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2. Authors: JB Kumer, JL mergenthaler, AE Roche and R Rairden, all with LMATC, and Robert Chatfield with ARC

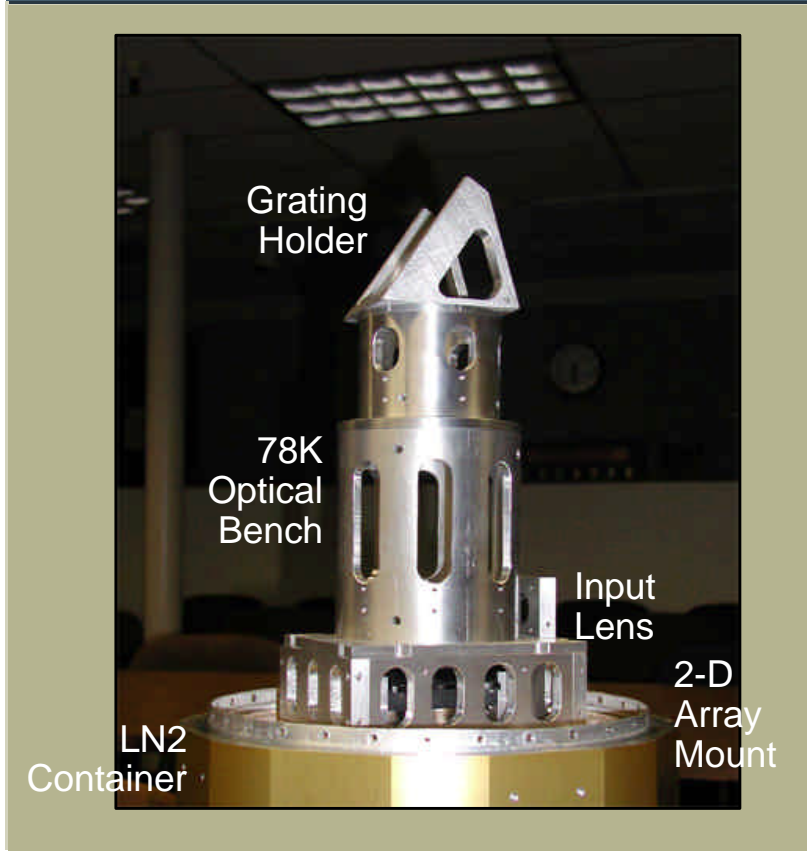
3. Tropospheric infrared mapping spectrometers (TIMS) for Air Quality measurements

4. Abstract:

We have been awarded a NASA Instrument Incubator Program (IIP) to develop grating mapping spectrometers (GMS) with very high spectral resolution, very low noise, and very wide field of view. These also would be very compact facilitating deployment in either a leo or geo application. The measurement set could be very comprehensive, addressing air quality, carbon species and climate change, or subsets of these. For this presentation we'll focus on the potential application of these GMS to provide an air quality subset of primary measurements consisting of CO partial columns, (vertical information), ozone partial columns and HCHO column. The measured spectra provide opportunity to retrieve secondary products including columns of CH₄, N₂O and CO₂, and improved retrieval of near surface H₂O. The CH₄ and CO₂ columns ratio can be used to retrieve vertically averaged tropospheric CH₄ mixing ratio. Spectral measurements would be acquired with several spectrometers. For the species as cited above these would include solar reflected spectra near 2.33 and 2.08 μm, and emissive spectra near 4.68 μm. Additional, optimal O₃ information could be obtained by adding another emissive region near 9.52 μm. For this application we'll discuss spectral regions, spectral resolution and noise for potential geo and leo applications. For these applications we'll describe the temporal and areal coverages and footprint sizes. We'll present retrieval results predicted by a linear error analysis for these applications. We'll present results from an in house lab demonstration GMS that is a predecessor to the IIP design.

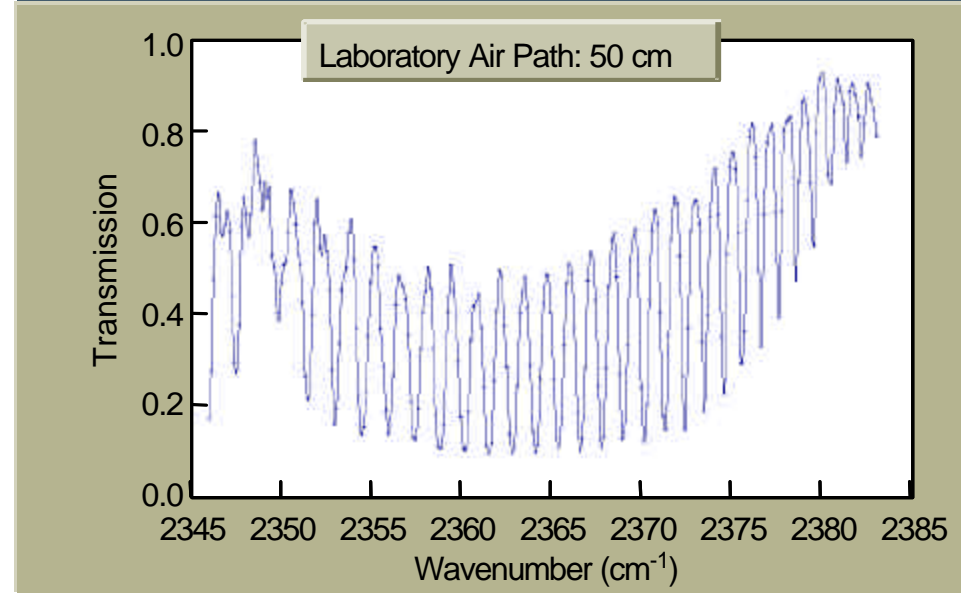
Lab demo grating mapping spectrometer (GMS)

0LN2 Cooled Demonstration Spectrometer Structure

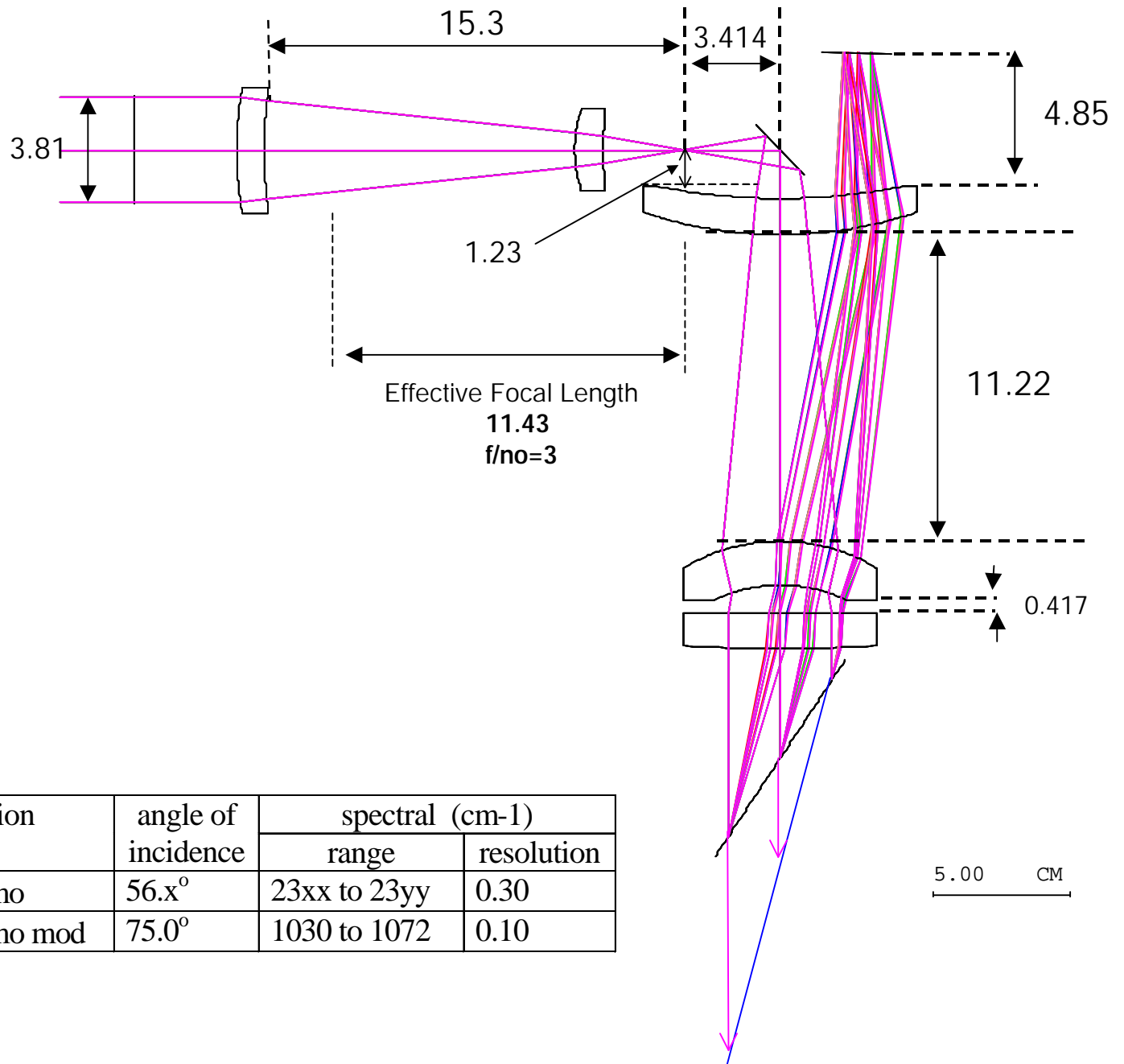


Hardware implementation of Lab demo SWIR GMS

0.3 cm⁻¹ Absorption Spectra of CO₂ 626 Fundamental Band Lines



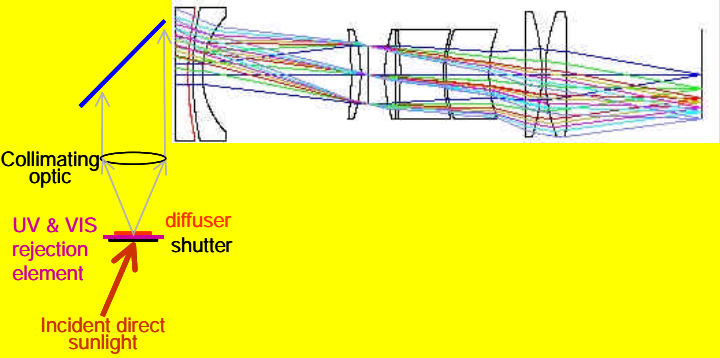
Lab demo SWIR GMS absorption spectra at spectral resolution $\sim 0.3 \text{ cm}^{-1}$ obtained for transmission through a 50 cm path of lab air



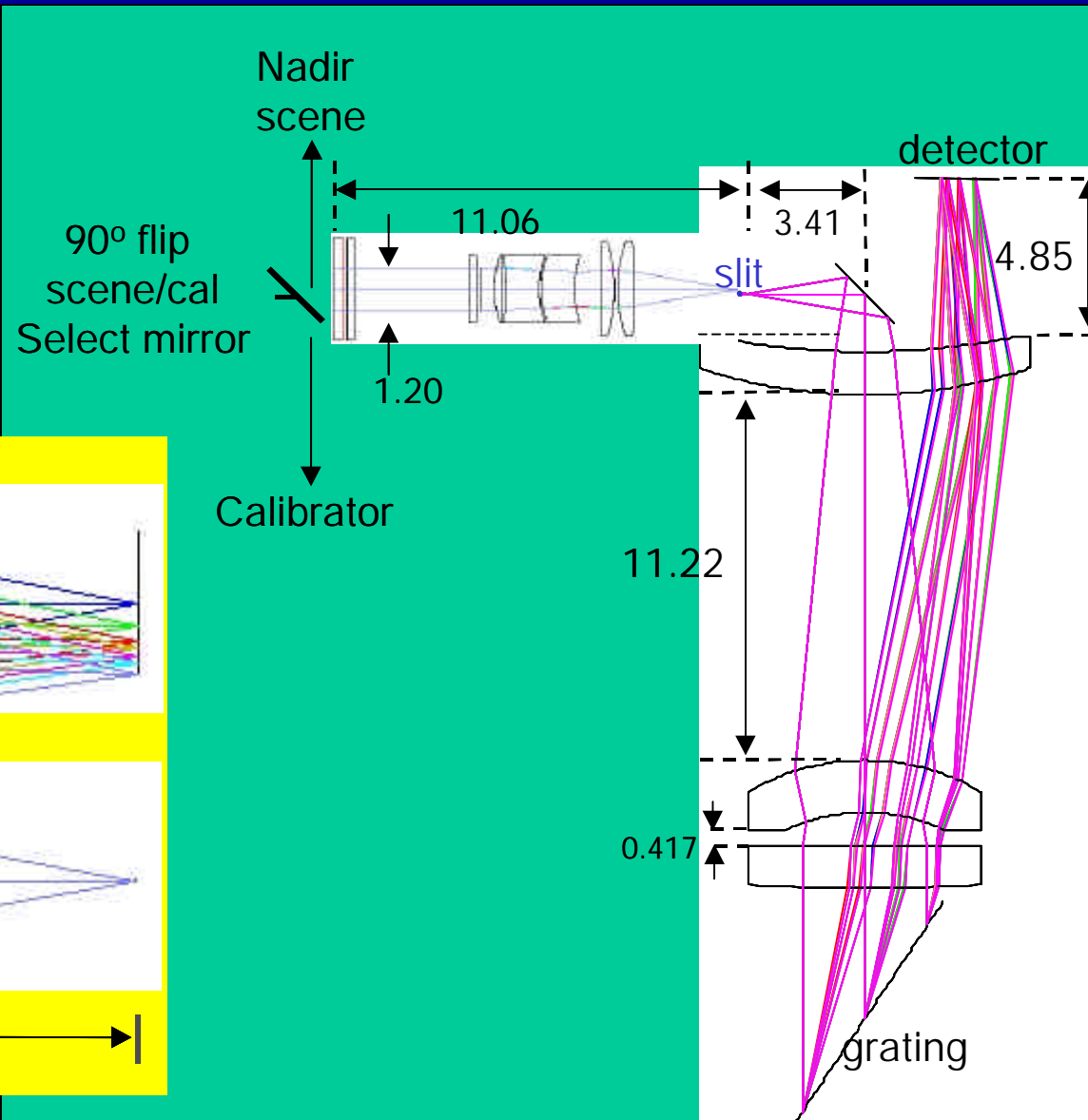
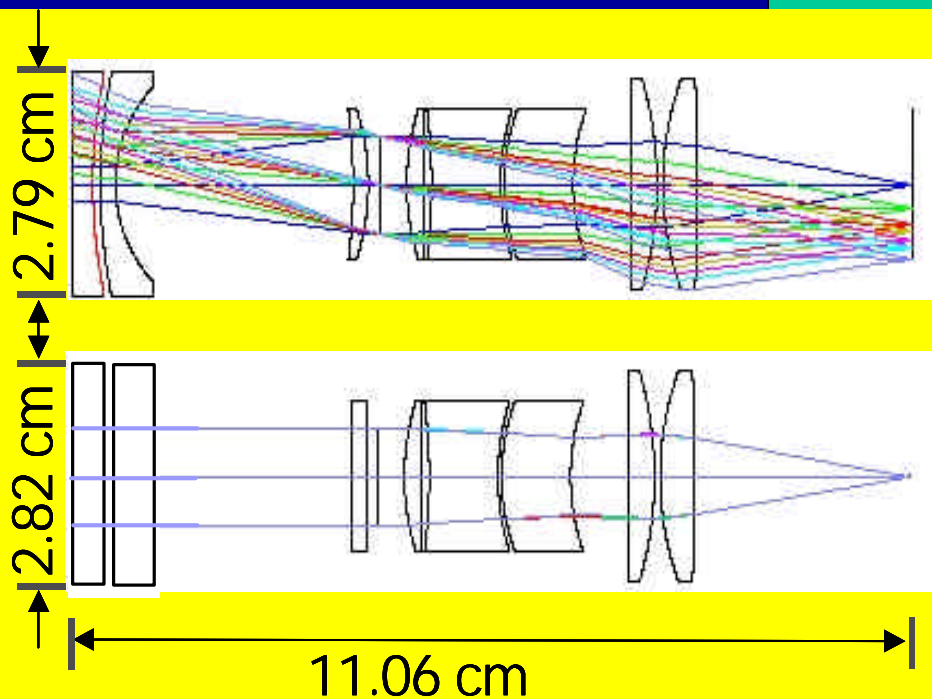
configuration	angle of incidence	spectral (cm-1)	
		range	resolution
4.2x μm lab demo	56.x°	23xx to 23yy	0.30
9.57 μm lab demo mod	75.0°	1030 to 1072	0.10

Lab demo optical design with crosstrack field widened input optics for spaceborne deployment

Solar spectral cal concept

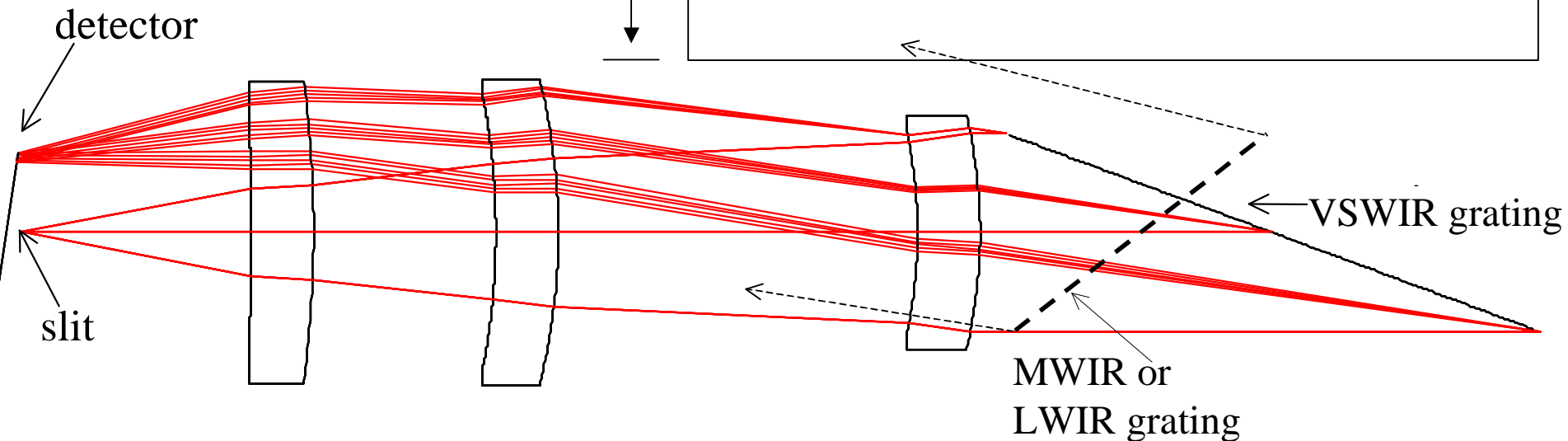


Two perspectives of anamorphic fore optics



The VSWIR spectrometer requirement for spectral resolution 0.10 cm^{-1} on the range $4281\text{ to }4301\text{ cm}^{-1}$, and with a 1.84 cm slit length, is by the far the most challenging to implement

5 cm scale



Measurement summary table

Spectral Region and priority	Approximate wavelength	Frequency resolution	NEdN ⁽¹⁾ goal & Threshold mW/(m ² sr cm ⁻¹)	Nadir ELF ⁽²⁾	Primary Measurement (potential measurement)	Consequent Additional Benefits
VSWIR 2ndary	2.09 μm	< 0.16 cm ⁻¹		1.6 km	column CO ₂ , clouds	ratio vs CH ₄ :CO ₂ columns for [CH ₄] ⁽³⁾
VSWIR 2ndary	2.25 μm	< 0.16 cm ⁻¹		1.6 km	column CH ₄ , N ₂ O, clouds	ratio CH ₄ :N ₂ O
VSWIR primary	2.33 μm	< 0.13 cm ⁻¹	0.04 & 0.10	1.6 km	column CH ₄ , CO, H ₂ O, clouds	BL ⁽³⁾ CO, CH ₄ , and H ₂ O columns, clouds & BL
SWIR 2ndary	3.33 μm	< 0.58 cm ⁻¹		3.2 km	CH ₄ , H ₂ O	good vertical info in this region
SWIR primary	3.56 μm	< 0.35 cm ⁻¹	0.0016 & 0.0050	3.2 km	HCHO, CH ₄ , N ₂ O, and maybe some O ₃ info	VOC's; high precision column info and some vertical info for HCHO, CH ₄ & N ₂ O
MWIR primary	4.65 μm	< 0.20 cm ⁻¹	0.006 & 0.012	3.2 km	CO, O ₃ and H ₂ O	CO profile ⁽⁴⁾ , tropospheric O ₃ and BL H ₂ O
LWIR ⁽⁵⁾ primary	9.5 μm	< 0.11cm ⁻¹	0.026 & 0.055	6.4 km	O ₃ partial columns (PCs)	PCs @ 0-6, 6-12 & 12-22 km

1 - @ 10% albedo for solar reflective & @ scene brightness 260 K for thermal

2 - ELF: Elemental (smallest sampled) footprint

AGF: aggregated footprint, nominally comprised of 12x12 VSWIR ELFs, co-registered with 6x6 SWIR and MWIR ELFs, and with 3x3 LWIR ELFs

3 - BL: Planetary Boundary Layer, also [CH₄] is total atmospherically averaged CH₄ mixing ratio

4 - CO profile and H₂O BL require retrieval that simultaneously utilizes the VSWIR and MWIR data

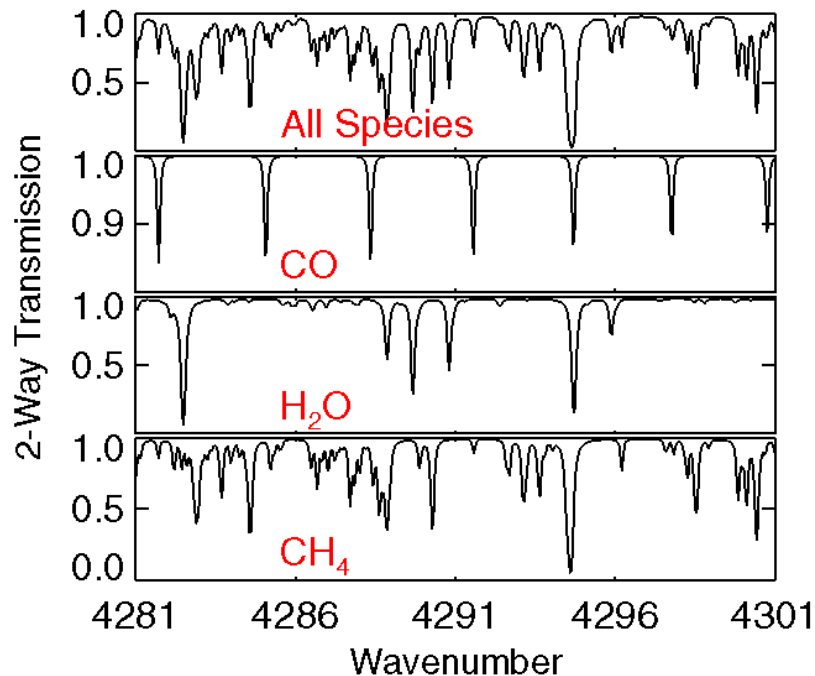
5 - Active cooling required; for others, shorter wavelength operation facilitates passive (radiative) cooling

example assumes (a) 829 km polar sun-sync orbit, (b) nadir centered swath width 25.45° on the earth, (c) end point zenith LOS @ surface 67.6°, (d) average crosstrack VSWIR ELF = 2.76 km, etc

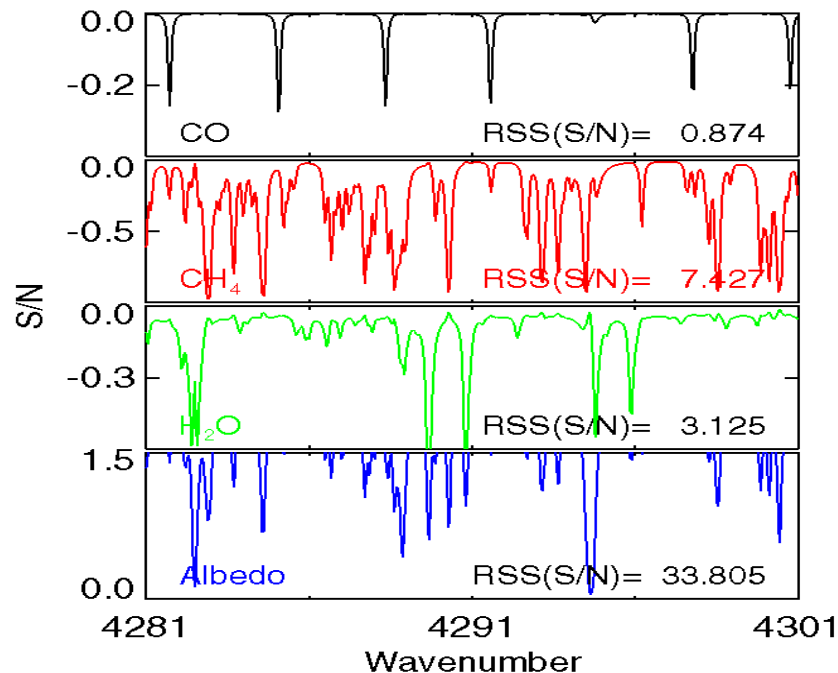
The measurements require 3 grating mapping spectrometers (GMS), one for the VSWIR, one for the SWIR and MWIR, and one for the LWIR

Solar reflective VSWIR region (~ 2330 nm) for CO

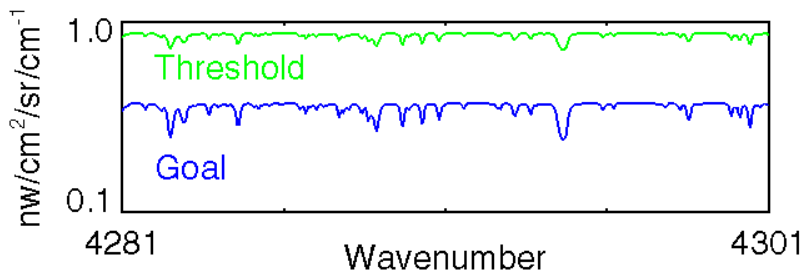
2-way transmission spectra, solar zenith angle = 45° and zenith angle for LOS to satellite = 45°



Spectral radiance changes (SRCs) in units S/N per 1% change in column, and/or albedo



Threshold & goal NEdN for aggregated footprint (AGF, xx.x km along track 7 average, yy.y km crosstrack)



linear error analysis (LEA) for columns & surface, A_{II} is the diagonal of the averaging matrix

Table of LEA results for 4281 to 4301 cm⁻¹

Geophysical parameter	Retrieval precision %	A_{II}	Rss_SNR
CO column	1.20	0.9977	0.874
CH ₄ column	0.17	1.0000	7.427
H ₂ O column	0.40	0.9993	3.125
albedo	0.044	1.0000	33.80

MWIR region (~ 4673 nm) for CO and O₃

Rss_NEdN is rss of threshold instrument noise
 NEdN and Noise Equivalent Temperature model
 Uncertainty NETU for an AGF where

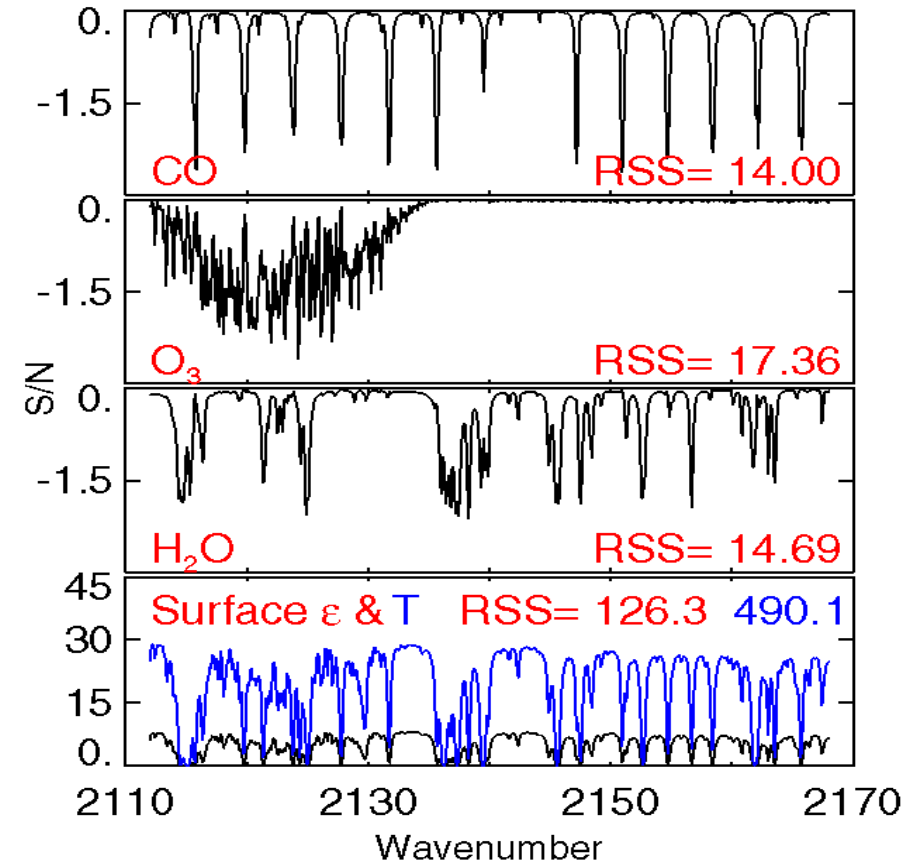
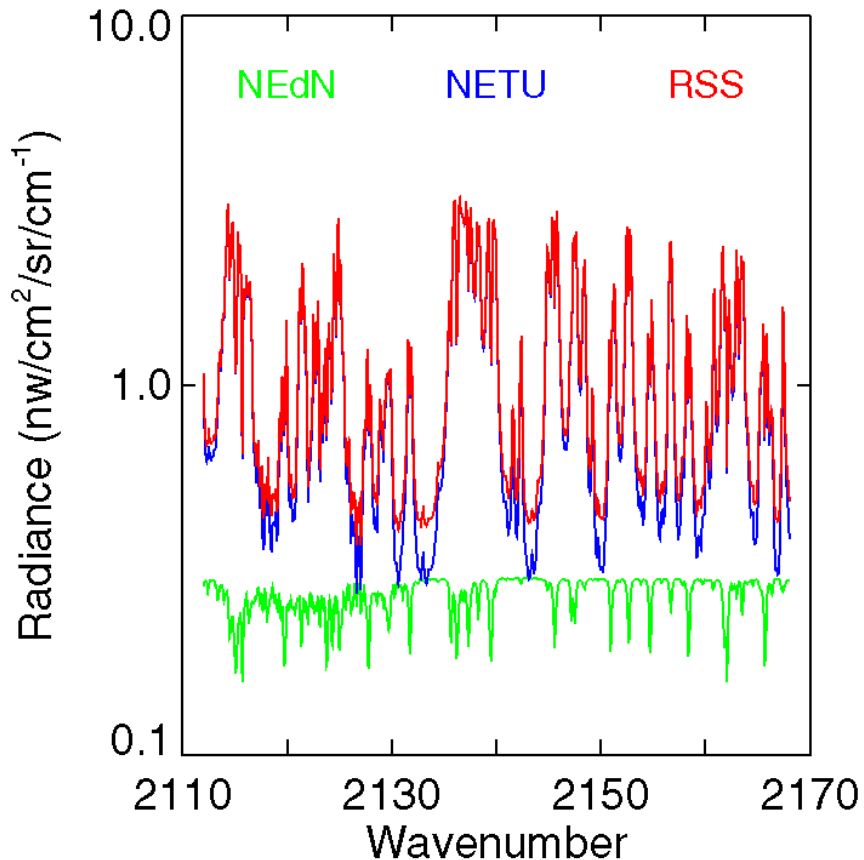
$$\text{NETU} = \Delta T (\Sigma (\partial N_{\text{rad}} / \partial T_j)^2)^{1/2}$$

For a temperature model with uncertainty $\Delta T=1\text{K}$
 on 2km layers

Spectral radiance changes (SRCs) resulting from
 1% changes in the columns of CO, O₃ and H₂O,
 and from 1% changes in surface emissivity, and
 1K change in surface temperature are shown

below for an AGF. (weaker CO₂ & N₂O contributions not shown here)

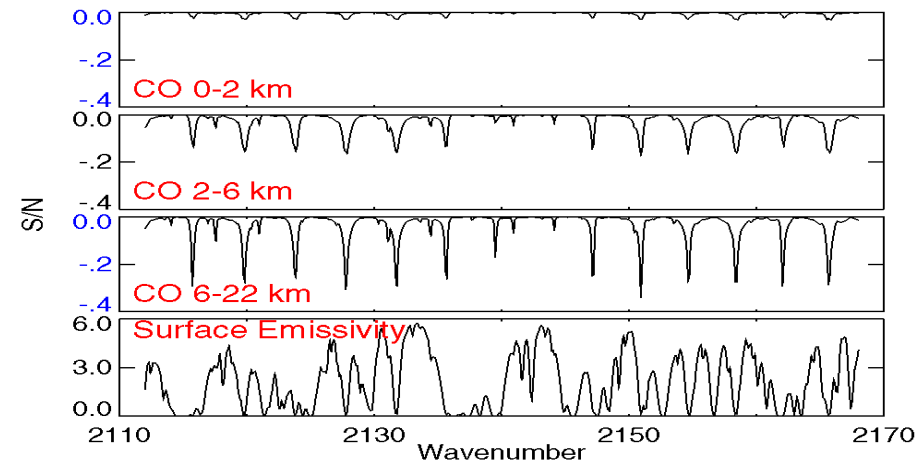
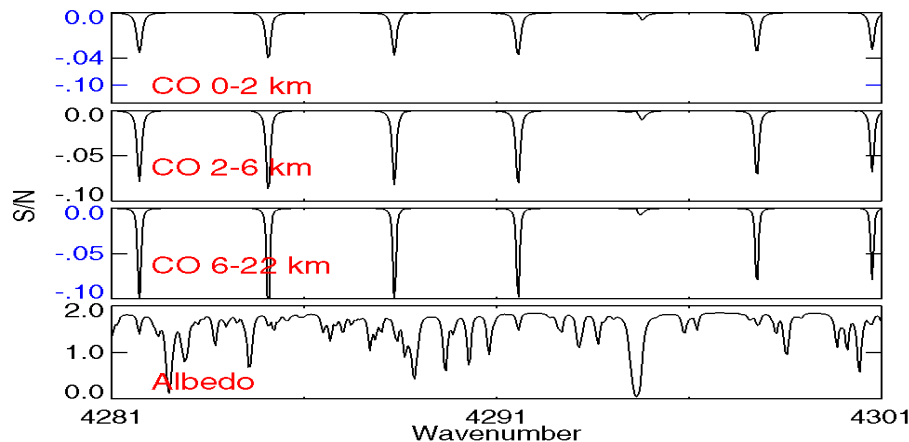
• **note the orthogonality of the species SRCs**



3-layer CO Retrieval

Following suggestion of our IIP co-operating scientist Robert Chatfield we executed the LEA on 3 layers that approximate independent layers for CO retrieval. the layers are selected as follows, each of the two upper layers should come as close as possible to having it's diagonal $A_{LAYER} = (DFS - A_{11})/2$ where $DFS = \Sigma A_{II}$ for a all layers of a 2km per layer model.

- On the left panel 2 figures with SRCs in the two spectral regions for 1% perturbations of CO partial columns and surface parameter perturbations of 1% emissivity & 1K temperature, and
- on the right panel tables of LEA results for day and night cases. Calculations apply for a 20km footprint.



Tables of LEA results for 3-layer CO retrieval

Daytime LEA results for layered CO retrieval			
parameter	Retrieval precision %	A_{II}	Rss_SNR
CO 0 – 2km	8.4	0.89	0.27
CO 2km – 6 km	4.3	0.97	1.13
CO 6 km – 22km	2.3	0.99	1.6
Surface reflectance	.03	1.0	71.5

Nighttime LEA results for layered CO retrieval			
parameter	Retrieval precision %	A_{II}	Rss_SNR
CO 0 – 2km	24	0.11	0.20
CO 2km – 6 km	6.7	0.93	1.09
CO 6km - 22km	2.5	0.99	1.56
Surface reflectance	0.59	1.0	63.0

LWIR region (~ 9515 nm) for O_3

Rss_NEdN is rss of threshold instrument noise
NEdN and Noise Equivalent Temperature model

Uncertainty NETU for an AGF where

$$NETU = \Delta T (\Sigma (\partial N_{rad} / \partial T_j)^2)^{1/2}$$

For a temperature model with uncertainty $\Delta T=1K$
on 2km layers

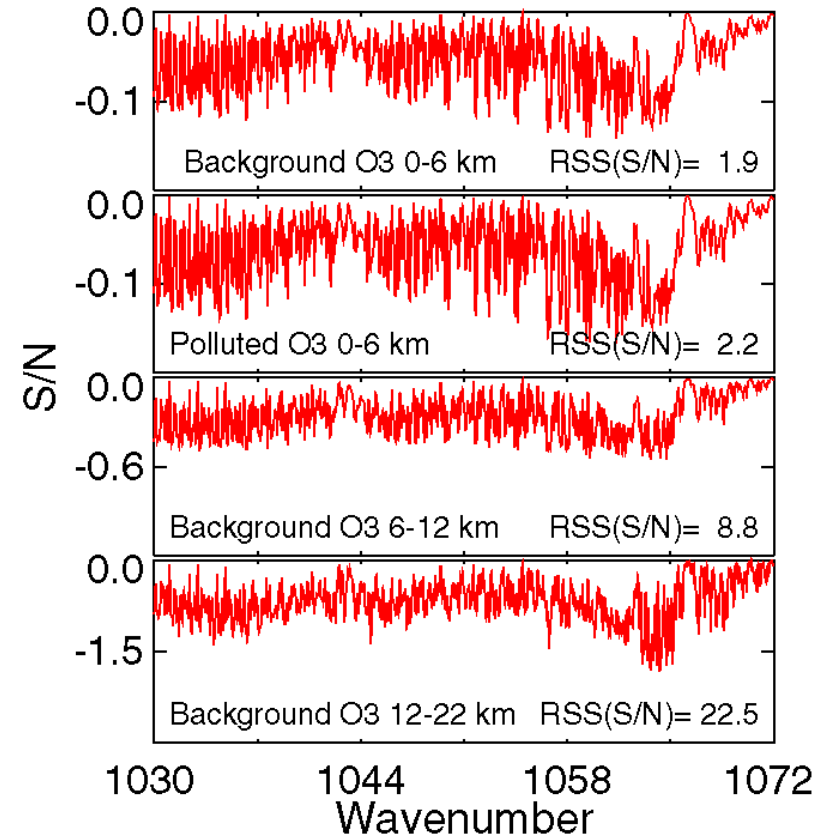
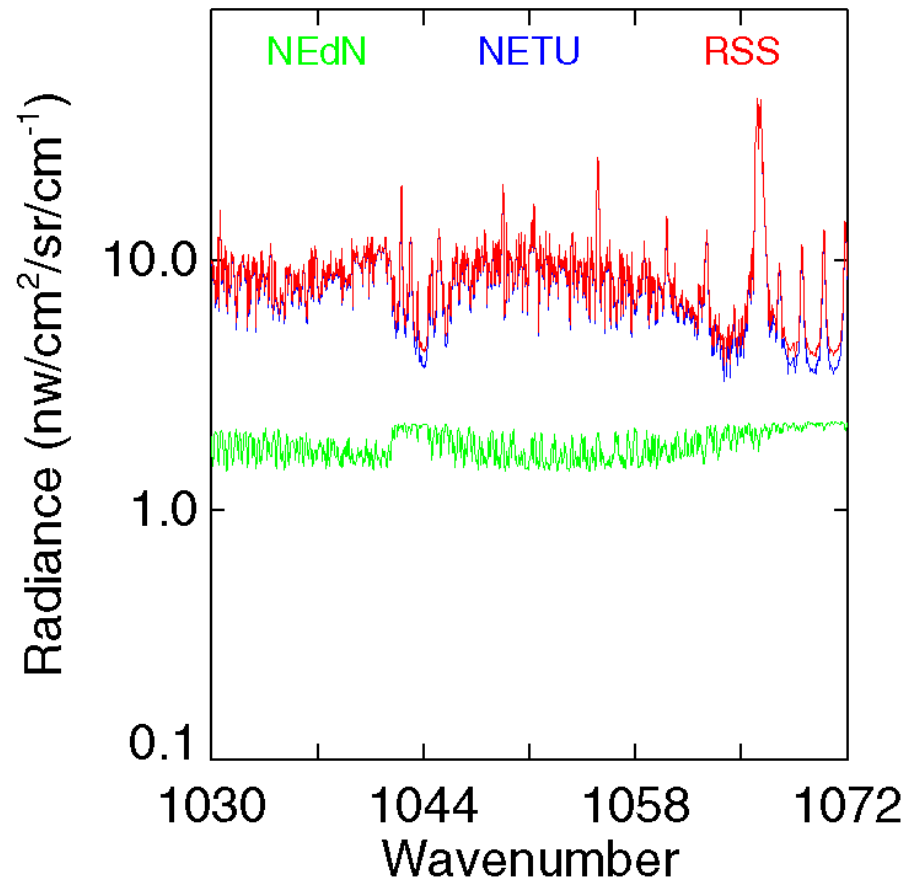
Spectral radiance changes (SRCs) resulting from
1% changes in partial columns of O_3

0 – 6km background, 20 ppbv in boundary layer

0 – 6km, polluted, 80 ppbv in boundary layer

6 – 12 km background case

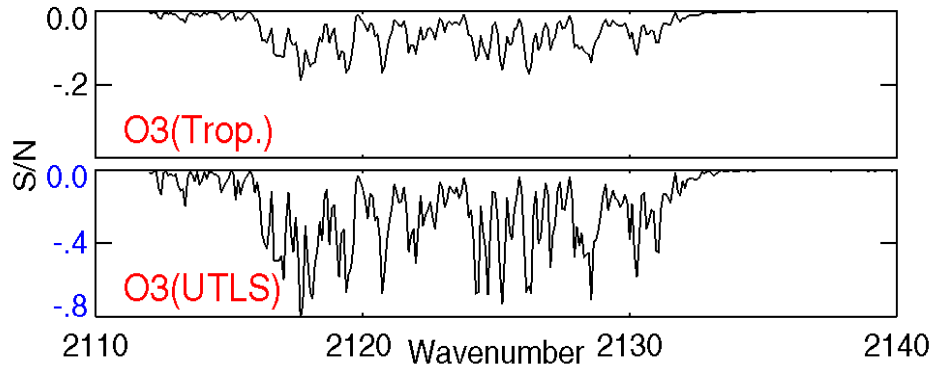
12 – 22 km background case



multi-layer ozone retrieval LEA on an AGF

2-layer retrieval LEA from MWIR data

- OMPS data product constraint
- On the top panel SRCs for 1% perturbations of ozone partial columns
 - 0 to 11 km and
 - 11 to 22 km
- and on the bottom panel tables of LEA results for day and night cases



MWIR LEA results for 2-layer O ₃ retrieval			
parameter	Retrieval precision %	A _{II}	Rss_SNR
O ₃ 0-11 km	6.10	0.996	1.12
O ₃ 11-22 km	1.44	0.979	4.66

3-layer retrieval LEA from LWIR data for background and polluted cases

LWIR LEA results for layered O ₃ retrieval			
parameter	Retrieval precision %	A _{II}	Rss_SNR
O ₃ 0-6 km, background	3.7	0.978	1.9
O ₃ 0-6 km, polluted	3.1	0.985	2.2
O ₃ 6-12 km, background	1.23	0.997	8.8
O ₃ 12-22 km	.269	1.0	22.5

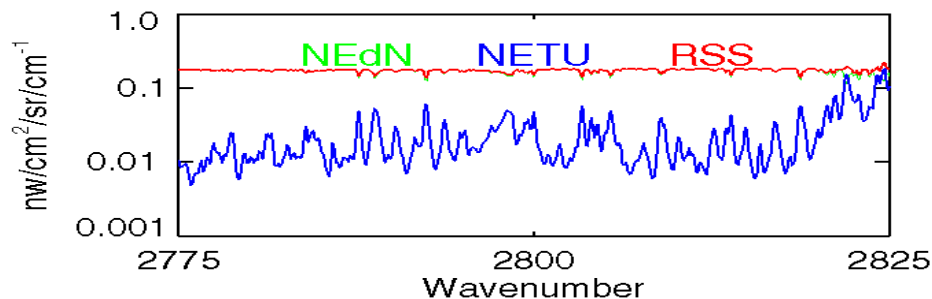
3-layer retrieval LEA from combined LWIR + MWIR data for background and polluted cases

LWIR + MWIR LEA results for layered O ₃ retrieval			
parameter	Retrieval precision %	A _{II}	Rss_SNR
O ₃ 0-6 km, background			
O ₃ 0-6 km, polluted			
O ₃ 6-12 km, background			
O ₃ 12-22 km			

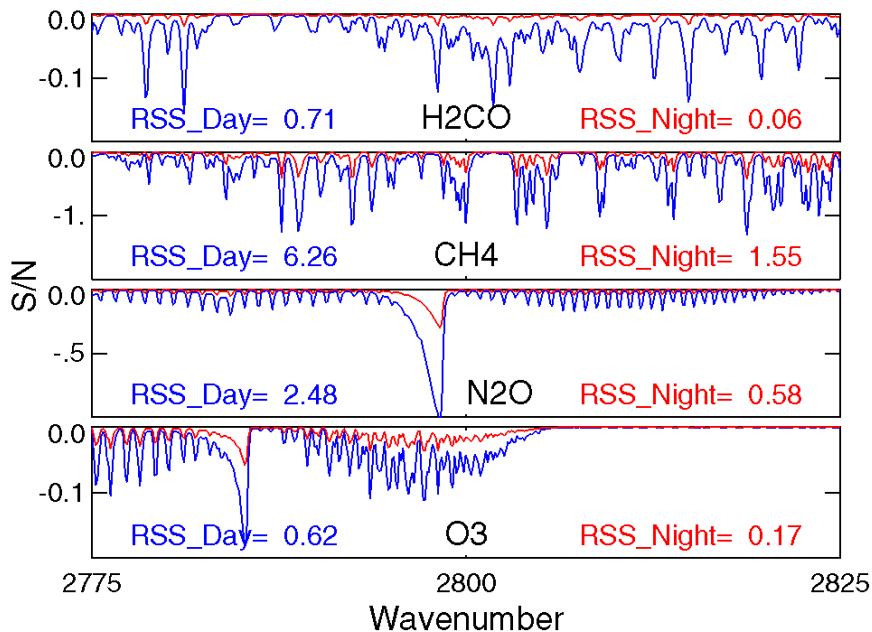
Note: Cases with no entry reflect that we were not able to finish the calculations prior to attending the 21 to 23 Feb 06 Workshop

SWIR region (~ 3571 nm) for HCHO column

Instrument NEdN, temperature uncertainty NETU and the Rss_NEdN



Day and night spectral radiance changes per 1K or 1% change in surface params or column, &/or for HCHO, CH₄, N₂O & O₃



LEA results for column for daytime case

Geophysical parameter	Retrieval precision %	A _{II}	Rss_SNR
HCHO column	1.92	0.994	0.71
CH ₄ column	0.27	0.999	6.26
N ₂ O column	0.42	0.999	2.48
O ₃ column	1.86	0.994	0.62
Surface temp	.11K	.999	91.3
albedo	0.44	0.997	19.47

LEA results for column for nighttime case

Geophysical parameter	Retrieval precision %	A _{II}	Rss_SNR
HCHO column	14.27	0.6723	0.06
CH ₄ column	0.63	0.999	1.55
N ₂ O column	1.52	0.996	0.58
O ₃ column	5.67	0.948	0.17

Summary of LEA for CO, O₃, HCHO and secondary species (1 of 2)

Geophysical parameter	Retrieval precision %		A _{II}		spectral region(s)
	day	night	day	night	
CO column	1.2		0.999		VSWIR
CO partial column (PC) 0-2 km	8.4	24.0	0.89	0.11	VSWIR and MWIR
CO PC 2-6 km	4.3	6.7	0.97	0.93	VSWIR and MWIR
CO PC 6-22 km	2.3	2.5	0.99	0.99	VSWIR and MWIR
O ₃ PC 0 – 11 km		6.1		0.996	MWIR
O ₃ PC 11 – 22 km		1.44		0.979	MWIR
O ₃ PC 0 – 6 km, background		3.7		0.978	LWIR
O ₃ PC 0 – 6 km, polluted		3.1		0.985	LWIR
O ₃ PC 6 – 12 km		1.23		0.997	LWIR
O ₃ PC 12 – 22 km		< 1.0		1.0	LWIR
O ₃ PC 0 – 6 km, background					MWIR and LWIR
O ₃ PC 0 – 6 km, polluted					MWIR and LWIR
O ₃ PC 6 – 12 km					MWIR and LWIR
O ₃ PC 12 – 22 km					MWIR and LWIR
O ₃ total column	1.86	5.67	0.994	0.95	SWIR
HCHO total column	1.92	14.3	0.994	0.67	SWIR
HCHO PC 0 – x km					SWIR
HCHO PC x – 22 km					SWIR
Secondary species					
CH ₄ column	< 1.0		1.0		VSWIR
H ₂ O column	< 1.0		0.999		VSWIR
albedo	<<1.0		1.0		VSWIR
H ₂ O PC 0 – 2 km					VSWIR and MWIR

Note: Cases with no entry reflect that we were not able to finish the calculations prior to attending the 21 to 23 Feb 06 Workshop

Summary of LEA for CO, O₃, HCHO and secondary species (2of 2)

Geophysical parameter	Retrieval precision %		A _{II}		spectral region(s)
	day	night	day	night	
Secondary species continued					
CH ₄ column	< 1.0	< 1.0	0.999	0.999	SWIR
N ₂ O column	< 1.0	1.52	0.999	0.996	SWIR
CH ₄ PC 0 – x km					SWIR
CH ₄ PC x – 22 km					SWIR
N ₂ O PC 0 – x km					SWIR
N ₂ O PC x – 22 km					SWIR
Surface temp					SWIR
albedo					SWIR
Surface temp					MWIR
emissivity					MWIR
Surface temp					LWIR
emissivity		0.067 ?		1.00	LWIR

Models for CO, O₃, HCHO

