# Atmospheric Composition Sounding

ESA Summer School
ESRIN
13th August 2010

Lecture 3 by B.Kerridge

Part 1: Solar Shortwave Nadir Spectrometry

Part 2: Integrated Approach to Composition Sounding

#### **Outline**

#### Lecture 3

#### Part 1 - Solar shortwave nadir spectrometry

- 1. Principles
- 2. Applications
  - a) uv ozone profiling
  - b) vis tropospheric NO<sub>2</sub> mapping
  - c) nir aerosol profiling
  - d) swir methane & CO
- 3. Summary and future advances

#### Part 2 - Integrated Approach to Composition Sounding

- mm-wave + ir limb emission
- limb + nadir
- ir + shortwave nadir
- 4. spectrometer + imager

#### **Conclusions**

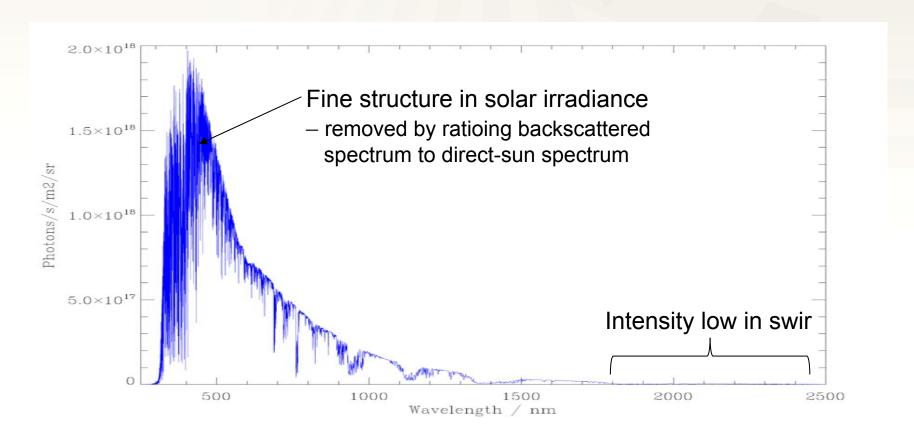
# Part 1 - Nadir Shortwave Spectrometry

- Sensitivity to near-surface layer
  - where primary emissions occur

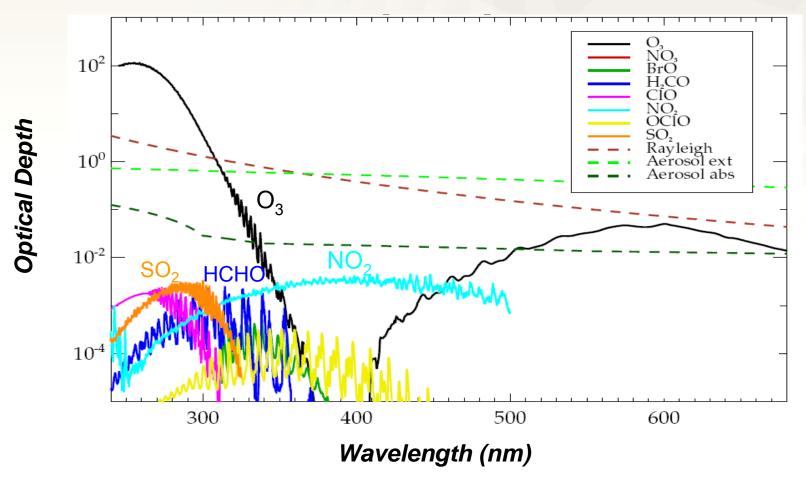
#### **Principles of Nadir Shortwave Spectrometry**

- Trace gas absorption signatures in spectra of backscattered sunlight
- Ozone absorption in Hartley band is strong and varies with wavelength
  - → Spectral intensity of backscattered uv radiation yields stratospheric profile information
- Ozone absorption signature in Huggins bands is less strong
  - → Temperature dependence adds ozone profile information in troposphere
- In near-uv/vis/near-ir, solar radiation can penetrate to surface
- For weak absorbers (eg NO<sub>2</sub>, SO<sub>2</sub>, HCHO), line-of-sight column proportional to depth of absorption features in reflectance spectrum.
- Conversion to vertical column requires knowledge of surface reflectance, scattering profile and other *prior* assumptions

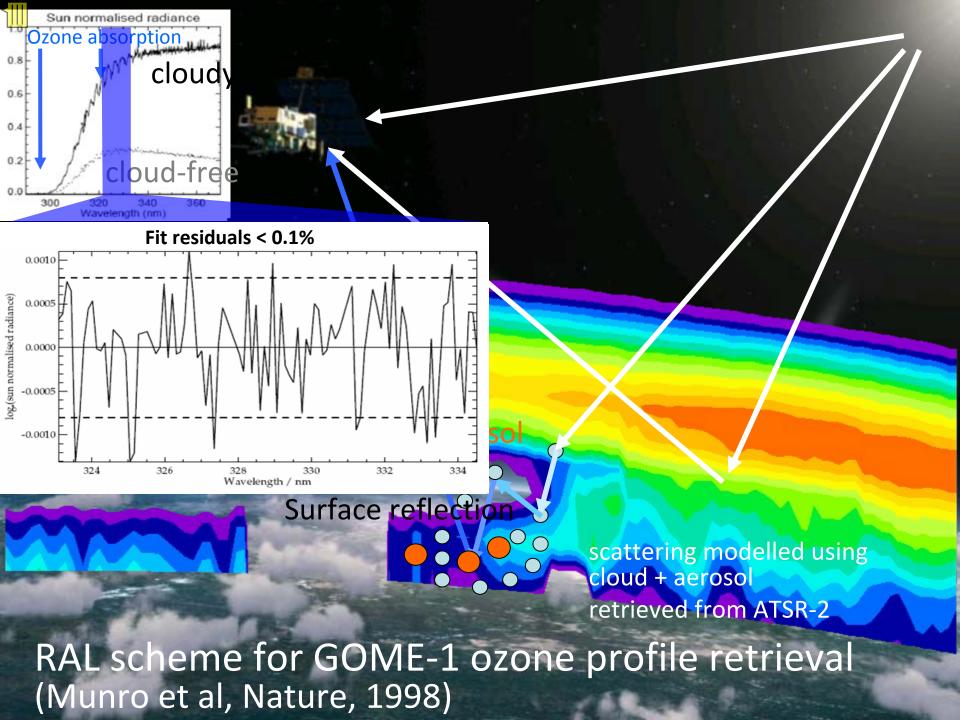
# **Spectral Intensity of Backscattered Solar Shortwave Radiation**



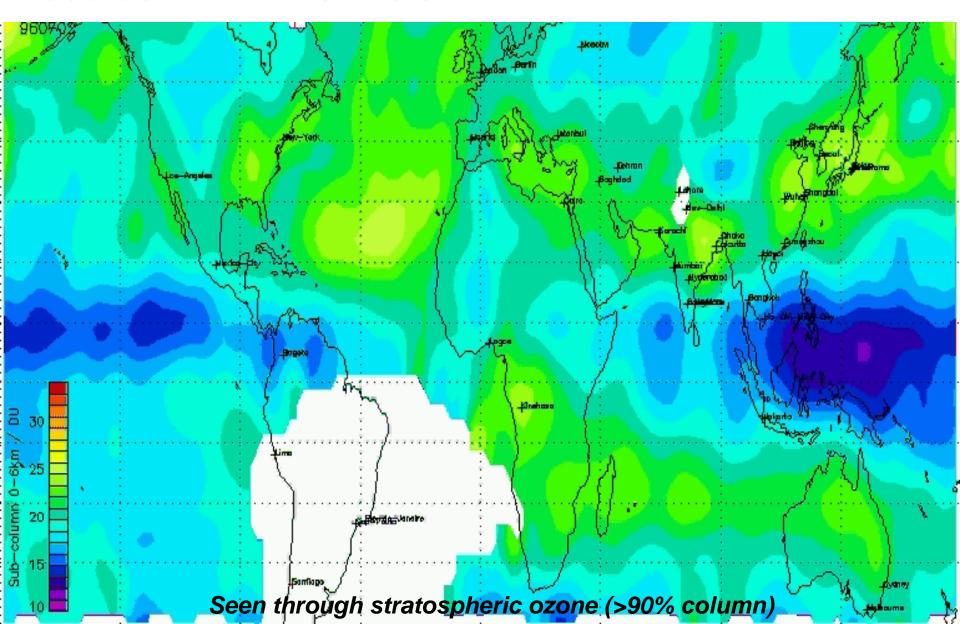
### Trace gas signatures in uv/vis region



→ RMS fitting precision of <0.1% necessary for tropospheric ozone & other gases

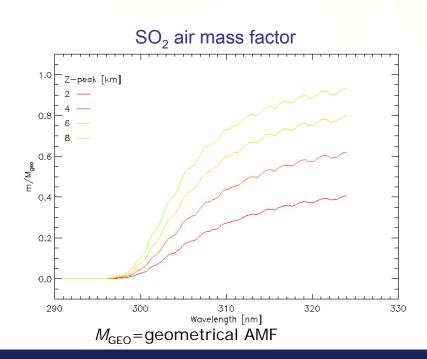


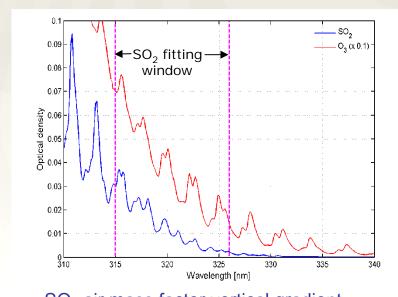
## **Evolution of Lower Tropospheric Ozone** 1996-99 from ERS-2 GOME-1 observations

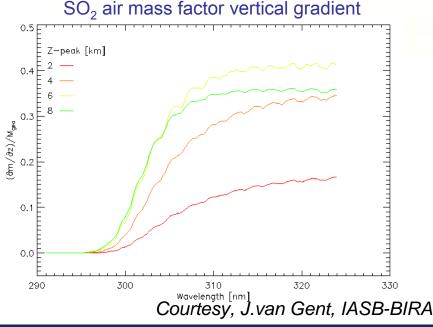


### Volcanic SO<sub>2</sub> plume

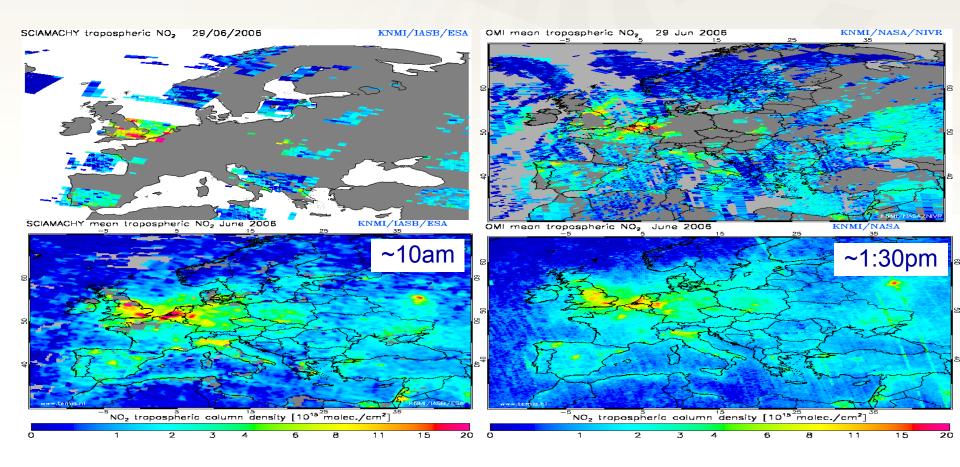
 Information on plume height available if perturbations to integrated column & plume height affect reflectance spectrum differently







## Comparison of Tropospheric NO<sub>2</sub> from SCIA and OMI

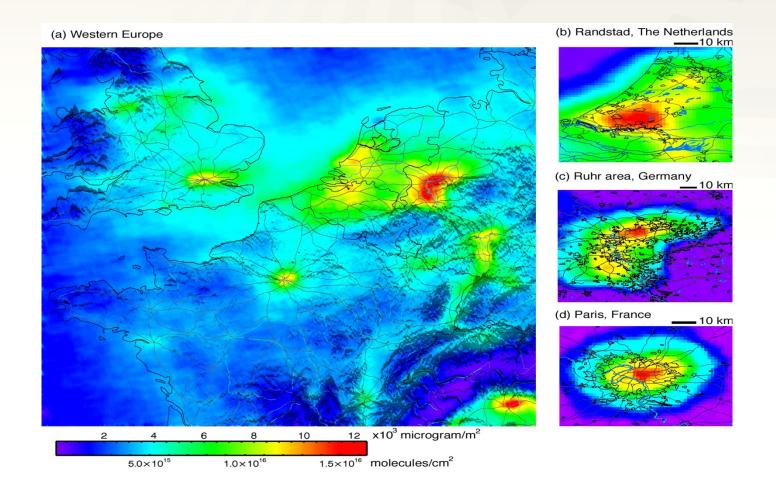


Courtesy: van der A and Dirksen, KNMI

(www.temis.nl)



# OMI Tropospheric NO<sub>2</sub> annual mean: Dec'04-Nov'05

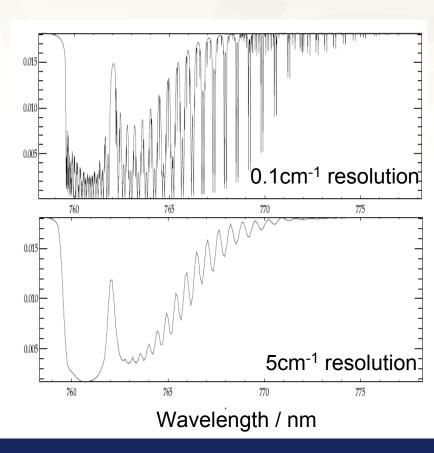


#### Simulations for O<sub>2</sub> A-band (764nm) for Sentinel-4 UVN

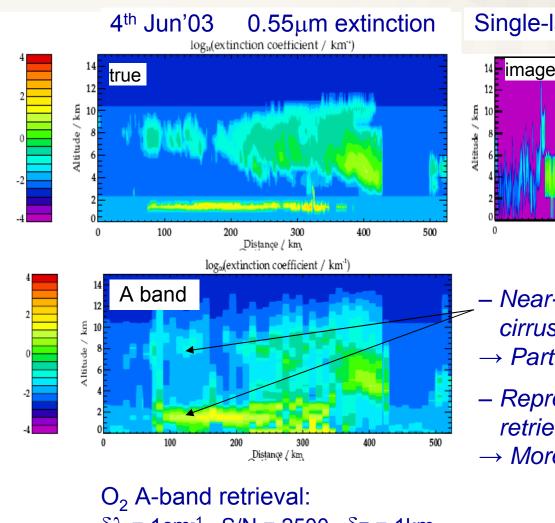
- O<sub>2</sub> A-band: opaque at line centres
  - Effective scattering height a strong  $fn(\lambda)$
  - O<sub>2</sub> mixing ratio known
  - → Retrieve scattering profile
- Sensitive to  $\delta\lambda$ , S/N and other errors
- Requirements assessed for height-resolved aerosol retrieval from Sentinal-4 UVN A-band

Siddans et al, EUM/CO/05/1411/SAT, 2007

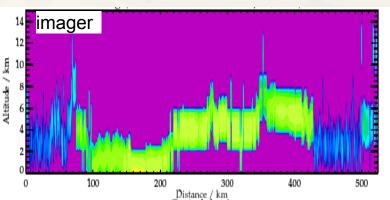
#### **Sun-normalised radiance**



#### Aerosol retrieval simulation for O<sub>2</sub> A-band (764nm)



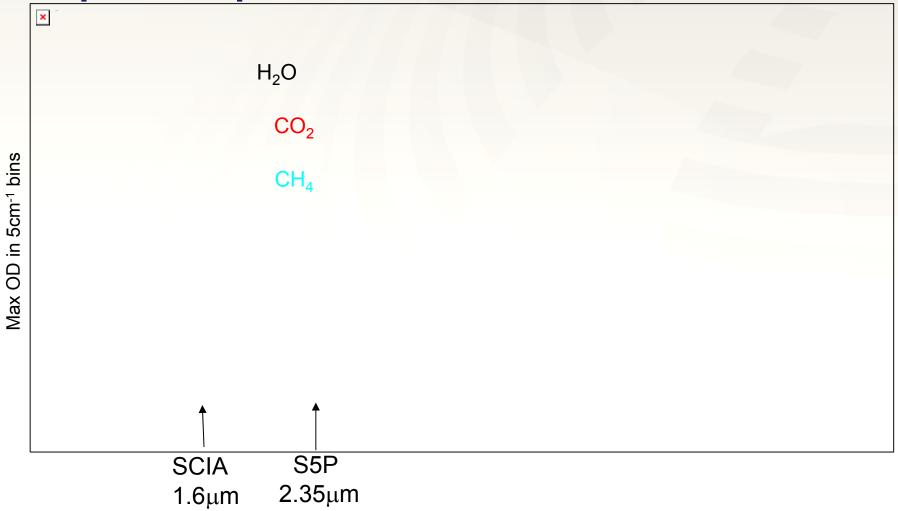
Single-layer multi-channel imager retrieval



- Near-surface aerosol discriminated from cirrus & aerosol in higher layers
- → Particulate sources & transport → AQ
- Represent scattering profile in trace gas retrievals
- → More retrieval of gaseous pollutants

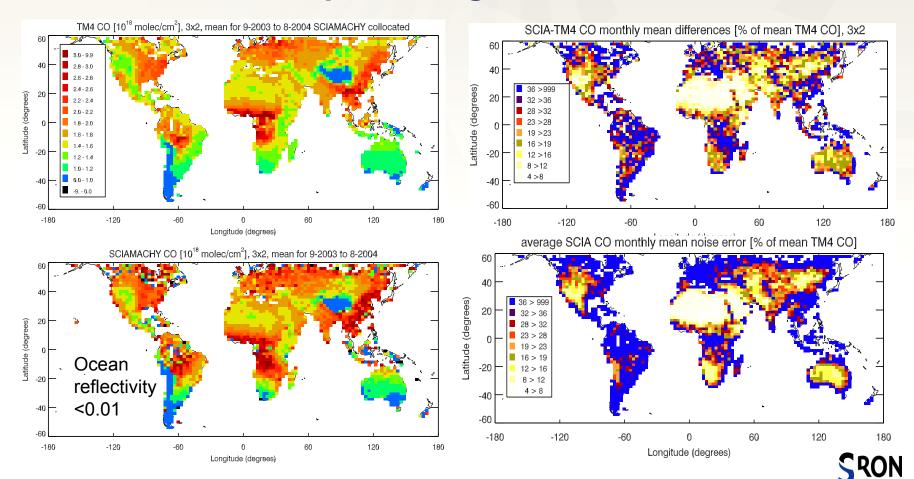
 $\delta \lambda = 1 \text{cm}^{-1}$ , S/N = 2500,  $\delta z = 1 \text{km}$ 

#### **Optical Depths in Short-wave IR**



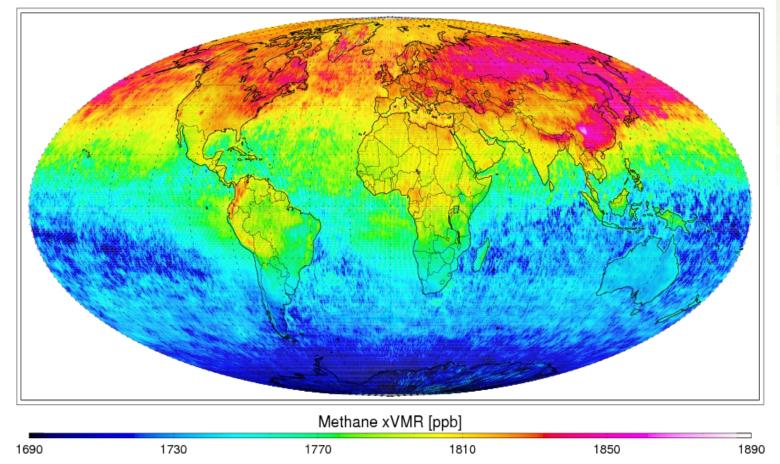
- In short-wave ir, spectral structure of vibration-rotation bands exploited, as in mid-ir.

# Comparison of SCIA & TM4 CO over land Annual mean: Sep'03 – Aug'04



- SCIA TM4 monthly mean difference spatially correlated with SCIA monthly mean noise
- SCIA errors dominated by 2.35  $\mu m$  detector noise  $\rightarrow$  large potential improvement for S5P & S5

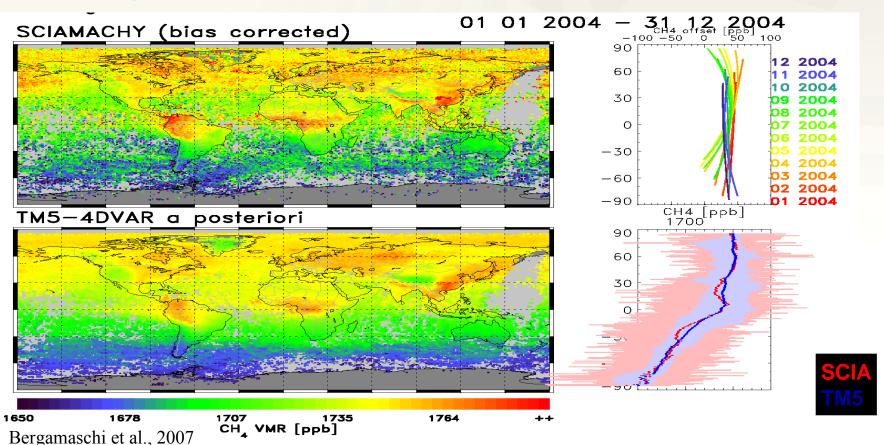
#### Global Mean CH<sub>4</sub> Distribution for 2003-4 from SCIAMACHY



- Fluctuations from uniform mixing are small
- → Accuracy requirements are challenging



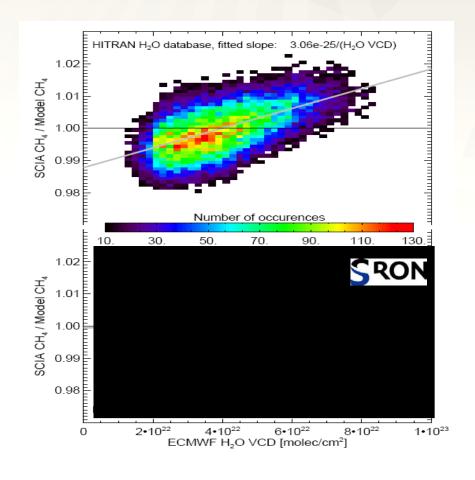
# Methane Annual Mean - 2004 Comparison of SCIAMACHY & TM5



SCIA seasonal / latitudinal bias w.r.t. surface obs



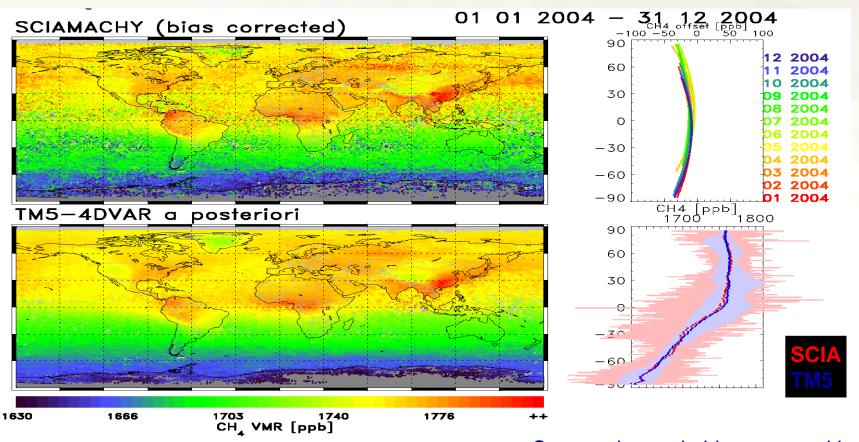
# Correlation of SCIA CH<sub>4</sub> retrievals with column water vapour



Frankenberg et al GRL 2008

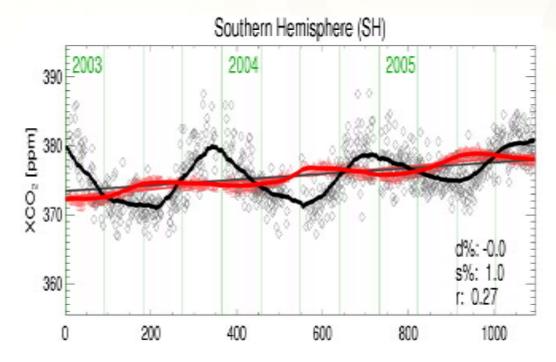


# **Methane Annual Mean - 2004** Comparison of SCIAMACHY & TM5

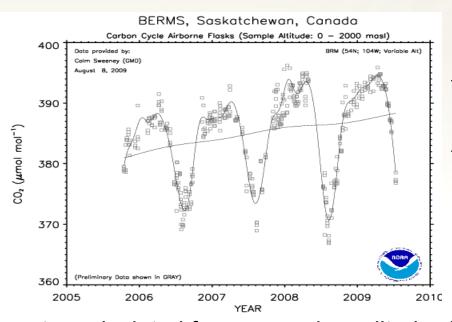


Seasonal varn. in bias removed by improved H<sub>2</sub>O (& CH<sub>4</sub>) spectral data

- SCIA measures CO<sub>2</sub> absorption simultaneously with CH<sub>4</sub> in 1.6μm band
- CH<sub>4</sub> column-average mixing ratio actually derived as ratio to CO<sub>2</sub>, which is much closer to being uniformly-mixed.
  - ratio approach allows some errors in knowledge of atmospheric physics and instrument to be accommodated in deriving CH<sub>4</sub>
- Q: Might perturbations from uniform-mixing be detectable for CO<sub>2</sub>?

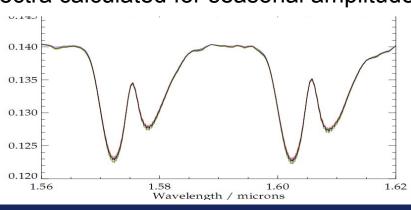


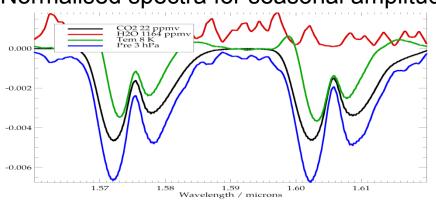
# Influence of geophysical factors on seasonal variation in 1.6µm reflectance spectrum



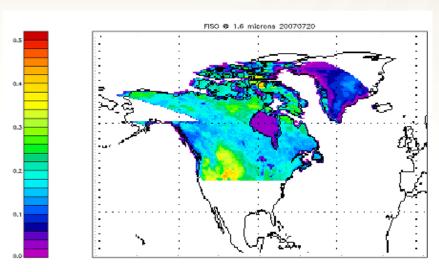
- -1.6μm reflectance spectrum influenced by geophysical factors additional to CO<sub>2</sub>
- –Detection of CO<sub>2</sub> seasonal variation (~few % pk-pk) depends on spectral correlation and how accurately these other factors can be known.

Spectra calculated for seasonal amplitudes Normalised spectra for seasonal amplitudes





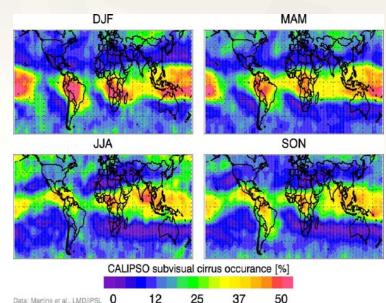
# Influence of geophysical factors on seasonal variation in 1.6µm reflectance spectrum (contd.)



Aerosol Optical Depth

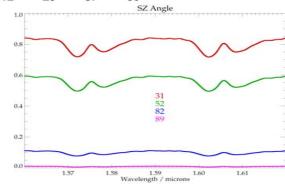
Wavelength / microns

BRDFs for season and location from MODIS.



Derivation of column-average vmr also depends on accurate knowledge of scattering ie:

- Solar zenith & viewing angle
- Surface BRDF
- Profiles of aerosol & thin cirrus
- 1.62 Residual cloud contamination

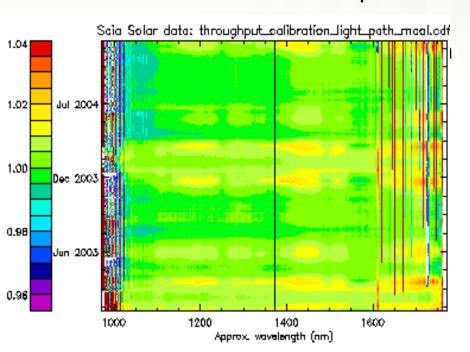


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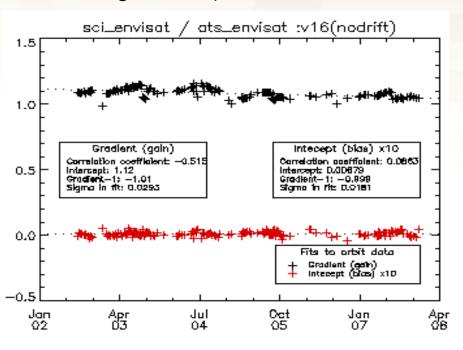
Atmospheric Composition Sounding: solar shortwave nadir spectrometry

# Influence of instrumental factors on seasonal variation in 1.6µm reflectance spectrum

#### SCIA normalised solar spectrum

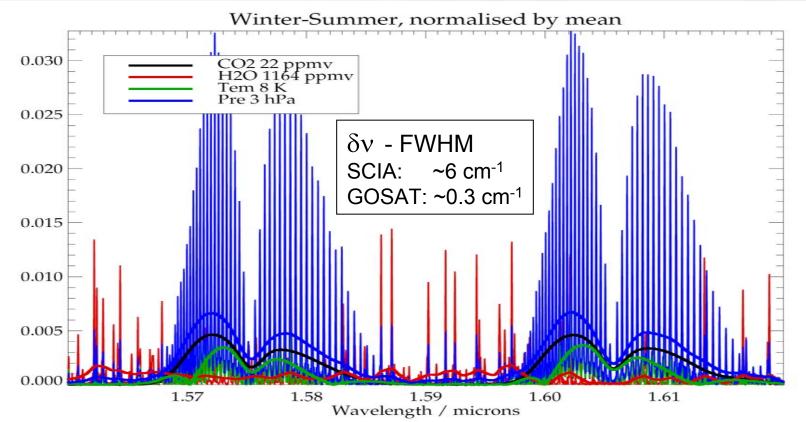


#### SCIA integrated 1.6µm reflectance v AATSR



• To detect regional perturbations from uniform mixing at accuracy (≤1%) needed for inverse modelling, near-perfect knowledge of other geophysical and instrumental factors is required.

#### Spectral signatures at resolutions of SCIA & GOSAT



- GOSAT: optimized for CO<sub>2</sub>
  - additional bands (2μm & IR); 20x higher spec. res., cloud imager
- GOSAT (FTS) and OCO-II (grating) should allow potential for CO<sub>2</sub> to be assessed more fully.

#### Advances: solar shortwave nadir-spectrometry

#### Improve accuracy:

Discriminate trace gases & aerosol more cleanly from cloud & surface

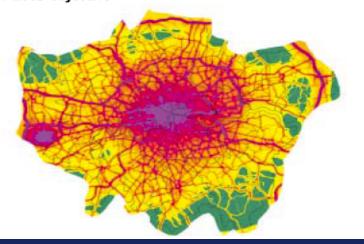
#### Improve height-resolution:

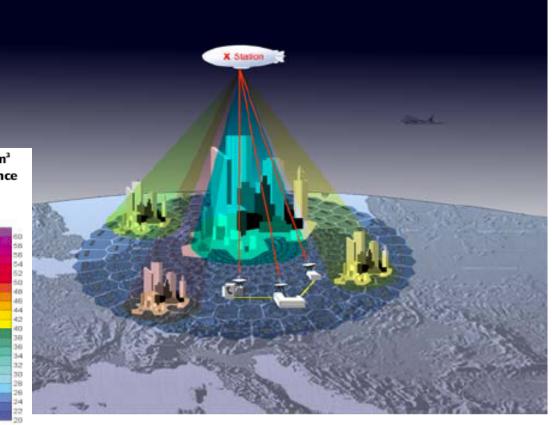
- Spectral resolution in O<sub>2</sub> A-band & swir vibration-rotation bands
- Improve sampling of lower trop. → monitoring/forecasting
  - Polar orbit:
    - smaller ground-pixel to see more often between clouds
    - sample several LTs: 9:30am (MetOp → S5/post-EPS) & 1:30pm (S5P → JPSS)
  - Geo orbit (S4/MTG-S)
    - denser spatio-temporal sampling of observable disk (if px size same as polar)
      - photon flux ~1600x smaller; compensated by t<sub>int</sub>, optics size & ground px size

### **Geostationary Platform in Stratosphere**

# Bridge the gap from street-level to satellite

Modelled 1999 annual mean  $NO_2$  concentrations in  $\mu g/m^3$  (poor weather year), above 40  $\mu g/m^3$  indicates exceedance of 2005 objective





Atmospheric Composition Sounding: solar shortwave nadir spectrometry

# Part 2 – Integrated Approach

#### 1. Complementarity of IR and mm-wave limb sounders

Target trace gases:

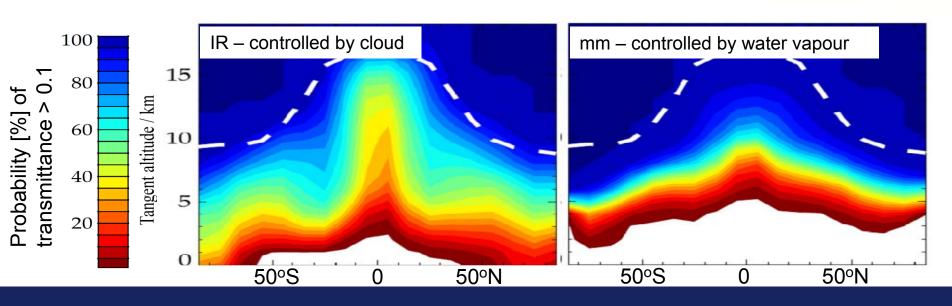
IR: CH<sub>4</sub>; organic compounds; nitrogen oxides mm-wave: CO; HCN & CH<sub>3</sub>CN (biomass burning indicators); halogens

Sensitivity to cirrus particle size

IR:  $R_e < 100 \mu m$ 

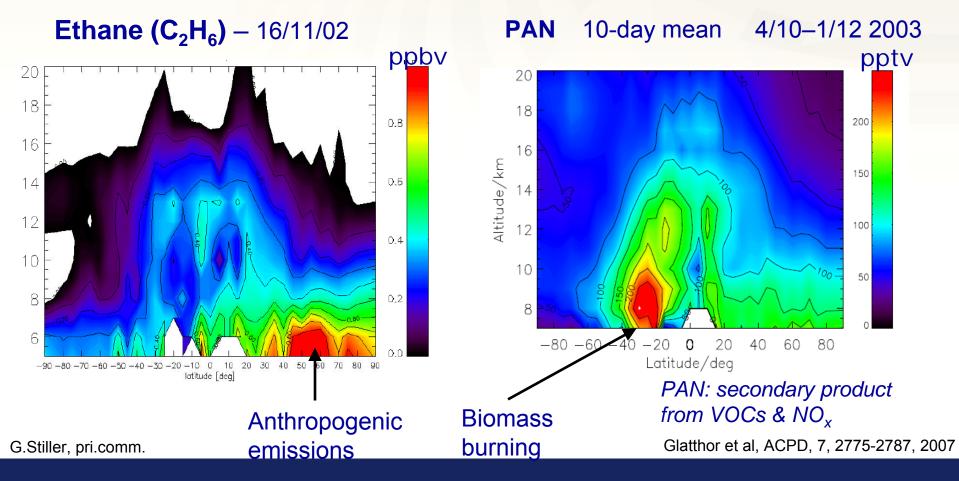
mm-wave:  $R_e > 100 \mu m$ 

→ Different penetration depths into troposphere



#### **Zonal-Mean Cross-Sections of Ethane & PAN from MIPAS**

• In addition to profiling many gases in the stratosphere, MIPAS can also probe the upper troposphere.

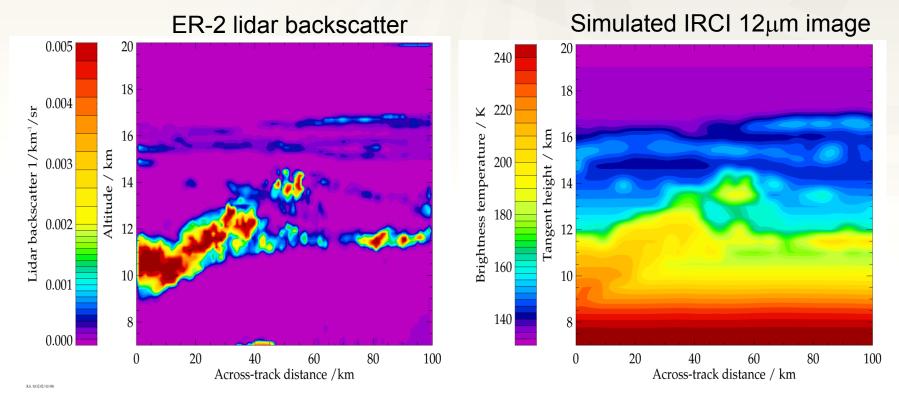


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Atmospheric Composition Sounding: integrated approach

B.Kerridge

### Thin cirrus layers near the tropical tropopause



- Thin cirrus layers influence water vapour transport through TTL
- Difficult to detect by satellite lidar but observable by high-resolution IR limb imaging
- These thin layers are transparent in mm-wave → retrieval of H<sub>2</sub>O & other gases unaffected
- Height of volcanic ash layer could also be determined precisely through IR limb imaging

#### 2. Limb – nadir combination



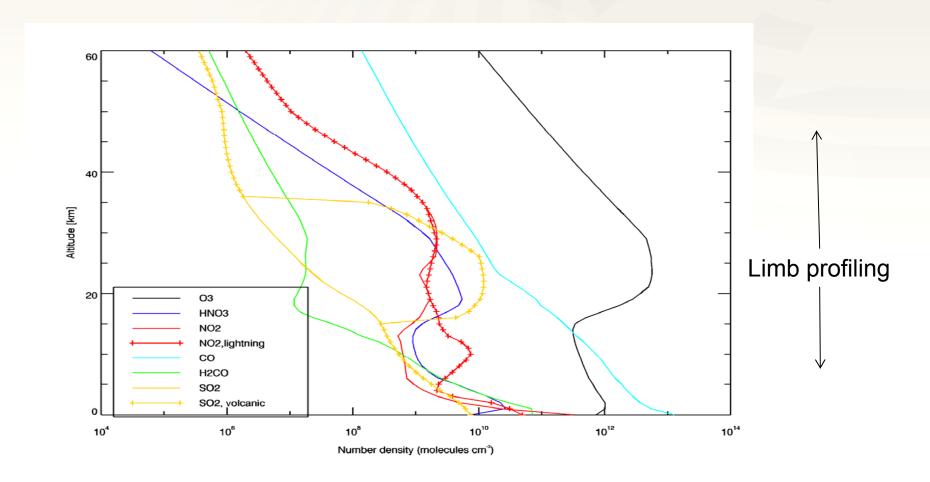
- Near-surface layer seen between clouds but
- Little or no vertical resolution

#### **Limb-emission sounding**

- High res. vertical profiling
- Tenuous trace gases detectable
- Cold space background
- Dense coverage cf solar occultation

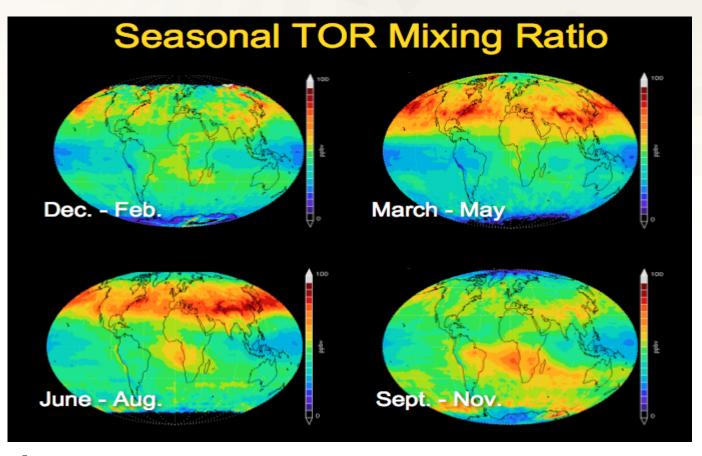


#### **Vertical Profiles: Number Density**



#### Limb – nadir combination (contd)

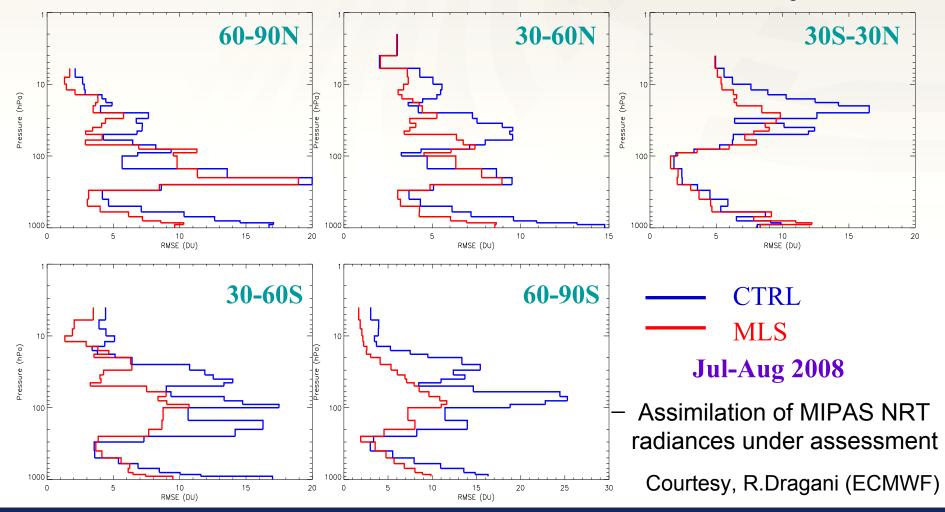
Aura MLS – OMI



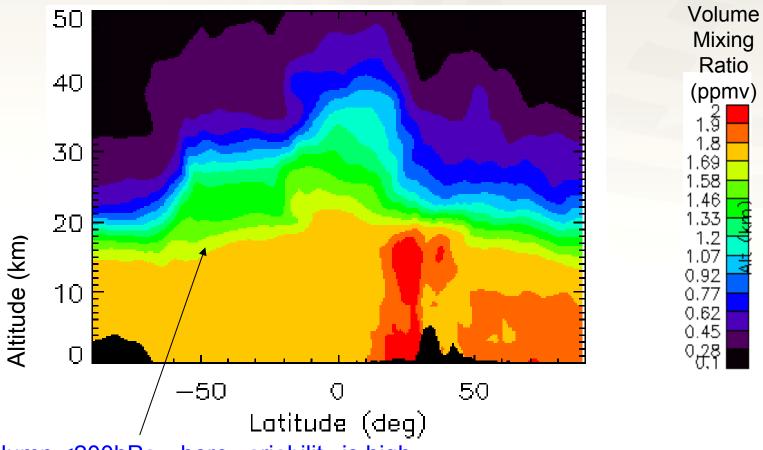
Schoeberl et al. 2007

### Impact of Limb Emission Data in Assimilation

ECMWF analysis – sonde RMSE comparison: Aura MLS O<sub>3</sub> NRT data

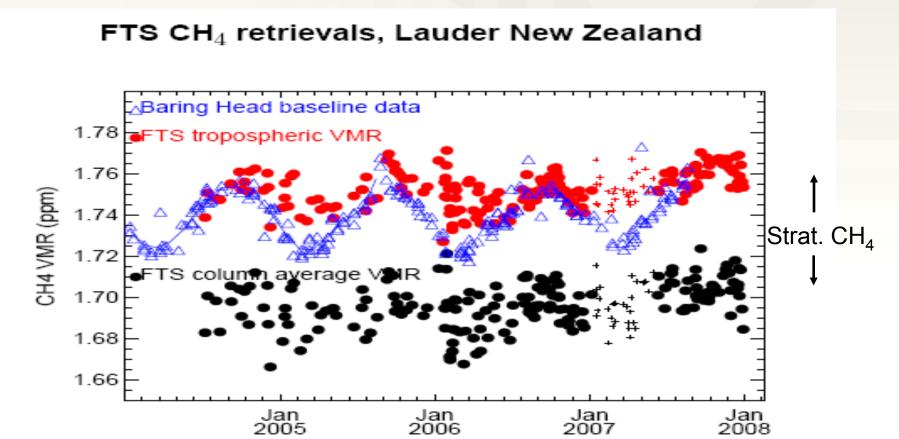


### **Methane Latitude-Height Cross-Section**



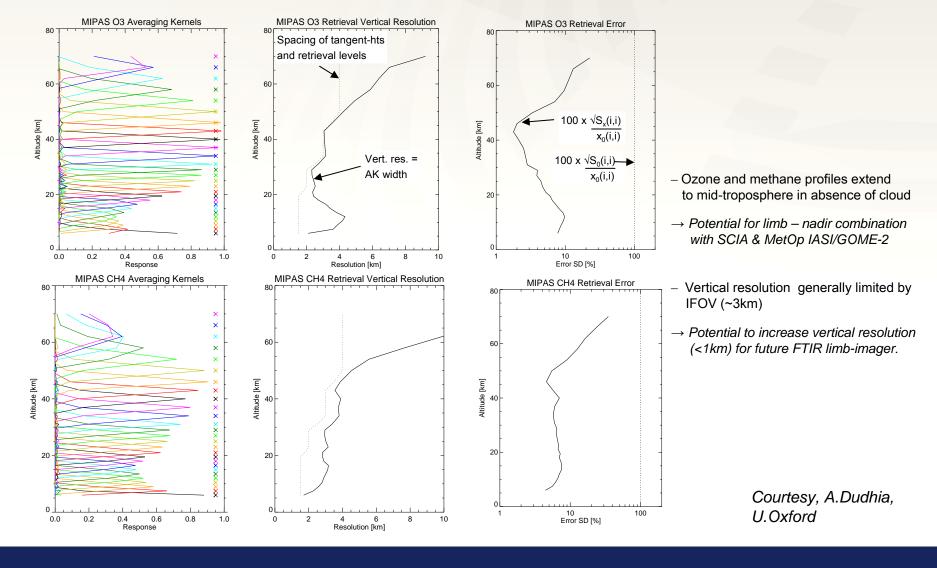
- ~10% of column <200hPa where variability is high
- → tropospheric column mean vmr "cleaner" than total column mean vmr for inverse modelling of methane surface sources

### Column-average CH<sub>4</sub> mixing ratio

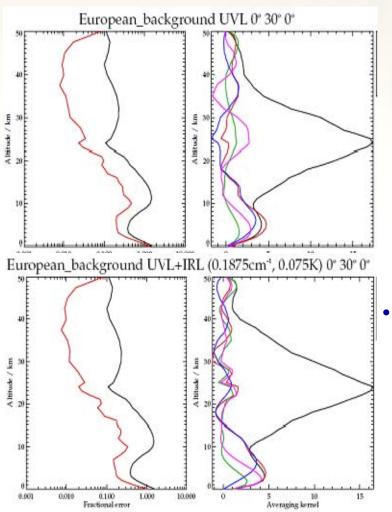


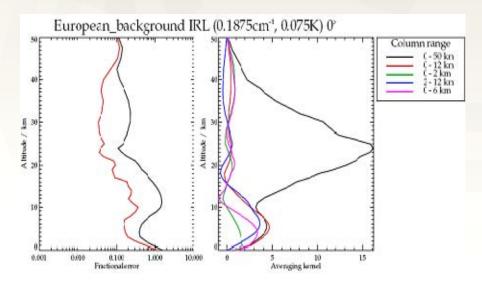
Tropospheric column averaged vmr from ground-based FTS closer to surface values and less variable than total column average vmr.

# O<sub>3</sub> & CH<sub>4</sub> Linear Retrieval Diagnostics for Envisat MIPAS – IR limb-emission sounder



### 3. Simulation of combined nadir/uv-ir O<sub>3</sub> retrieval



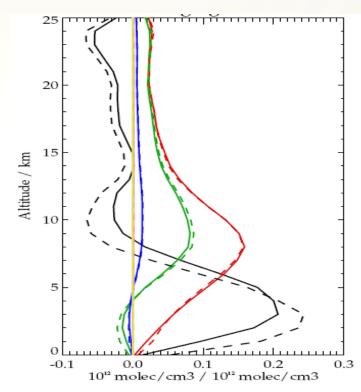


- Different height sensitivities in UV & IR
  - UV & IR kernels for 0-2km and 0-6km layers are sharpened by combining them
  - $\rightarrow$  should improve mid/lower trop.  $O_3$
  - eg GOME-2 + IASI combination



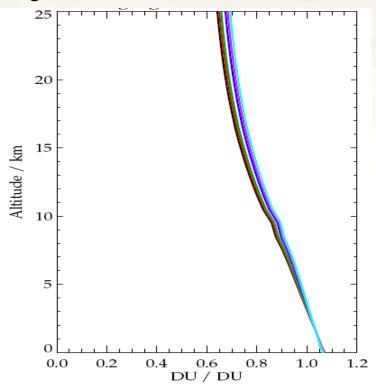
### Averaging Kernels for IR & SWIR CH<sub>4</sub> retrieval

 IASI averaging kernels using 1240-1290 cm<sup>-1</sup>



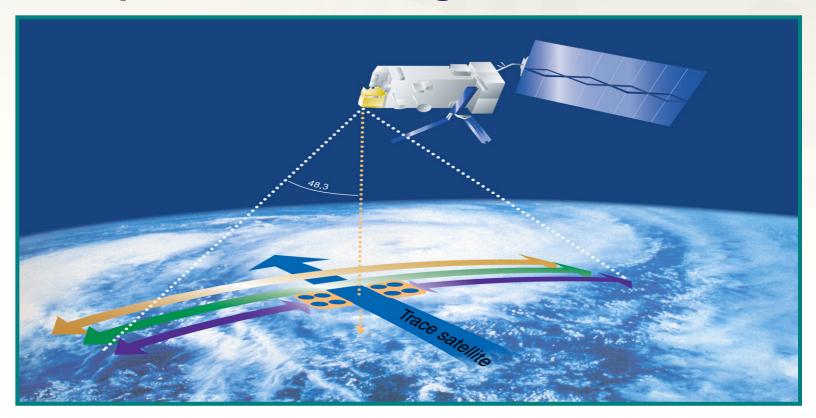
- Assumes 0 (solid) or 10K (dashed) air/surface temperature contrast
- > IASI has height-resolution in troposphere

 SCIA 1.6 micron averaging kernels for integrated column retrieval



- For surface albedo 0.16 (typical vegetated land)
- SCIA more sensitive near surface over land

### 4. Spectrometer - Imager

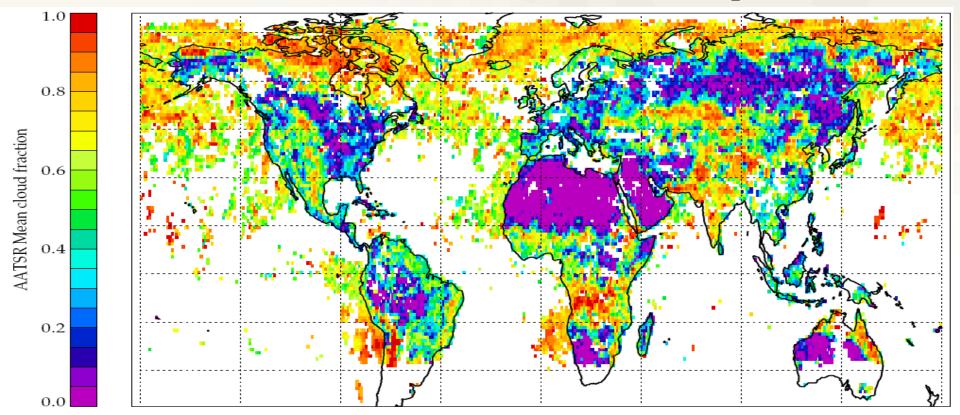


- Cloud and surface properties affect radiative transfer in non-linear ways
- Many scenes viewed by spectrometers are inhomogeneous
- Co-located imager → sub-pixel distributions of cloud, aerosol & surface properties
- eg Envisat & MetOp



#### AATSR cloud fraction for SCIA scenes which pass CH4 QC

SCIA QC includes cloud screening based on CO<sub>2</sub> column

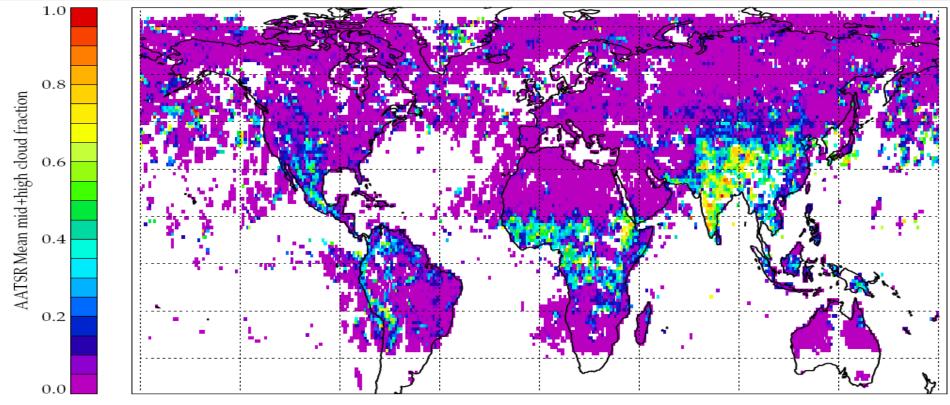


- ~Half SCIA's swath covered by AATSR swath (512km)
- Where AATSR cloud fraction is high, SCIA sensitivity to boundary layer CH<sub>4</sub> is low

#### $\left\{ \left\| \left\| \right\| \right\| \right\}$

### AATSR mid/high level cloud fraction in SCIA scenes

Fraction of SCIA scene occupied by cloud <650 hPa.</li>



- Sensitivity to mid tropospheric CH<sub>4</sub> compromised eg over Indian sub-continent.
- Co-located AATSR data can identify SCIA scenes affected by cloud
- Partially cloudy scenes could be post-processed using cloud properties from AATSR to characterise better SCIA's vertical sensitivity to CH₄.

#### **Conclusions**

- There is a strong scientific imperative to sound atmospheric composition from space, to complement surface & airborne observations.
- The challenge is to resolve atmospheric structure on finer scales while maintaining and improving accuracy.
- Coupling between layers is crucial, both for science & for retrieval/assimilation
- Advanced techniques are in development to exploit better the data from existing and planned satellites.
- New satellite missions are needed to address major scientific issues and also to serve new operational applications (GMES Atmosphere Service).
- These will be designed to exploit new technology and to combine optimally different observing techniques.

