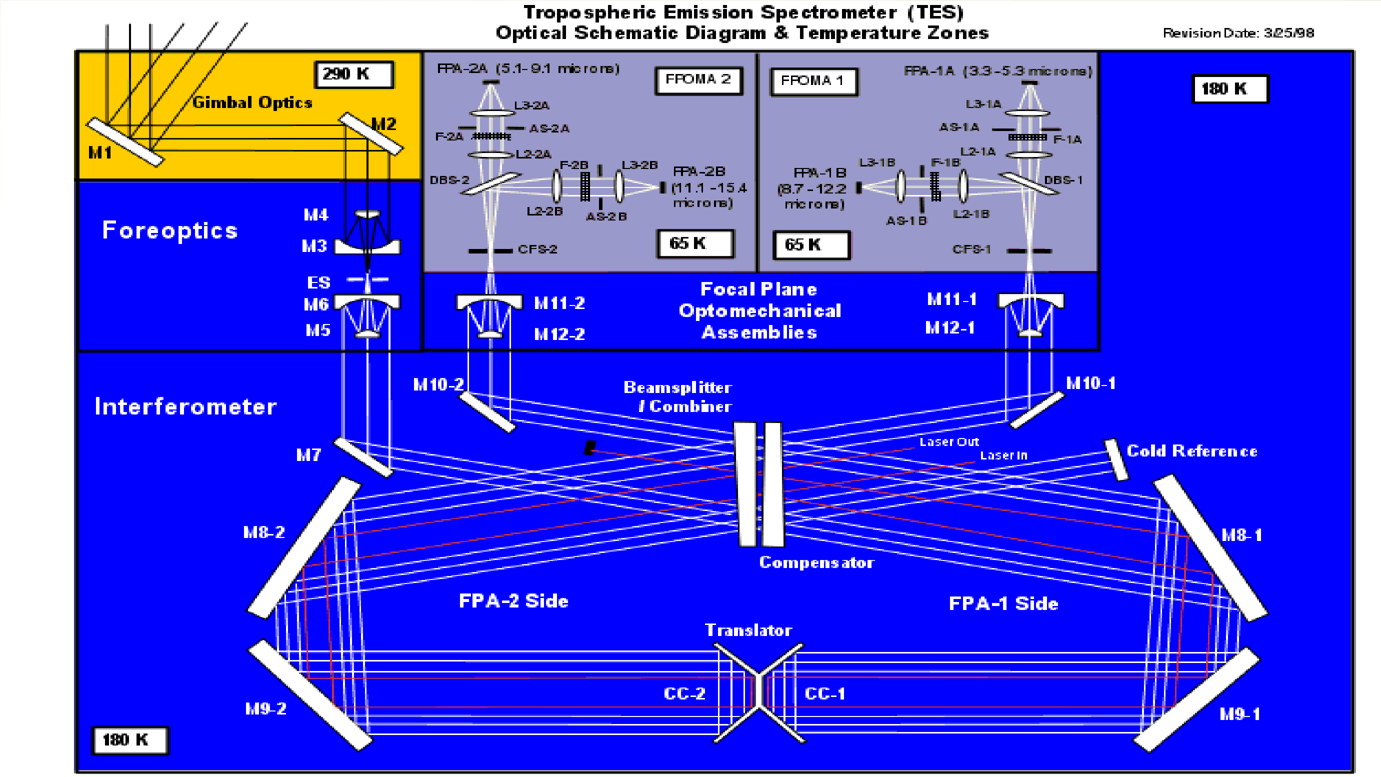
– Generally good agreement in CO morphologies: day/night & IASI/MOPITT
– IASI CO lower over southern ocean

TES Observing Geometry



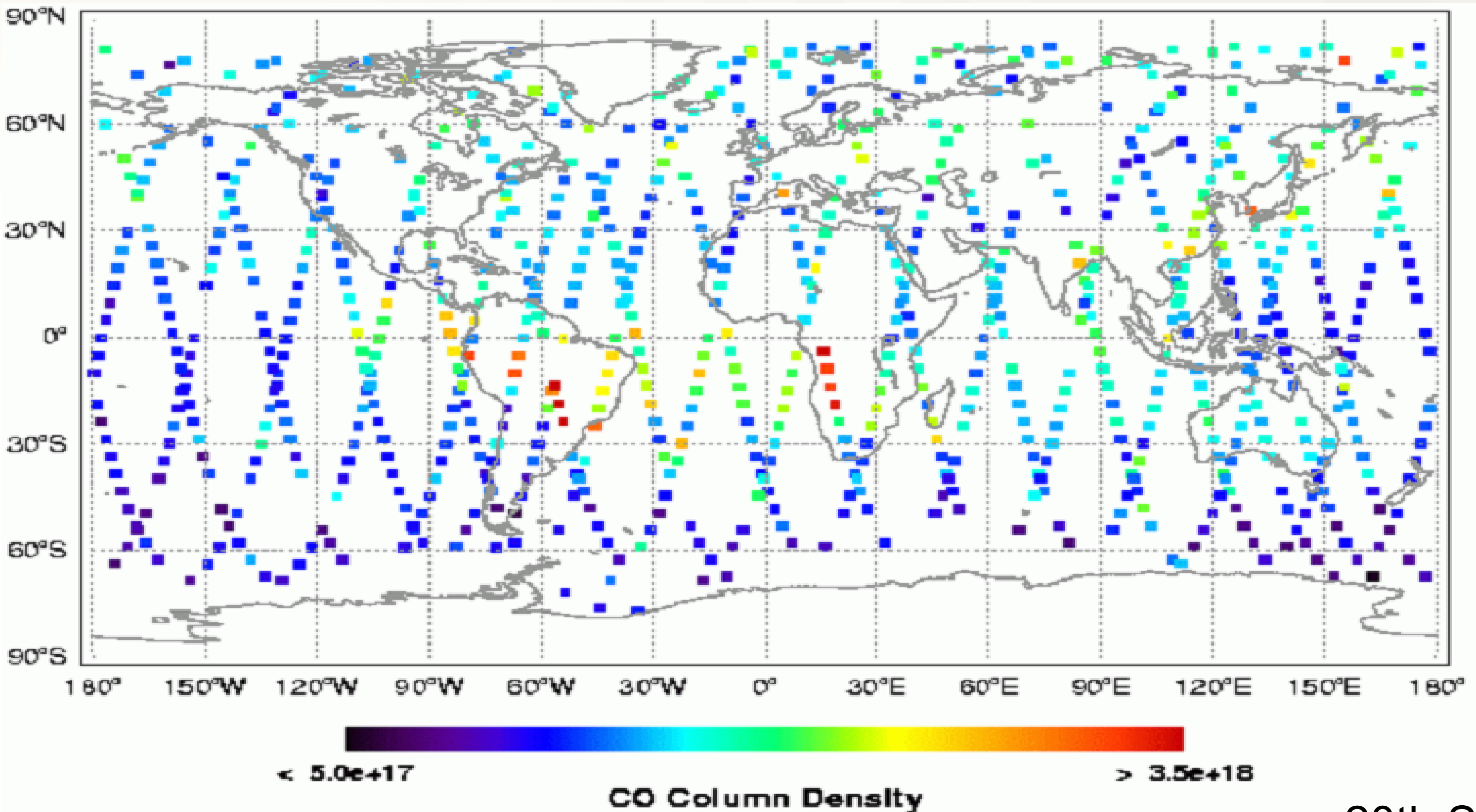

LIMB PROJECTION
NADIR PROJECTION
Flight Path perpendicular to page
Flight Path
7.5 mrad
7.5 mrad
~ 33 km altitude
~ +4.2 km
16 km aimpoint
Optic Axis
2.3 km
0.75 mrad
0.53 km
0.75 mrad
0 km altitude
~ -4.2 km
23 km
5.3 km
Vertical FOV ~ 13.2 mrad
In-track swath ~ 13.2 mrad

TES Optical Schematic



– Fore-optics & interferometer cooled to 180K
– 4 FPAs cooled to 65K

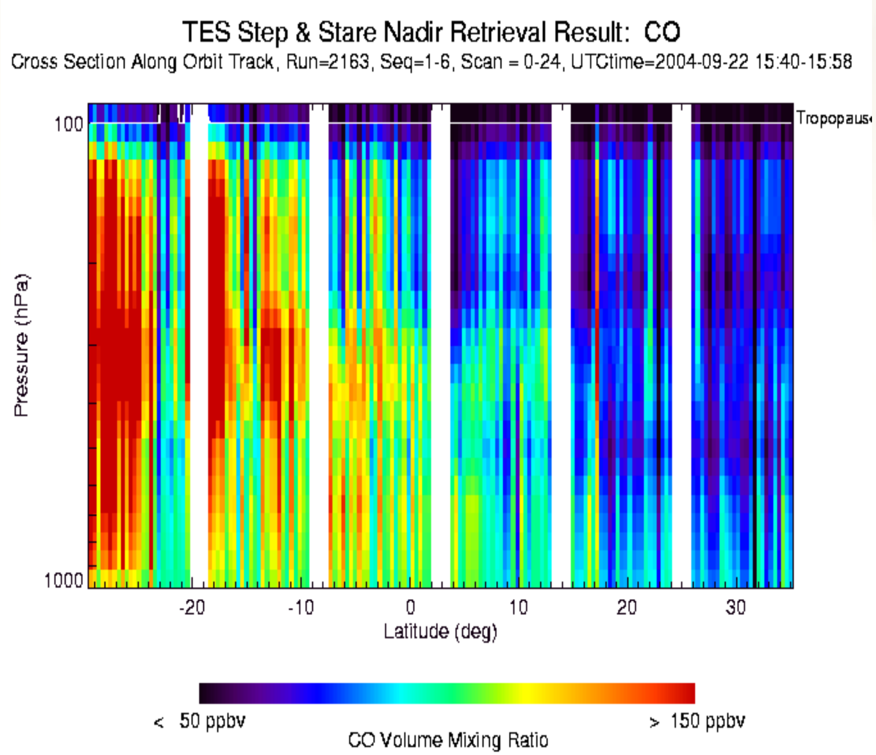
Height-integrated CO retrieved from TES 4.7μm

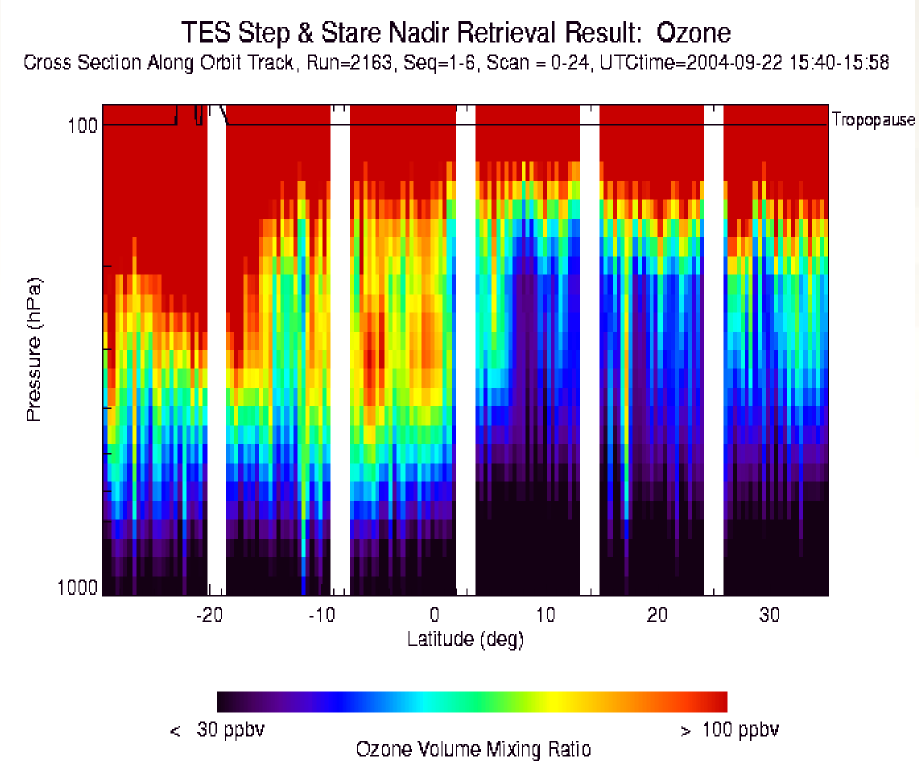


20th Sept.'04

TES does not scan across-track, so daily coverage sparser than IASI

CO & O_3 cross-sections along-track retrieved from TES



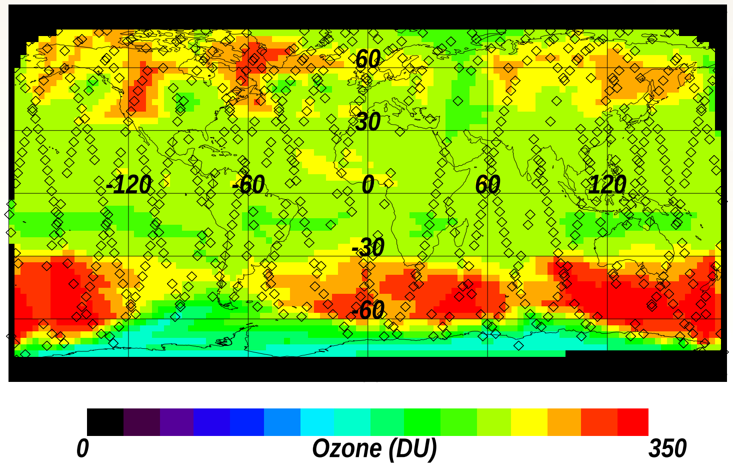


22nd Sept.'04

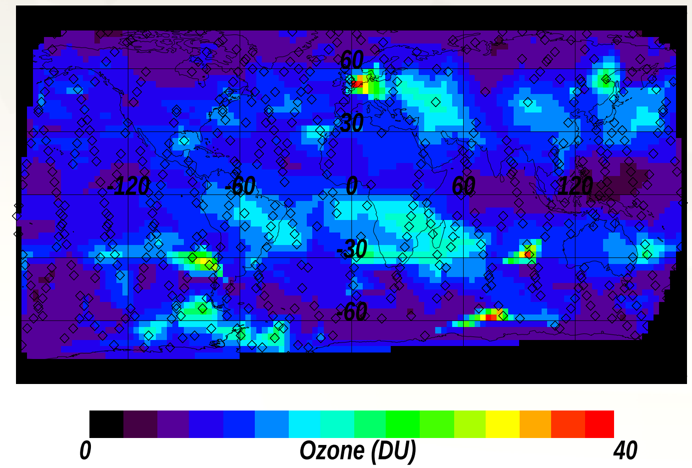
- *Height-resolved* distributions of CO and O_3 retrieved in the troposphere
- Plumes centred ~300hPa (ie mid-troposphere) from tropical biomass burning
- O_3 a secondary product of burning; not emitted directly
- O_3 structure retrieved below sharp gradient in upper troposphere

O_3 height-integrated layer distributions retrieved from TES

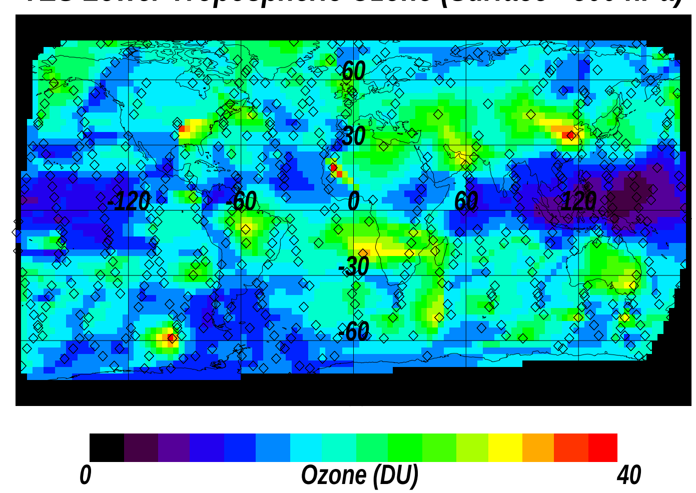
TES Stratospheric Ozone (Tropopause - TOA)



TES Upper Tropospheric Ozone (500 hPa - Tropopause)



TES Lower Tropospheric Ozone (Surface - 500 hPa)



Typically ~90% of O_3 column in stratosphere
→ accurate stratospheric retrieval a pre-requisite for tropospheric retrieval

– Height integration sensitive to tropopause pressure

– Some realistic features seen in trop. O_3 maps

Additional Trace Gases Potentially Detectable by TES

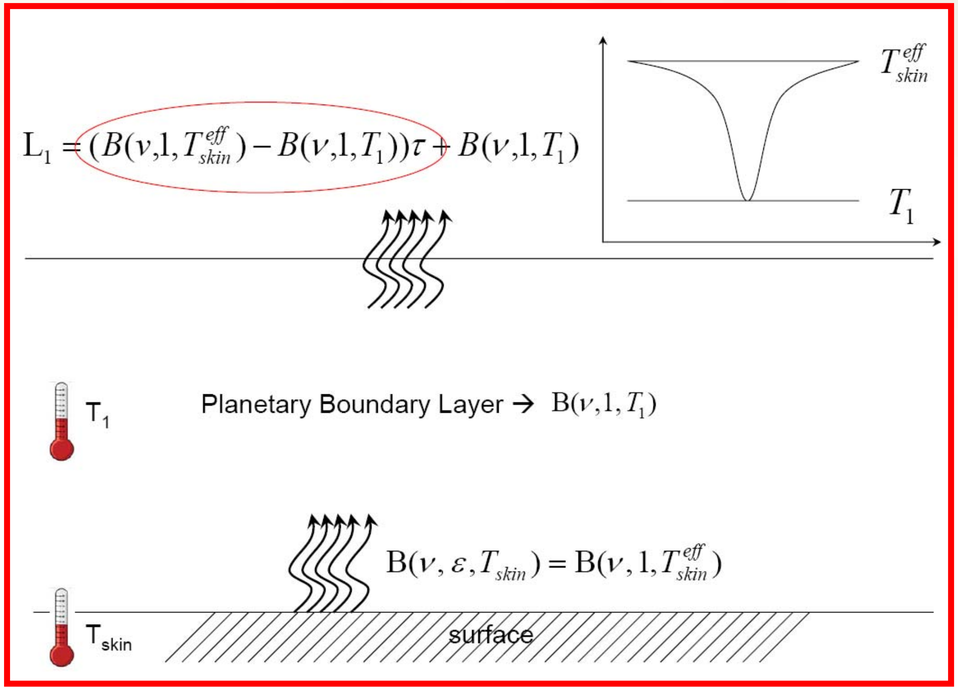
Chemical Group	Common Name	Formula	Product Source	
H_xO_y	Hydrogen Peroxide	H_2O_2		L
	Mondeuterated Water Vapor	HDO	N	L
Carbon Compounds	Ethane	C_2H_6		L
	Acetylene	C_2H_2		L
	Formic Acid	HCOOH	N	L
	Methyl Alchohol	CH_3OH	N	L
	Peroxyacetyl Nitrate	$CH_3C(O)OONO_2$		L
	Acetone	$CH_3C(O)CH_3$		L
	Ethylene	C_2H_4		L
Nitrogen Compounds	Peroxynitric Acid	HO_2NO_2		L
	Ammonia	NH_3	N*	L
	Hydrogen Cyanide	HCN		L
	Dinitrogen Pentoxide	N_2O_5		L
Halogen Compounds	Hydrogen Chloride	HCl	N*	
	Chlorine Nitrate	$ClONO_2$		L
	Carbon Tetrachloride	CCl_4		L
	CFC-11	CCl_3F		L
	CFC-12	CCl_2F_2		L
	HCFC-21	$CHCl_2F$		L
	HCFC-22	$CHClF_2$		L
Sulphur Compounds	Sulphur Dioxide	SO_2	N	L
	Carbonyl Sulphide	OCS	N	L
	Hydrogen Sulphide	H_2S	N*	L
	Sulphur Hexafluoride	SF_6		L

* Volcanic/Industrial/Biomass Burning plume column densities only

TES can detect additional, tenuous trace gases more easily than IASI due to ~5x higher spectral resolution

Surface – air temperature contrast

$$\Delta T = T_{skin}^{effective} - T_1$$



$T_1 = T_{skin}^{effective}$ → no spectral information from the first layer

$T_1 < T_{skin}^{effective}$ → Absorption from the first layer (usual case during daytime)

$T_1 > T_{skin}^{effective}$ → Emission from the first layer (temperature inversion; night-time mainly)

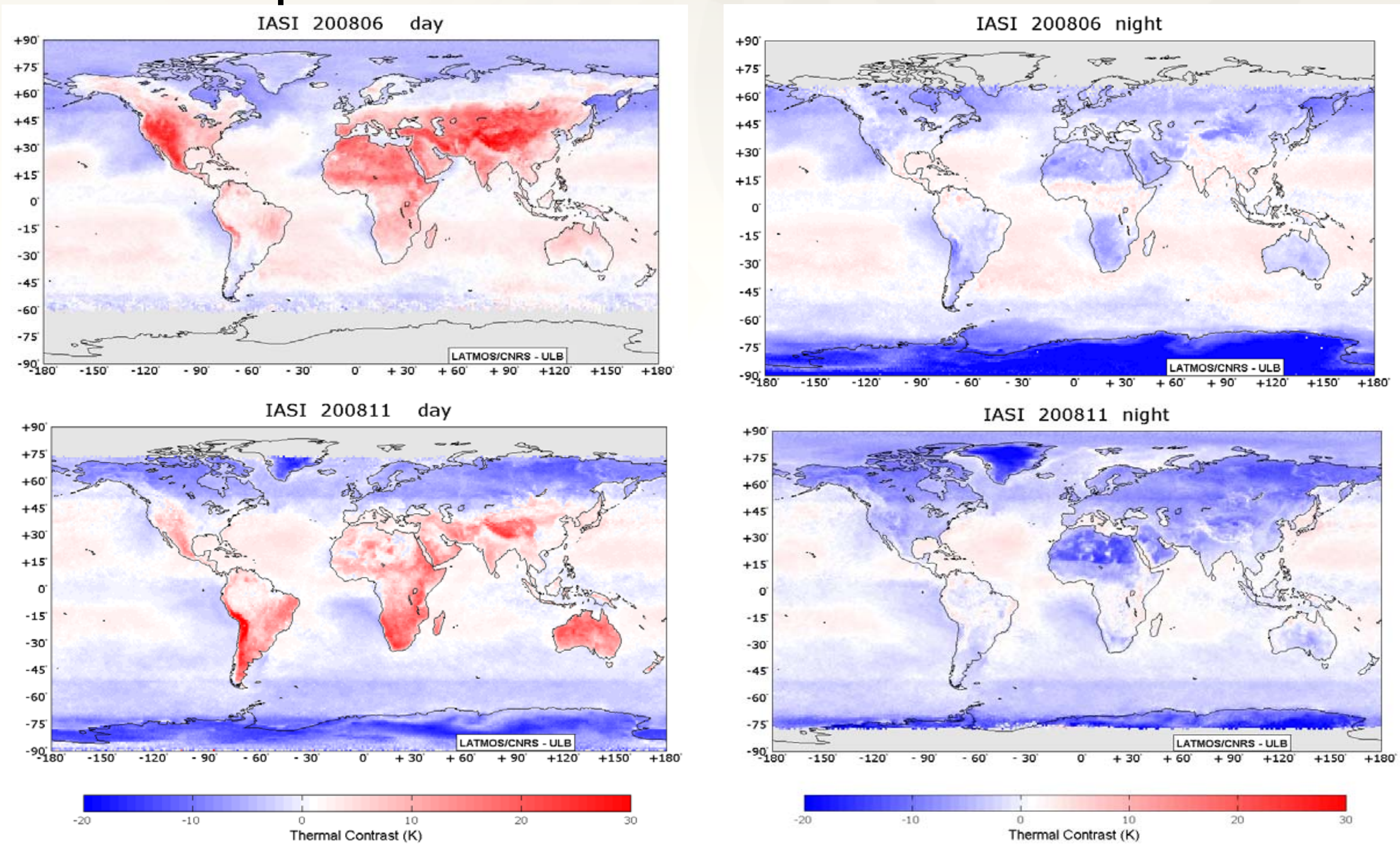
Courtesy P-F Coheur, ULB

Surface – air temperature contrast (contd.)

9:30 AM - Eq | **9:30 PM - Eq**

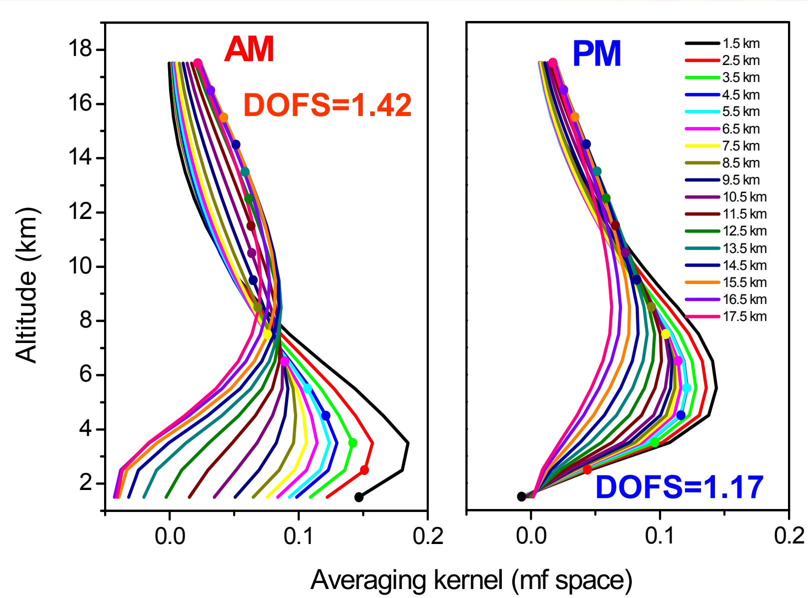
June

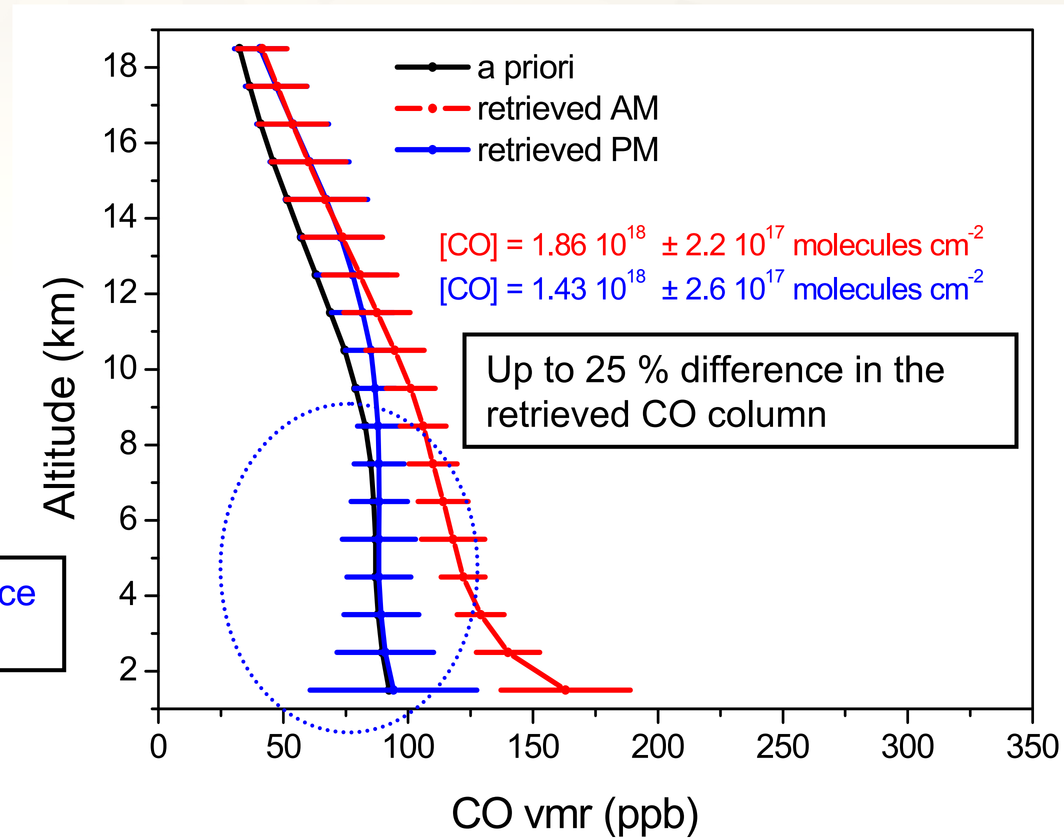
Nov.



Courtesy P-F Coheur, ULB

Example: IASI CO retrievals over Teheran on clear day



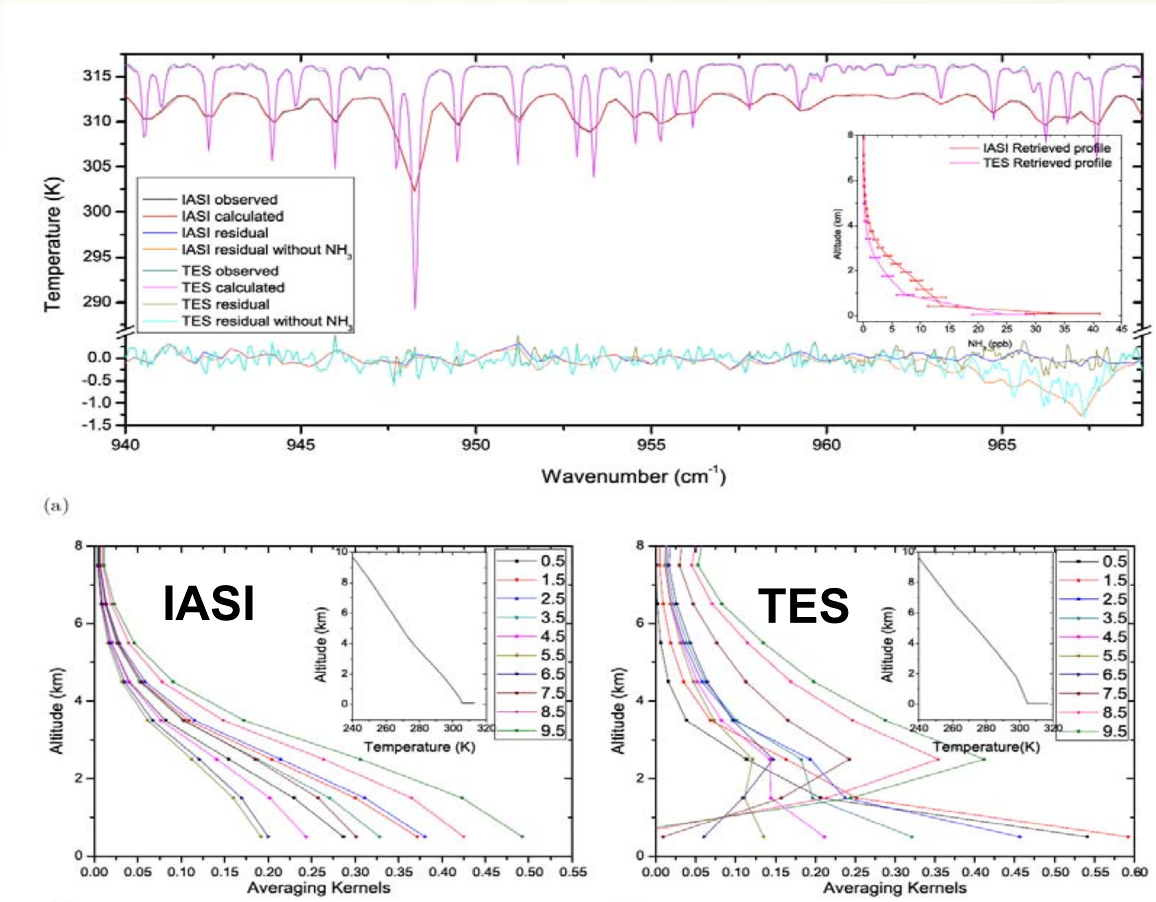


Vanishing sensitivity at the surface due to low thermal contrast

Courtesy P-F Coheur, ULB

NH_3 retrievals above the San Joaquin Valley (IASI and TES)

Case 1: POSITIVE thermal contrast (day)



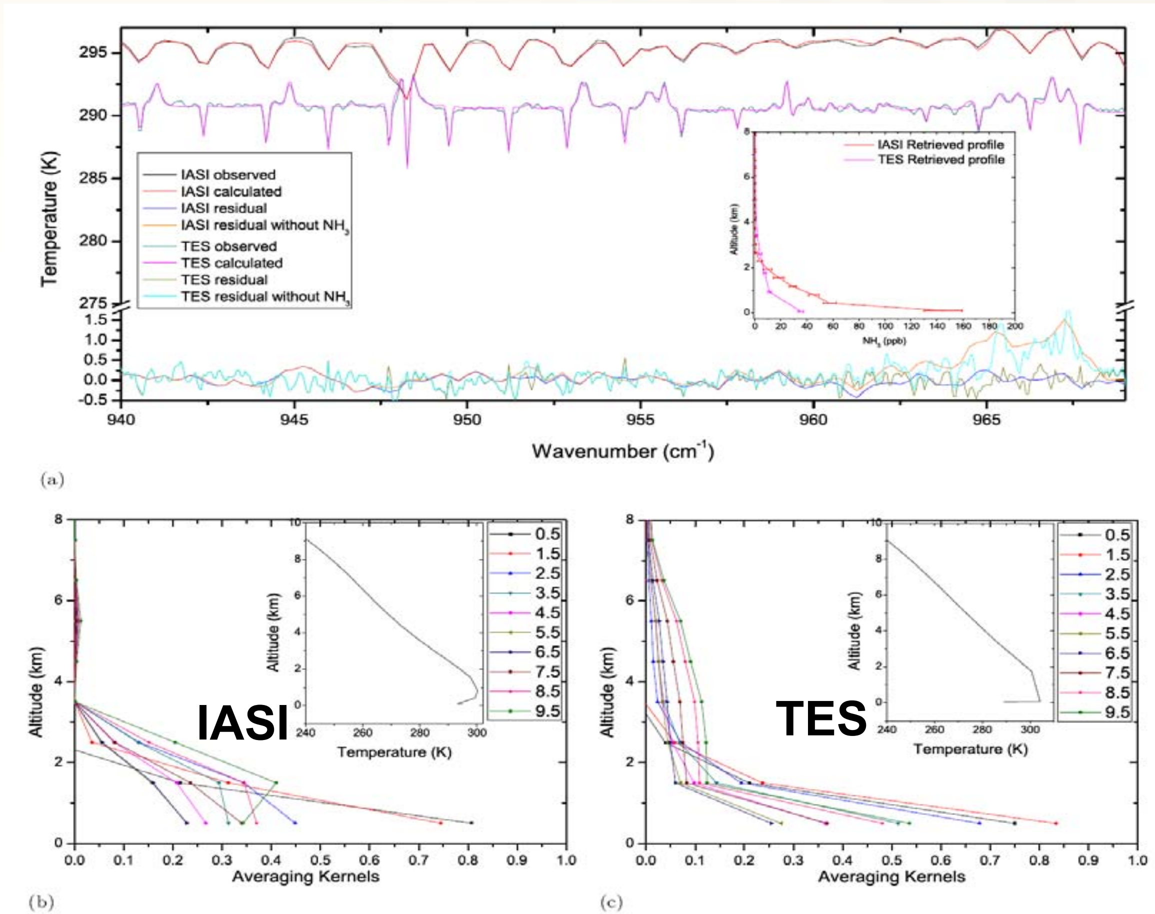
NH_3 *absorption* in TOA radiance spectrum

Sensitivity to near-surface layer

Clarisse et al., submitted to JGR 2009

NH_3 retrievals above the San Joaquin Valley (IASI and TES)

Case 2: Temperature inversion (night)



NH_3 *emission* in TOA radiance spectrum

Sensitivity to near surface layer

Clarisse et al., submitted to JGR 2009

Summary & Future Advances

1. Nadir IR spectrometry demonstrated to be a powerful tool for sounding the troposphere from space:
   a) Temperature and humidity profiling for NWP
   b) Global observations of mid-tropospheric distributions of methane, carbon monoxide and ozone

2. Potential for CH_4 emissions and air quality (CO & O_3) applications will depend on attainable accuracy and height-resolution
   – eg accounting for cloud, surface reflectivity/heterogeneity & *continua*

3. Research ongoing with IASI & TES data to:
   a) Determine sensitivity to boundary layer
   b) Detect additional trace gases

4. Advances foreseen for possible future missions:
   a) Increase spectral resolution
      → Improve *accuracy* and *vertical resolution* (NB CO)
      → Additional trace gases (eg organic compounds)
   b) Increase spatio-temporal sampling
      → More observations per day between clouds
      → Identify and quantify emission sources & plumes more precisely.