More Spectroscopy Than You Ever Hoped to Hear About

Tony Clough

Advanced High Spectral Resolution Infrared Observations
EUMETSAT
16 September 2008

Collaborators

- **Water Vapor Line Parameters**
  - **Laurent Coudert**
  - **Jean-Marie Flaud**
  - **Linda Brown**
  - **Bob Gamache**

- **Carbon Dioxide Line Parameters**
  - **Jean-Michel Hartmann**
  - **Niro**
  - **Tashkun**
  - **Jean-Marie Flaud**

LBLRTM Considerations

- **LBLRTM Issues**
  - **Changing water in a layer > changes layer boundary altitudes > changes level temperatures**
    - **Simultaneous temperature and water vapor retrievals are effected**
    - **Fix boundary altitudes on input (hydrostatic equation not satisfied)**
  - **AJ: self broadening of water vapor lines is not treated**
  - **Upwelling Radiance Calculations: Currently NO capability to include downwelling radiance at upper boundary**
    - **Not a problem for TOA**
    - **Problem for HIS, e.g. ozone**
    - **Problem for AJ**

What is ‘Truth’?

- **Spectral Residuals are Key!**

- **Consistency within a band system** ← ?
  - ν_2 band to investigate consistency for H_2O

- **Consistency between bands**
  - IASI ν_2 and ν_3 bands to investigate consistency for CO_2

- **Consistency between species**
  - TES: temperature from O_3 and H_2O consistent with CO_2 ; N_2O

- **Consistency between instruments**
  - IASI
  - AIRS
  - ACE
  - TES
  - MIPAS
  - SHIS
  - NAST-I
  - AERI

Temperature Retrievals

- **Carbon Dioxide**
  - **Niro et al. Line Coupling- implications for co2 continuum**
    - **Accuracy of collision rates**
    - **Limitations of impact approximation**
    - **Significant impact on our understanding of absorption far from band center**
  - **Chi factor- duration of collision effects**
  - **Line intensities- MIPAS line strengths**
    - **Tashkun, Teffo, Flaud et al.**
  - **H_2O broadening of CO_2**

CO_2 Line Coupling : Effect on Spectra

- **Line Parameters:**
  - Niro, F., K. Jucks, J.-M. Hartmann, Spectra calculations in central and wing regions of CO2 IR bands. IV : Software and database for the computation of atmospheric spectra: J Quant Spectrosc Radiat Transfer., 95, 469-481.
  - P, Q, & R line coupling for bands of importance
  - Niro et al. code modified to generate first order line coupling coefficients, y_i.
  - Works in regular line by line mode with LBLRTM
  - Temperatures: 4

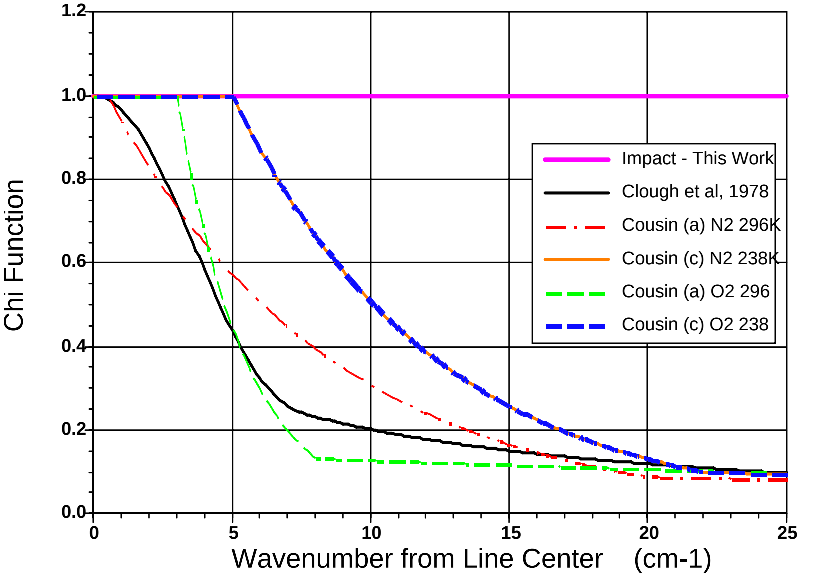
- **Line Shape:**
  - Impact Approximation
  - Duration of collision effects under study

- **Continuum:**
  - χ Factor
  - Sampled 2 cm^{-1}
  - New definition required
  - Temperature dependence ??

Chi Factor

Line Coupling Duration of Collision

Clough Burch/Benedict based on 3 band



Line Coupling

Lorentz (Impact)

$$k_i(\nu) = \frac{1}{\pi}\frac{S_i}{(\nu-\nu_i)^2+\alpha_i^2}\left[\alpha_i + y_i(\nu-\nu_i)\right]$$

Line coupling coefficient: y_i

$$k(\nu) = \sum_i \frac{1}{\pi}\frac{S_i\,\alpha_i}{(\nu-\nu_i)^2+\alpha_i^2} + \sum_i \frac{1}{\pi}\frac{S_i\left[y_i(\nu-\nu_i)\right]}{(\nu-\nu_i)^2+\alpha_i^2}$$

$$\textit{far from line center}: (\nu-\nu_i) >> \alpha_i \qquad \textbf{\textit{e.g. continuum}}$$

$$= \sum_i \frac{1}{\pi}\frac{S_i\,\alpha_i}{(\nu-\nu_i)^2} + \sum_i \frac{1}{\pi}\frac{S_i\left[y_i(\nu-\nu_i)\right]}{(\nu-\nu_i)^2}$$

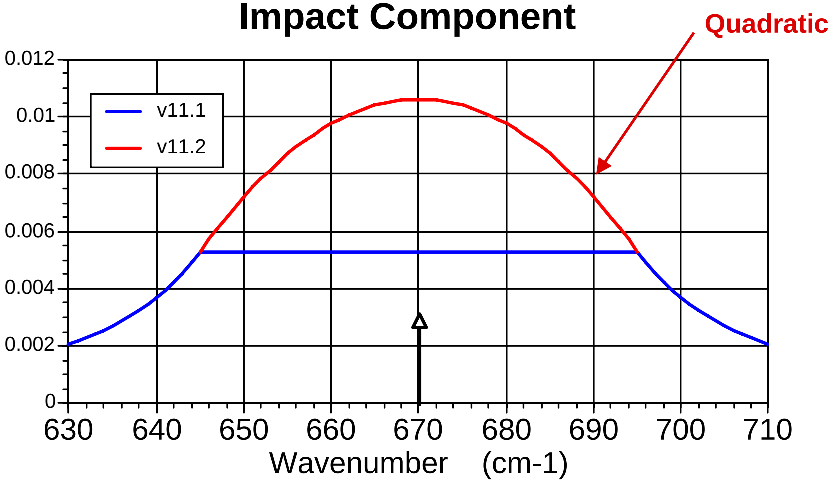
$$\textit{let} \qquad \nu_i = \nu_o + \delta_i \qquad \textit{far from band center with} \quad (\nu-\nu_o) >> \delta_i$$

$$= \frac{1}{\pi}\frac{1}{(\nu-\nu_o)^2}\sum_i S_i\,\alpha_i + \frac{1}{\pi}\frac{1}{(\nu-\nu_o)^2}\sum_i S_i\,y_i\,\delta_i$$

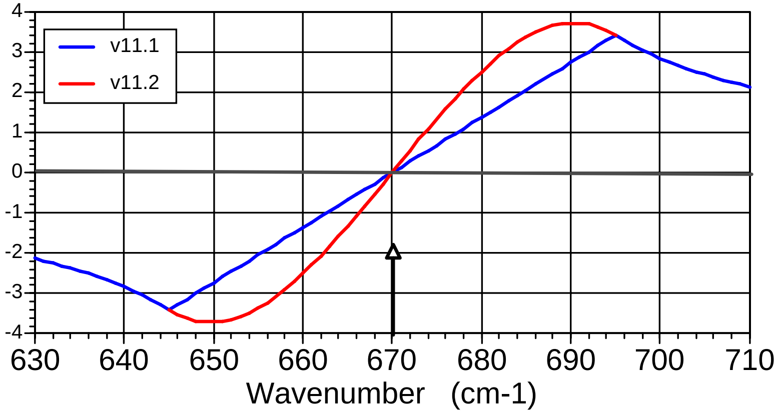
New Definition for Continuum Function

Single Line

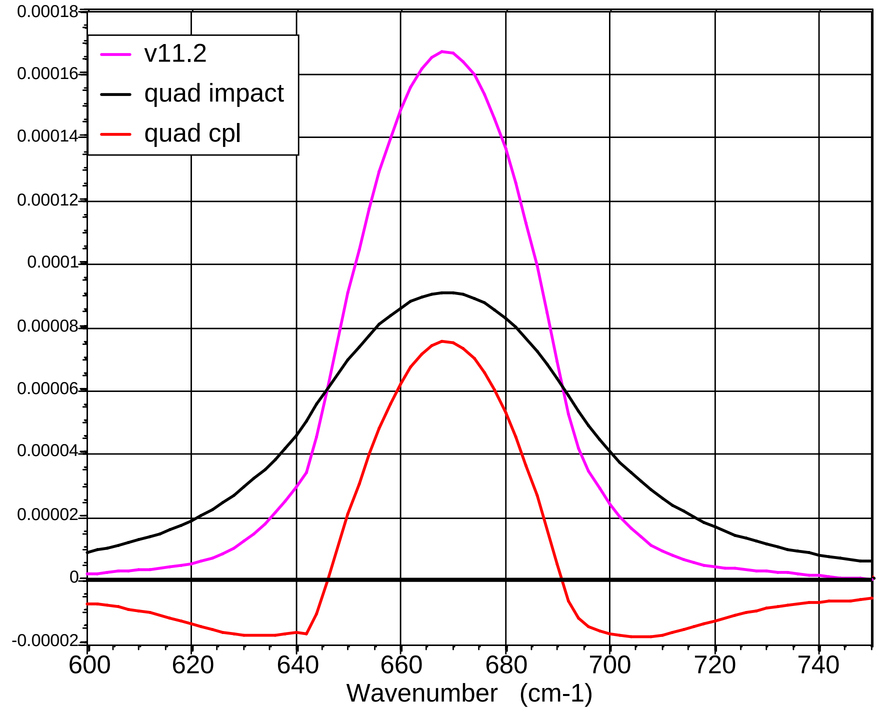
Impact Component



Line Couple Component



Q-Branch

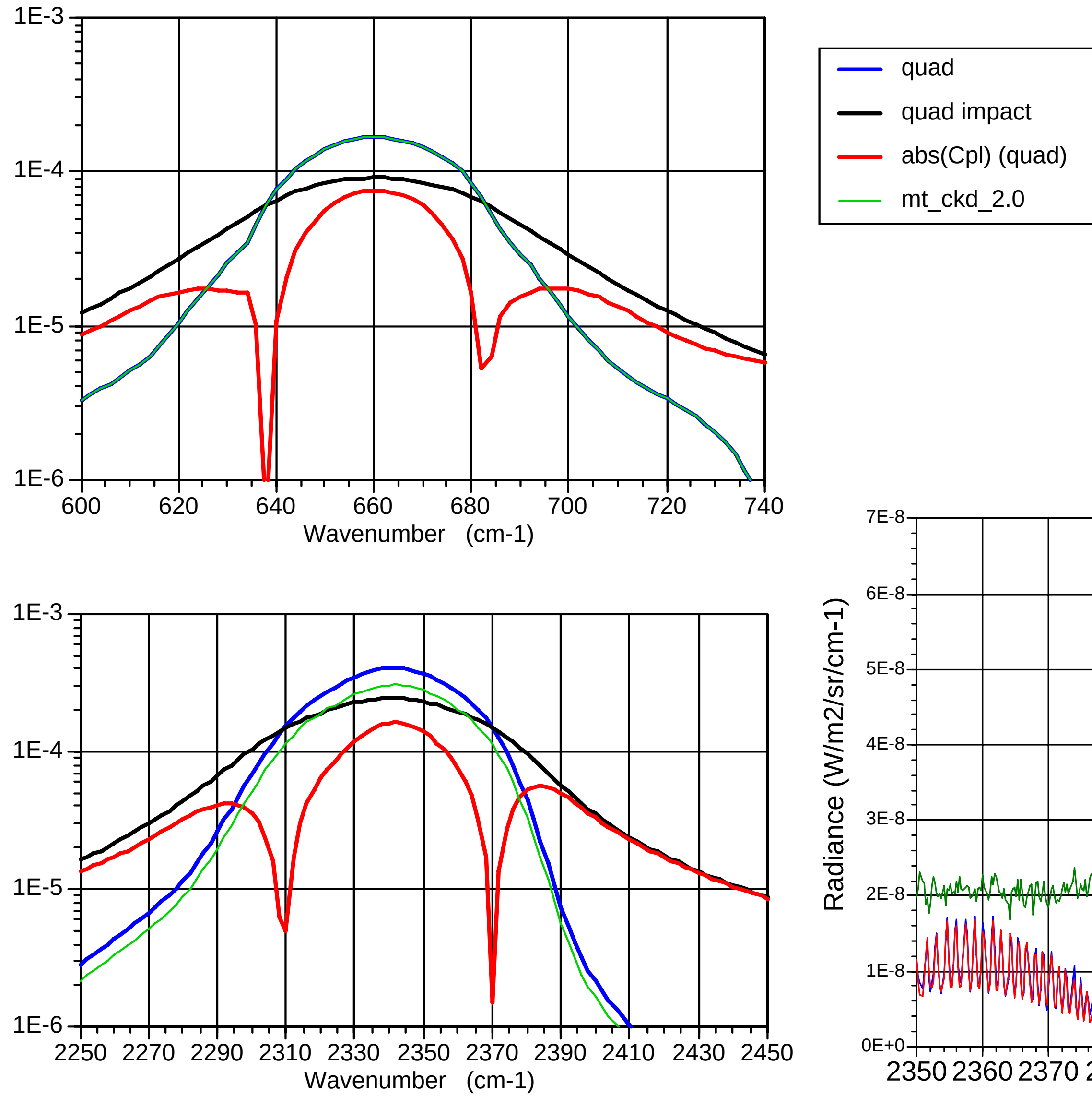


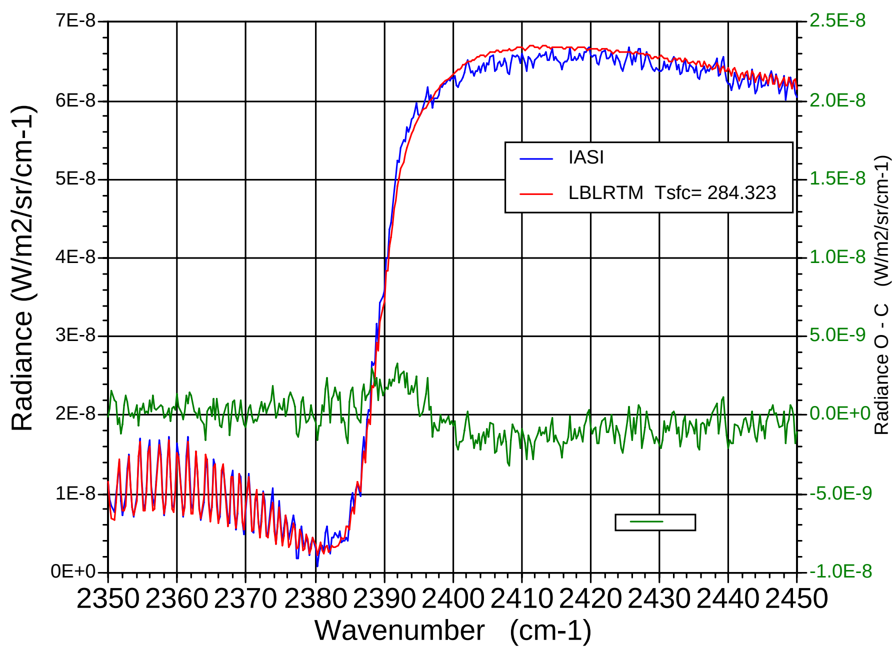
CO2 Continuum

Symmetrized Power Spectral Density Function

ν_2

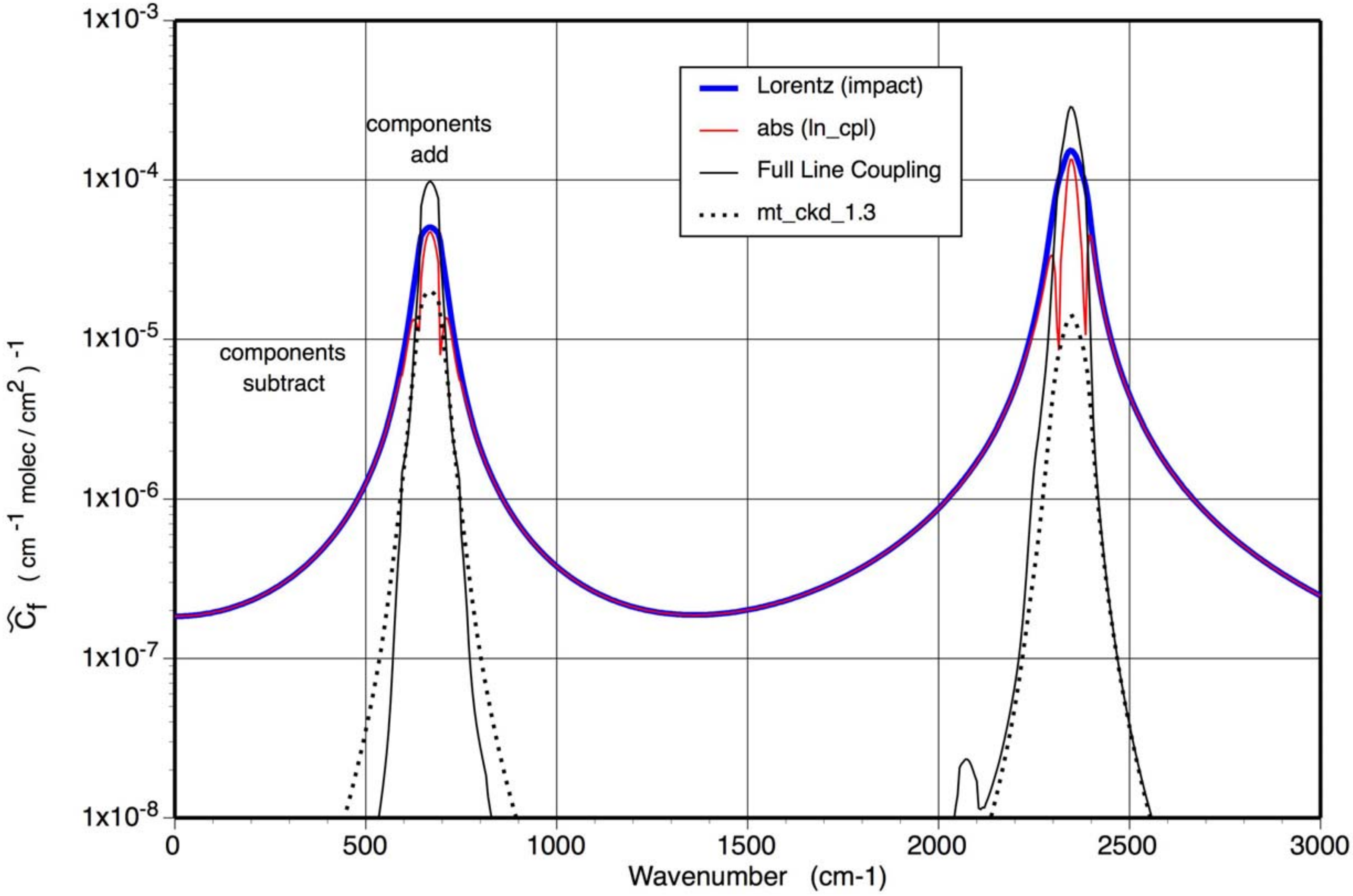
ν_3





CO2 Continuum

Symmetrized Power Spectral Density Function



Introduction

IASI

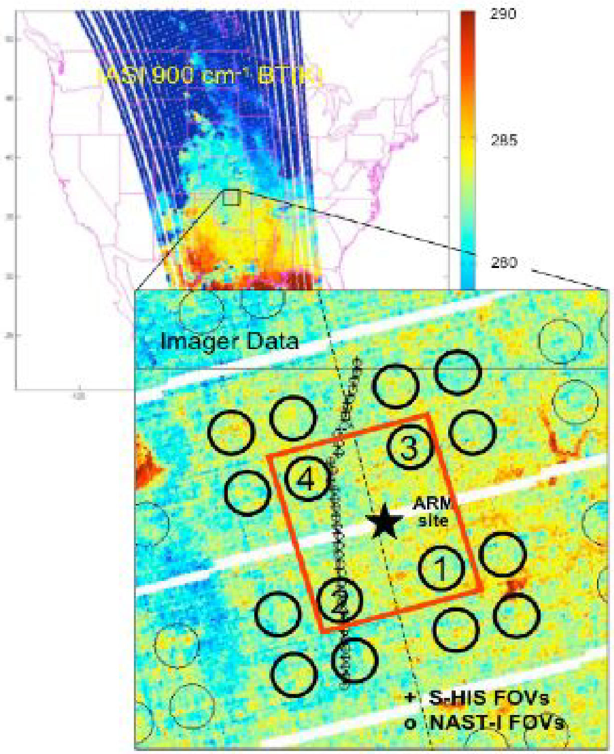
Scan Rate	8 secs
Scan Type	Step and dwell
Pixel IFOV	0.8225°
IFOV size at Nadir	**12 km**
Sampling at Nadir	18 km
Earth View Pixels / Scan	2 rows of 60 pixels each
Swath	± 48.98°
Swath	± 1066 km
Spectral Range	645 to 2760 cm-1
Resolution (hw/hh)	**0.25 cm-1**
Lifetime	5 years
Power	210 W
Size	1.2 m x 1.1 m x 1.3 m
Mass	236 kg
Data rate	1.5 Mbps
Radiometric Calibration	**< 0.1 K**

- **The IASI programme is led by**
- **Centre National d'Études Spatiales (CNES) in association with EUMETSAT.**
- **Alcatel Alenia Space is the instrument Prime Contractor.**

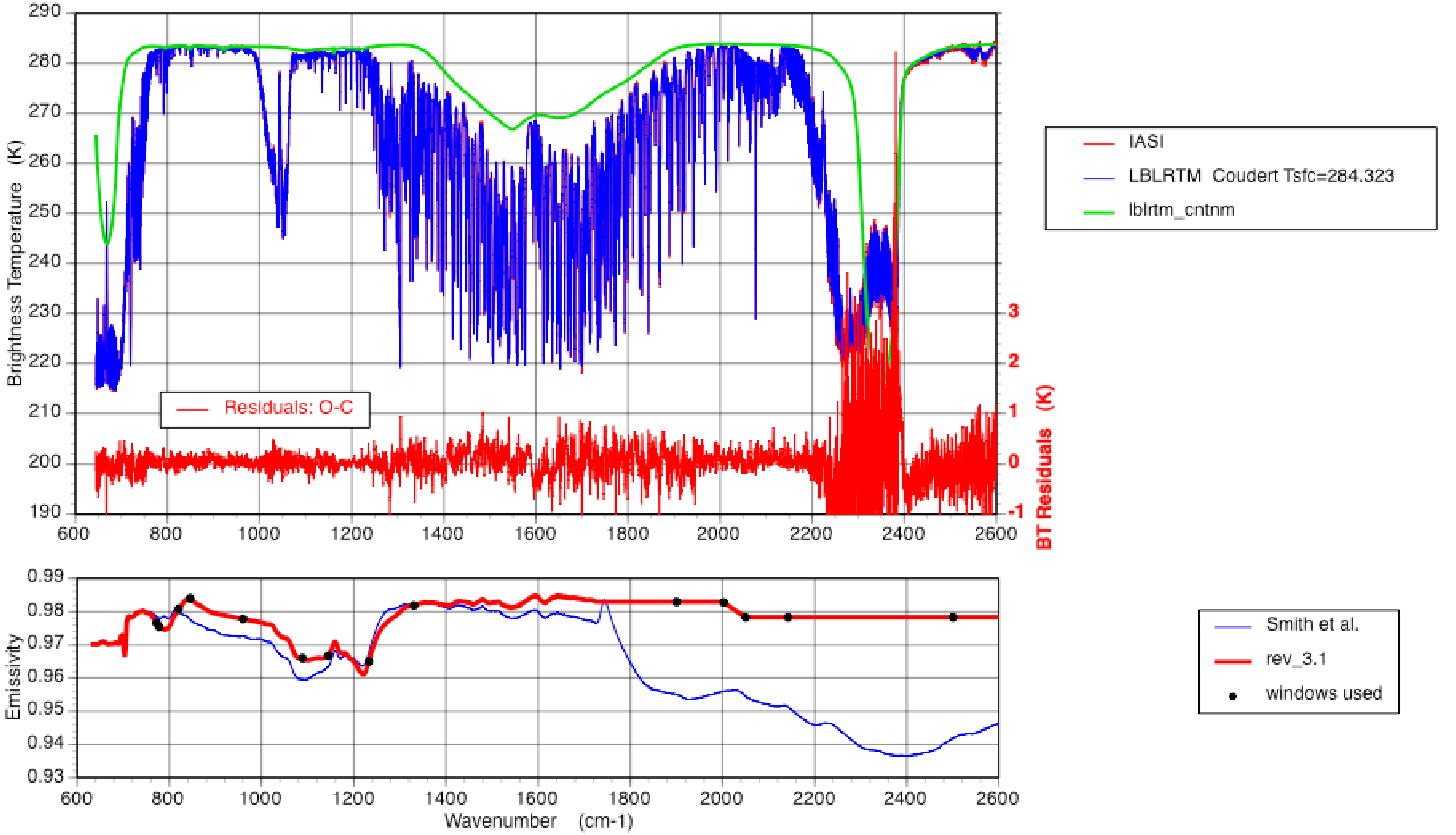
Joint Airborne IASI Validation Experiment

JAIVEx 19 Apr 2007

CART-site (03:35 UTC)



IASI JAIVEx 19 April

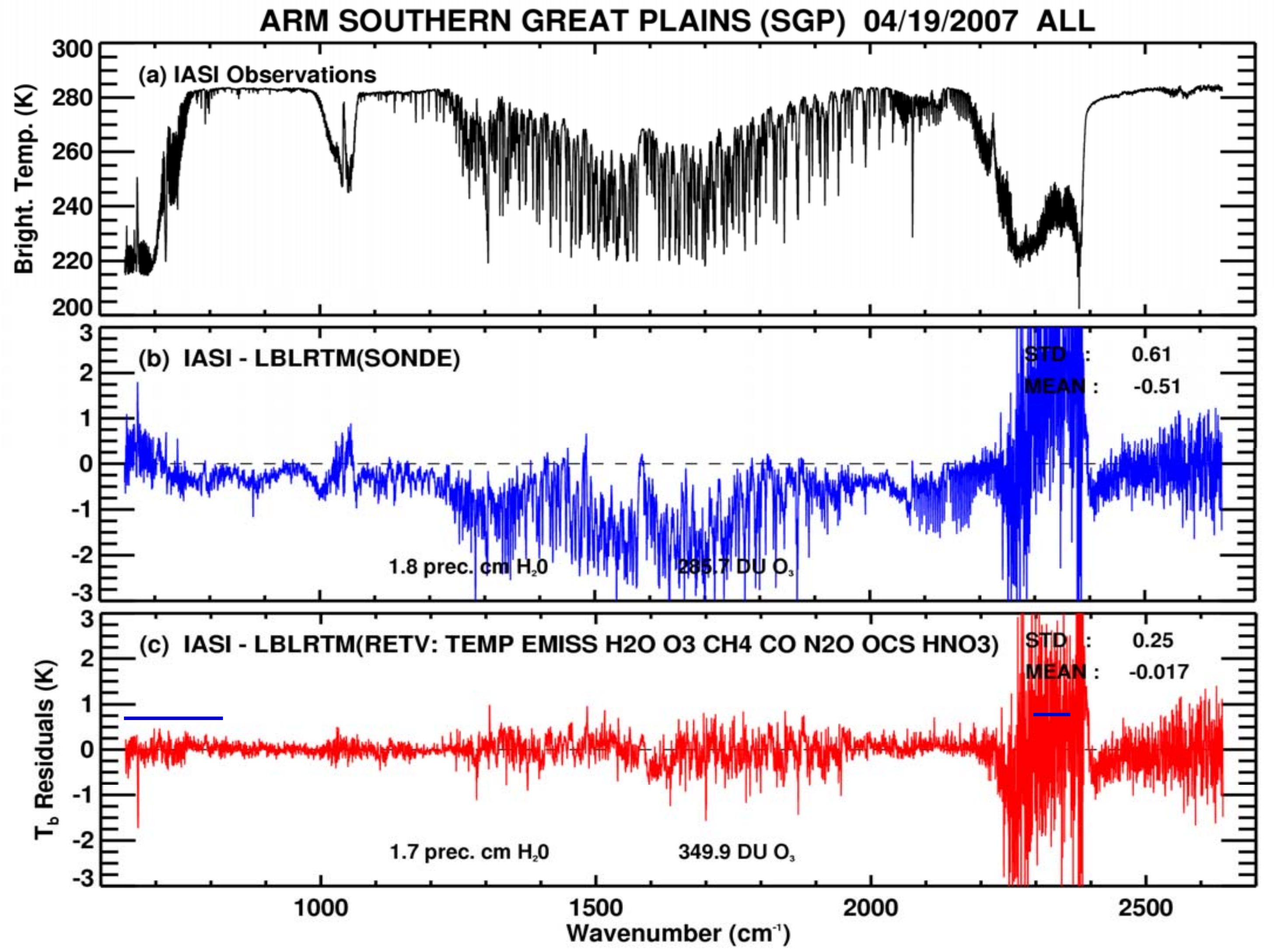


IASI/LBLRTM Validation

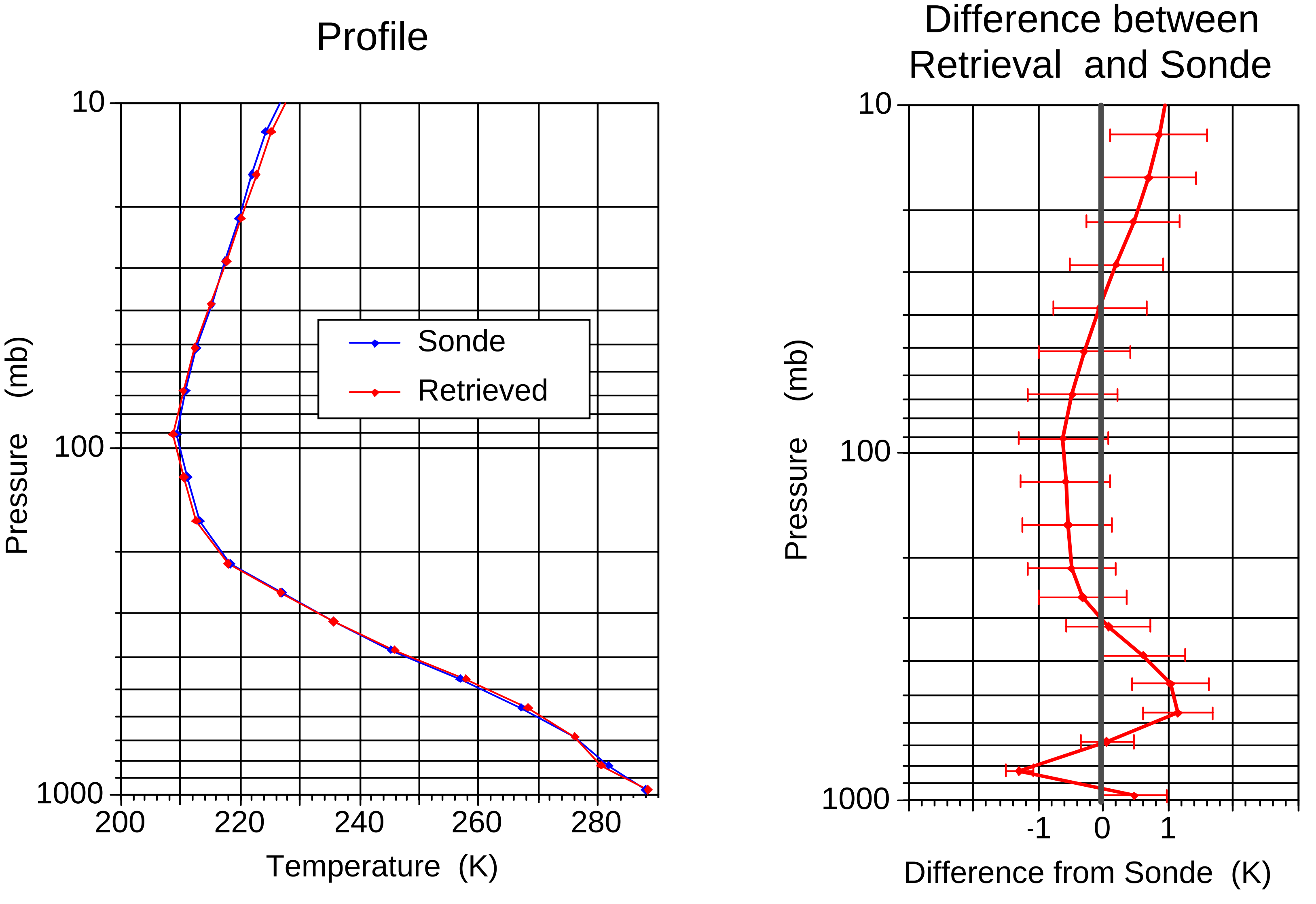
IASI

SONDE

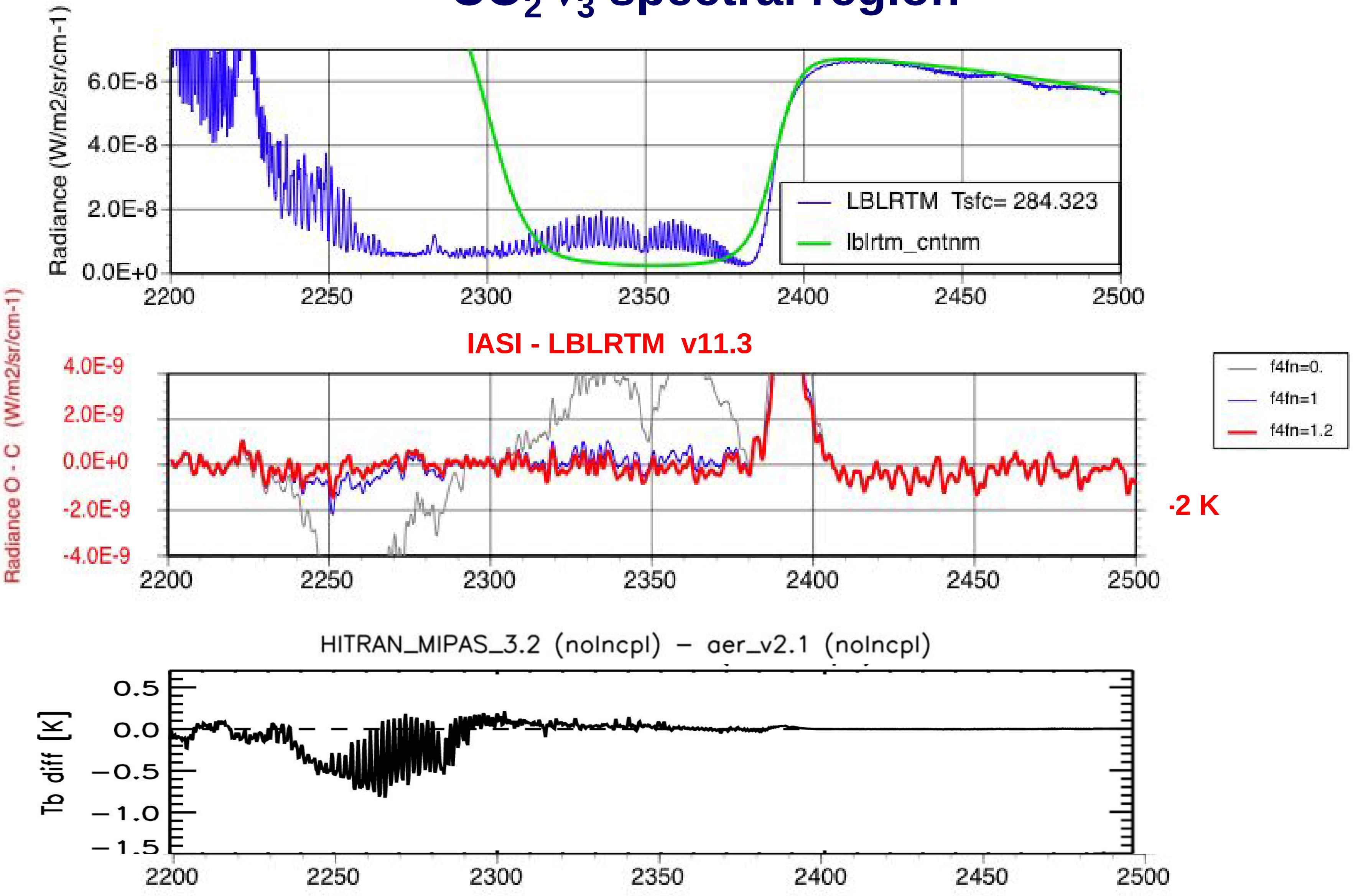
RETV



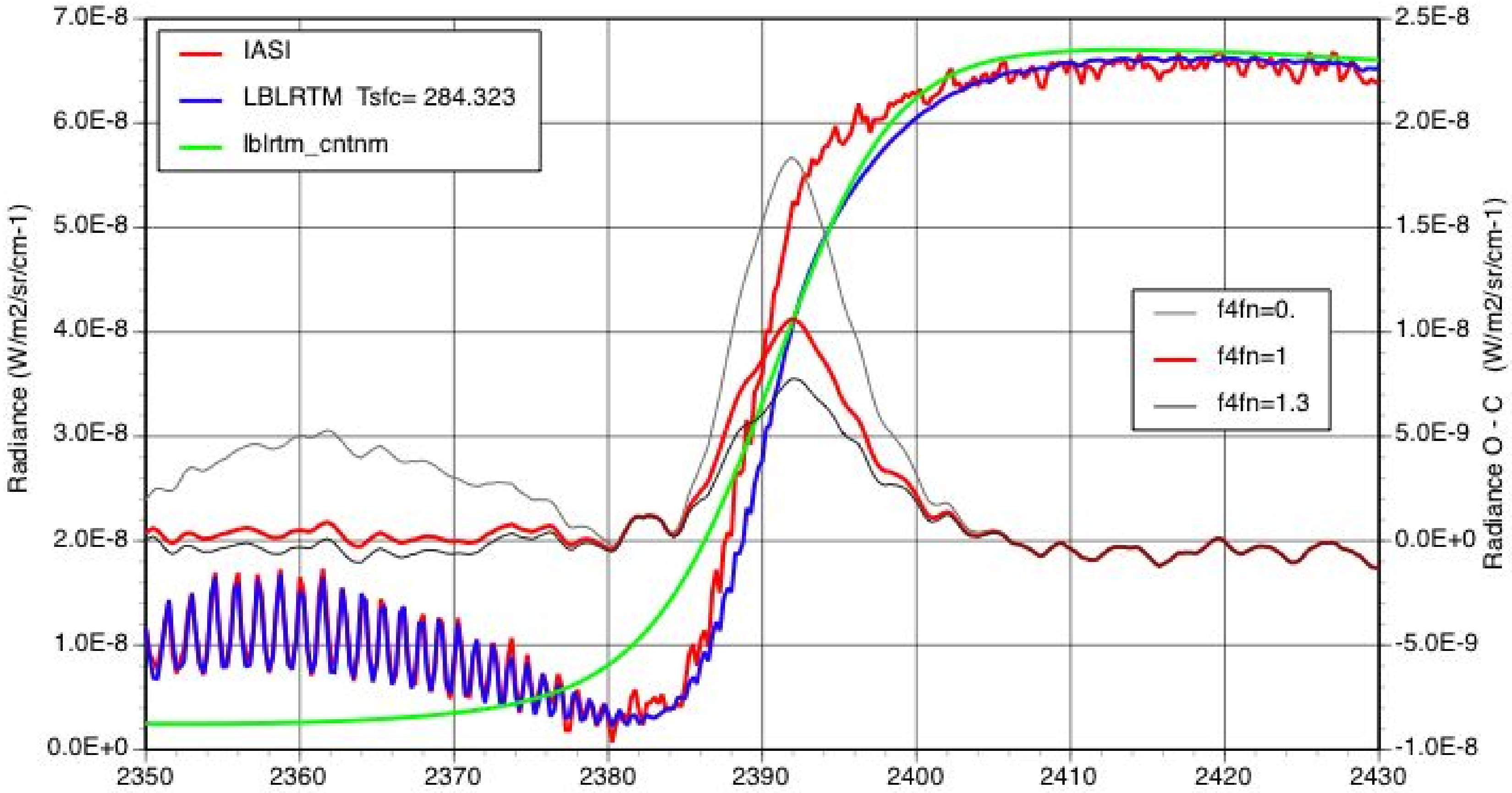
Temperature



CO_2 ν_3 spectral region



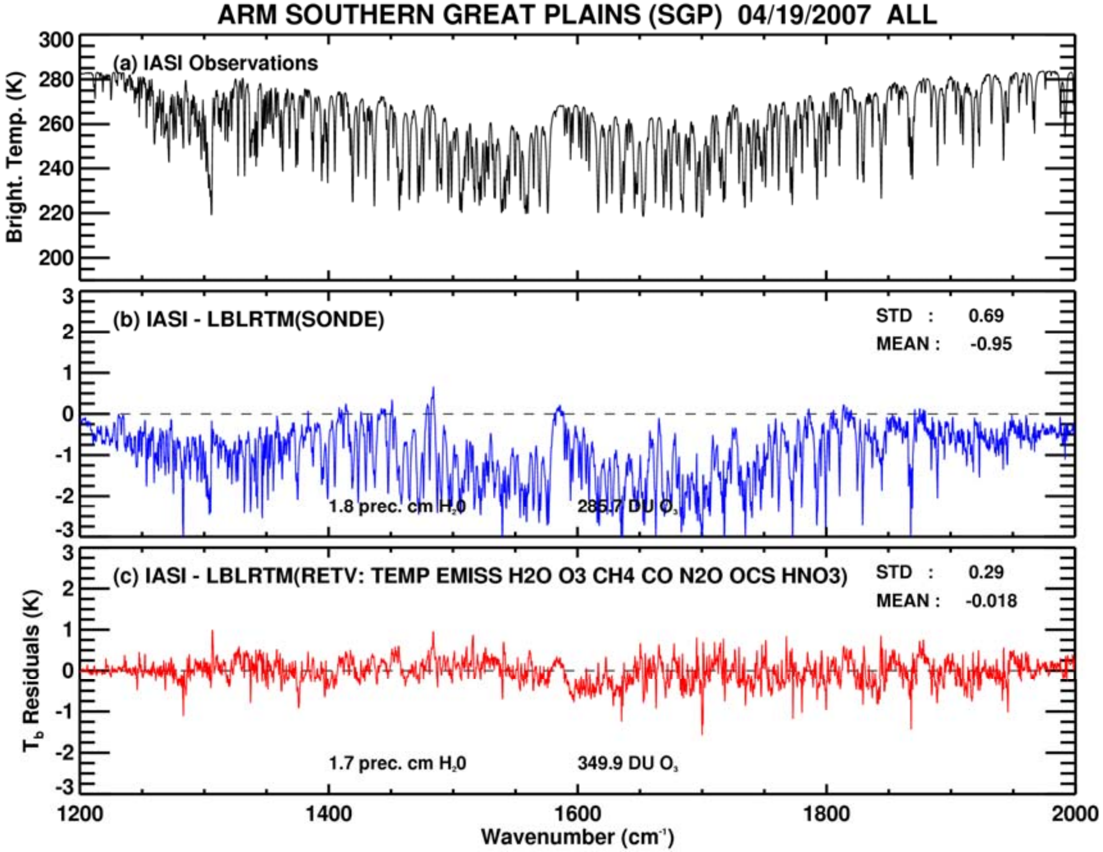
‘Bandhead’ CO_2 ν_3 spectral region

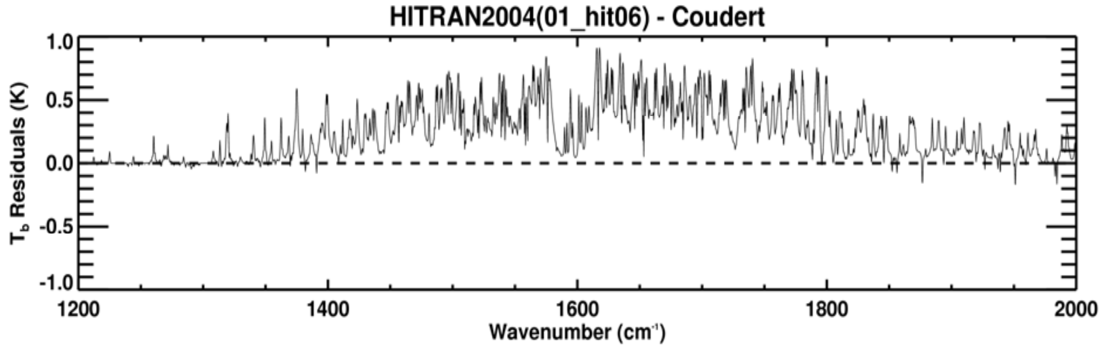


Water Vapor Retrievals

- **Water Vapor**
  - **Variability: Horizontal / Vertical / Time**
  - **Residuals are consistently greater than IASI noise**
  - **Coudert et al. Line Strengths**
  - **Line Widths**
  - **Continuum**
    - **Provides the extra absorption previously provided by the ‘super Lorentzian’ chi factor**
    - **Based on dipole allowed transitions with widths ~ 50 cm-1**
    - **Same line shape is used for every line from the Microwave to UV**
  - **Implications from downwelling spectra at the ARM NSA site.**

Water Vapor ν_2 Region



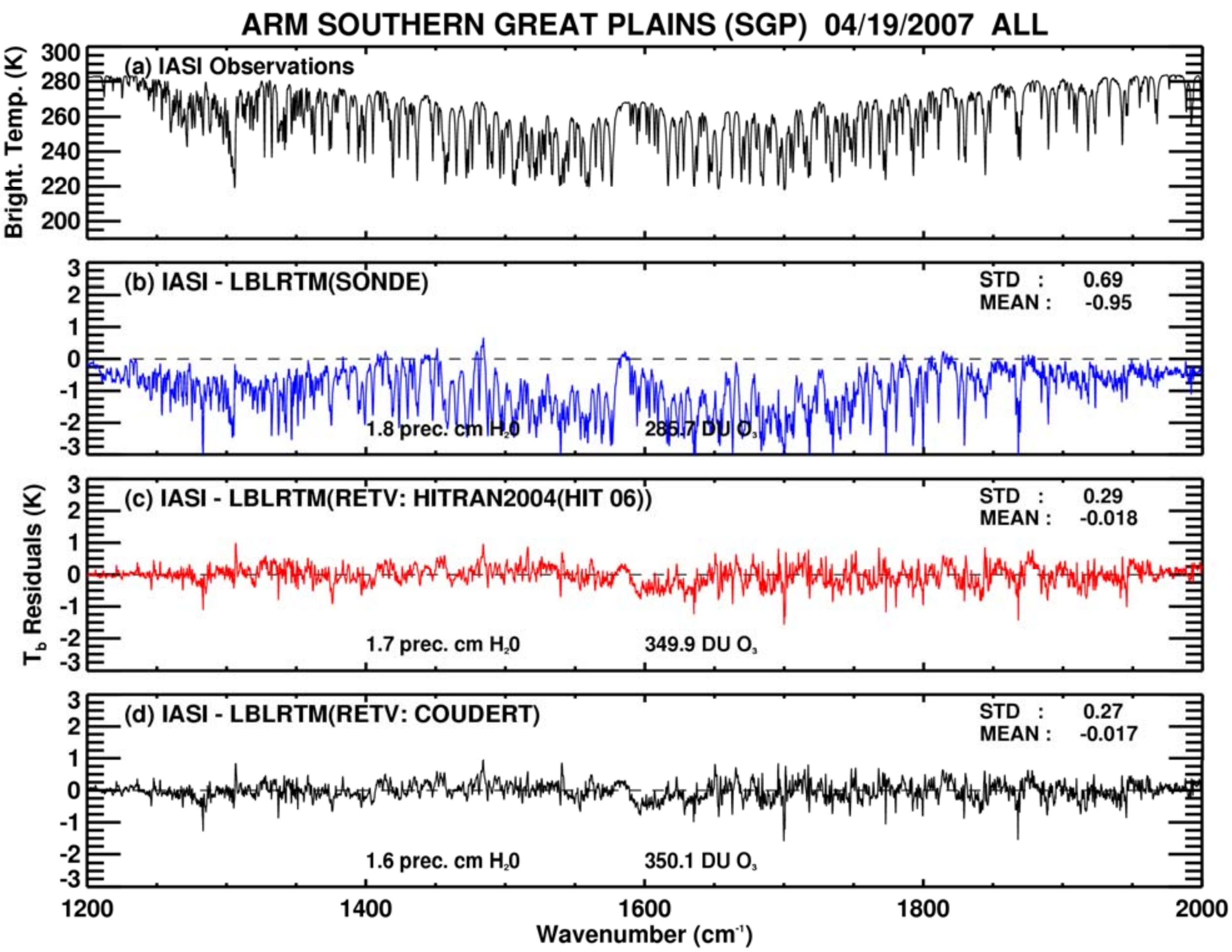


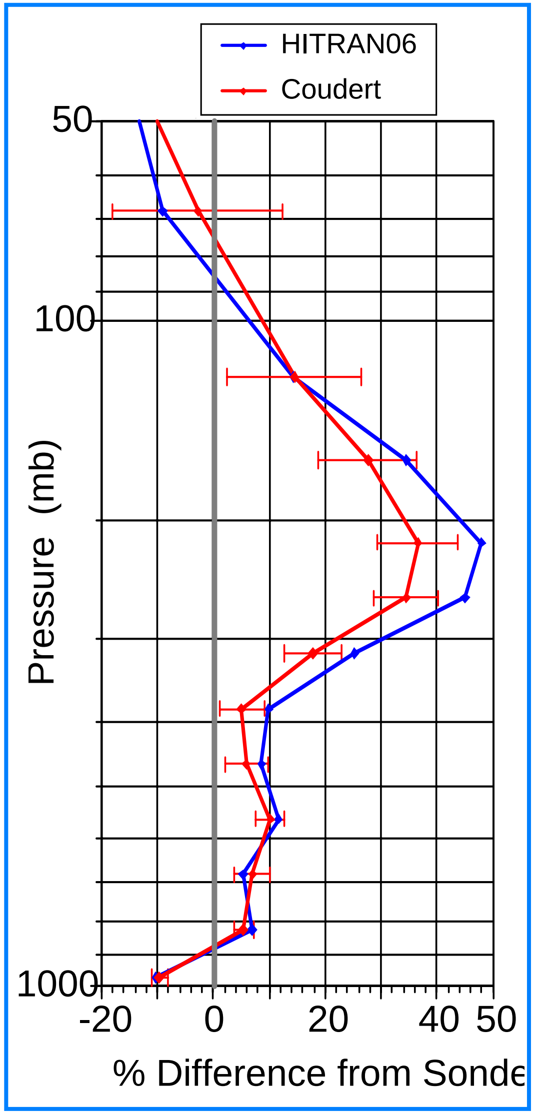
Larger residuals remain:

- **IASI Noise: ~0.15K**
- **Atmospheric state: retrieved**
- **Likely Spectroscopy**

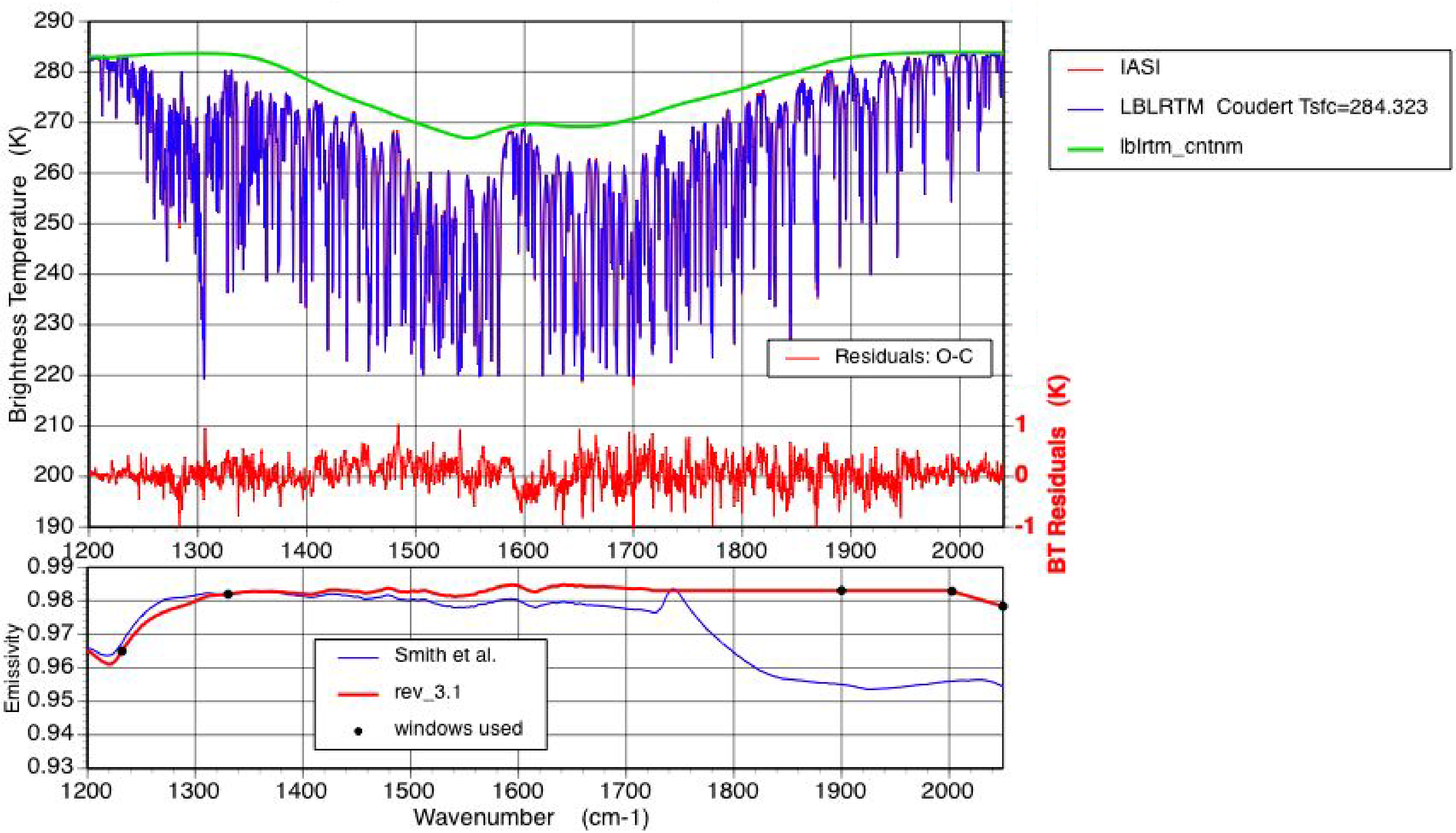
Coudert water vapor intensities?

Water Vapor ν_2 Region : Impact of Coudert Intensities

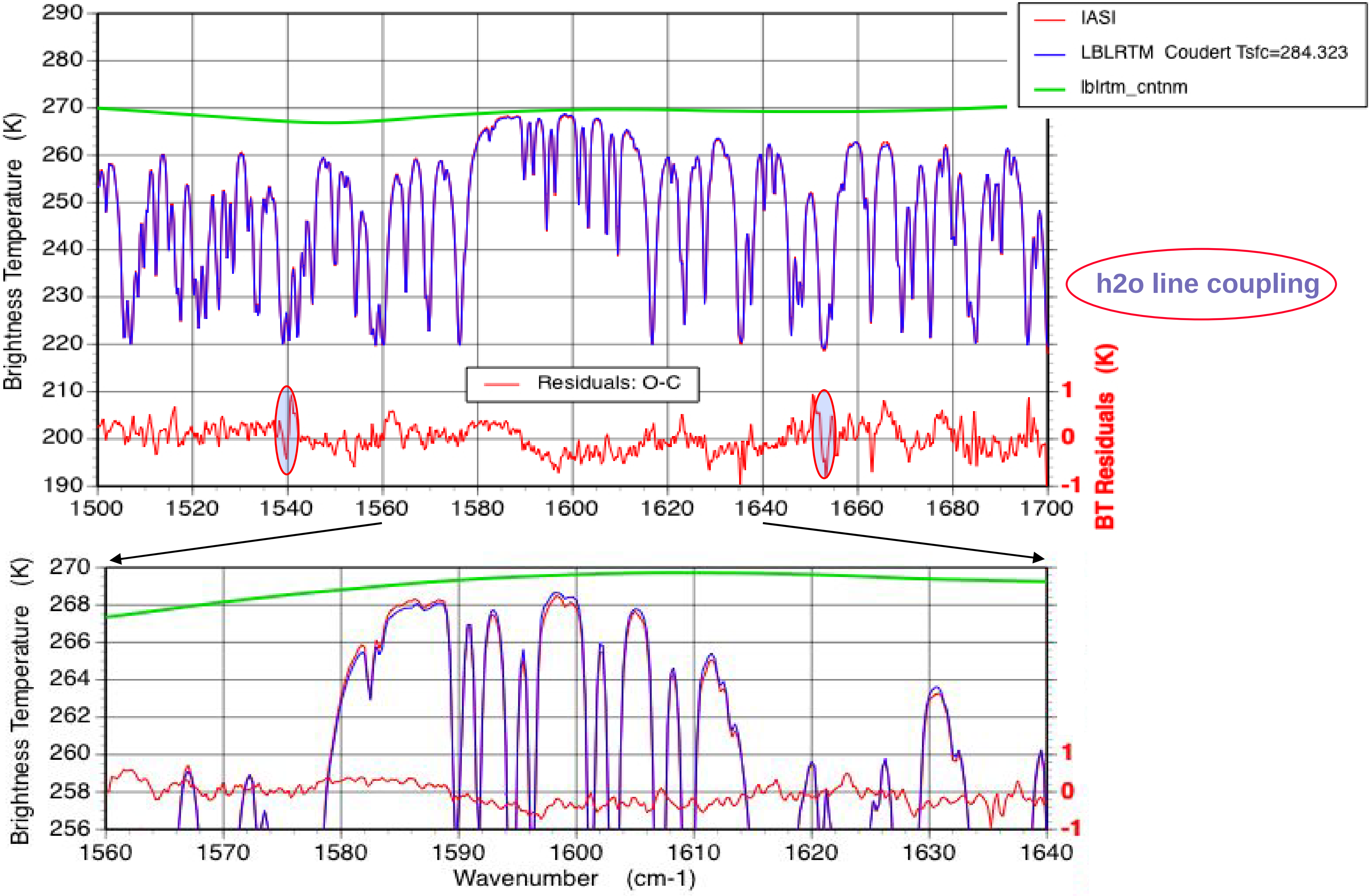




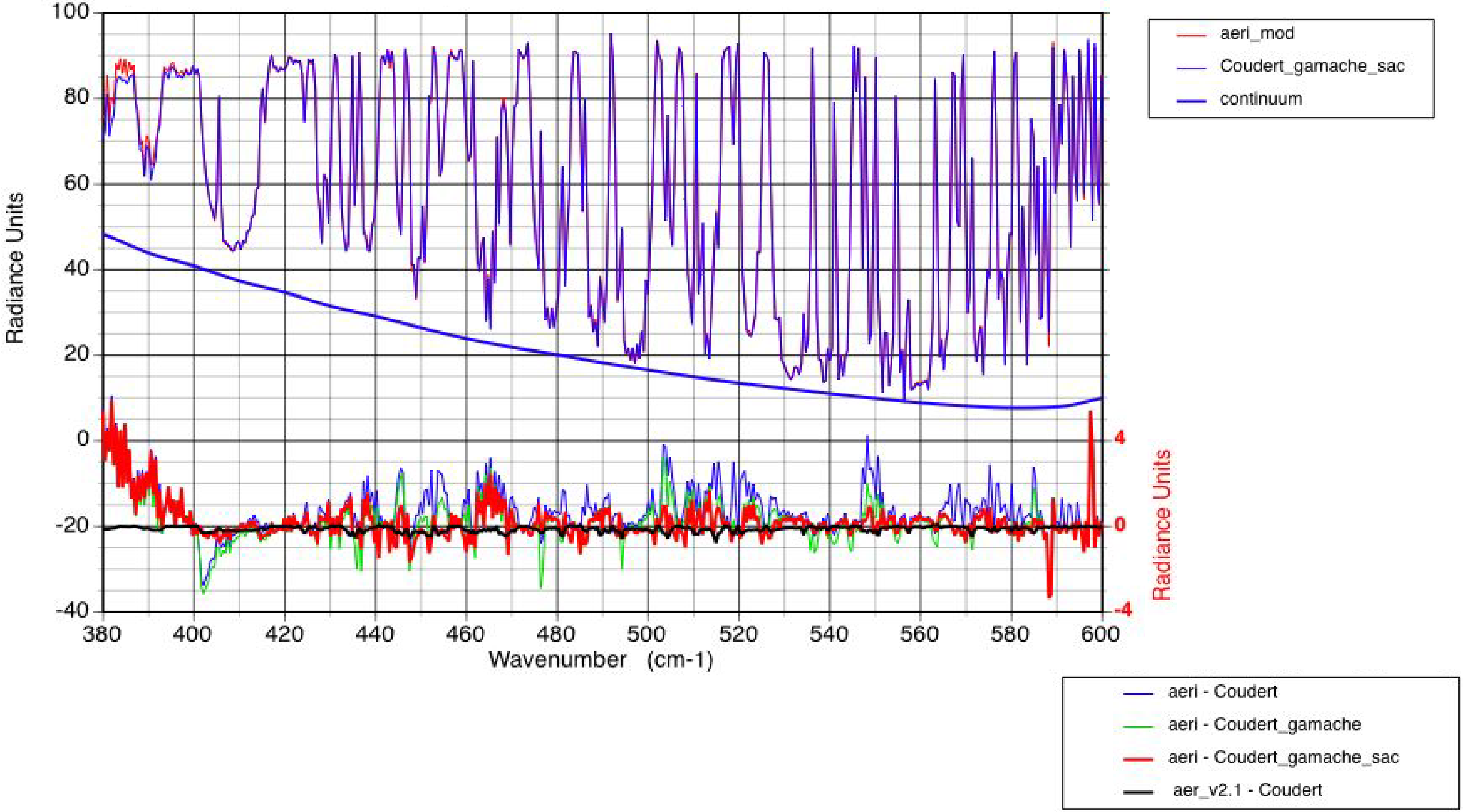
IASI 19 April
Water Vapor



Detail of Band Center



AERI Downwelling Radiances
ARM NSA Site



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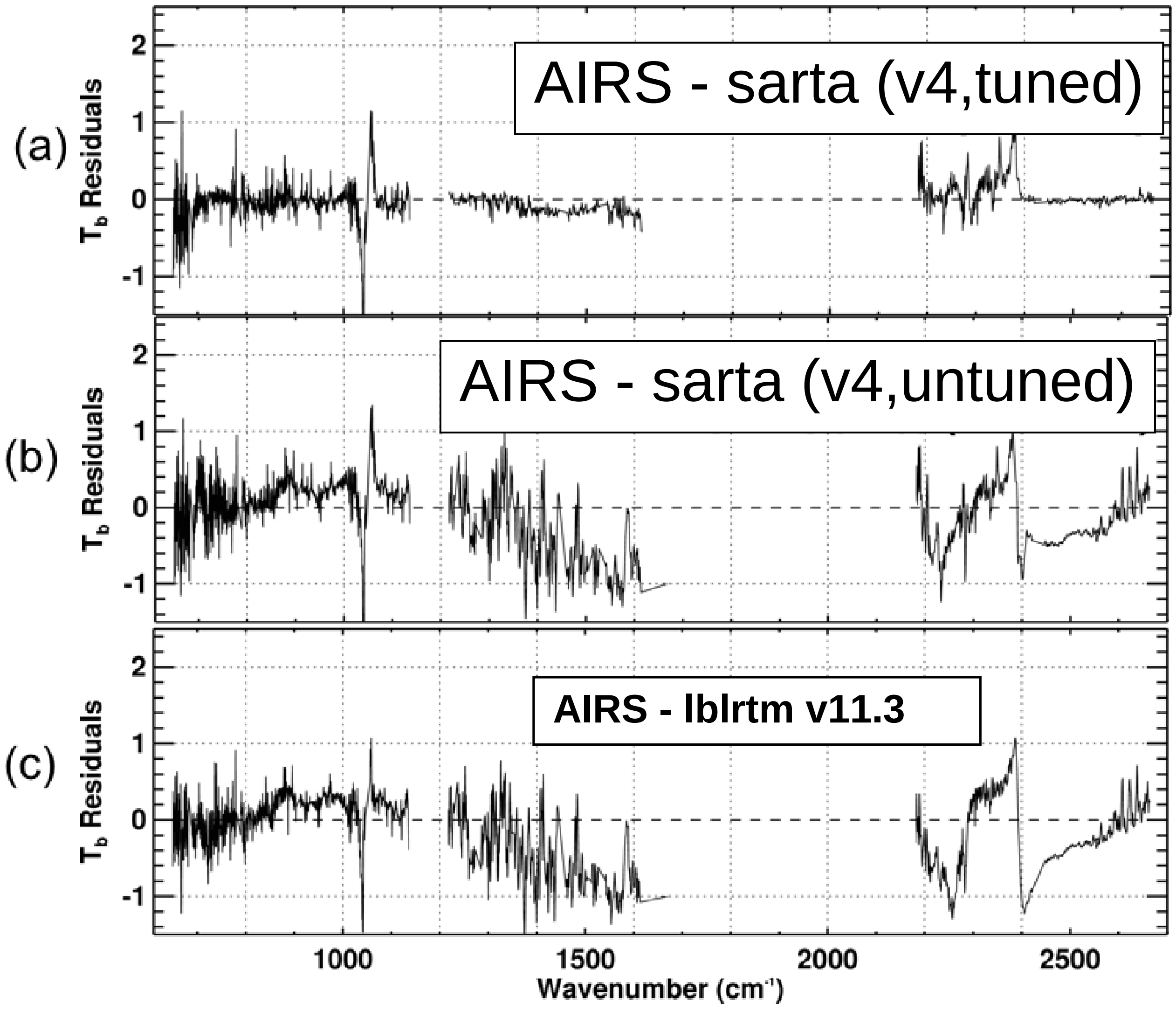
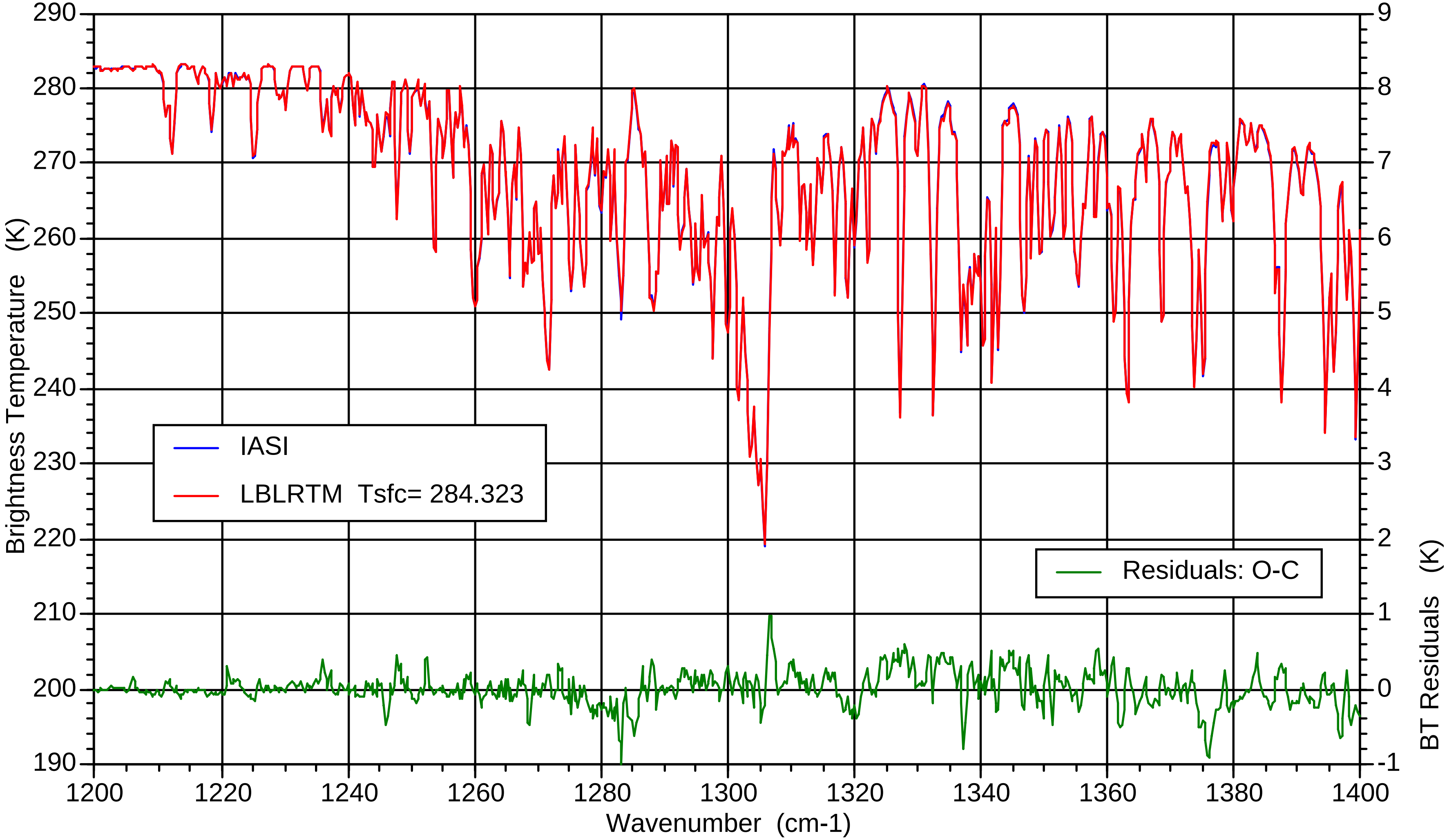


METHANE


290
280
270
260
250
240
230
220
210
200
190
9
8
7
6
5
4
3
2
1
0
-1
Brightness Temperature (K)
BT Residuals (K)
IASI
LBLRTM Tsfc= 284.323
Residuals: O-C
1200
1220
1240
1260
1280
1300
1320
1340
1360
1380
1400
Wavenumber (cm-1)

Summary

- Carbon Dioxide:
  - Line Coupling is the key!
  - Relaxation Matrix needs adjustment

    and/or
  - Duration of Collision Effects need to be included
  - CO_2 Continuum requires modification
  - ν_2 and ν_3 approaching consistency

    Tashkun ν_3 line parameters to be evaluated
  - ν_2 Q-Branch not yet consistent

Summary

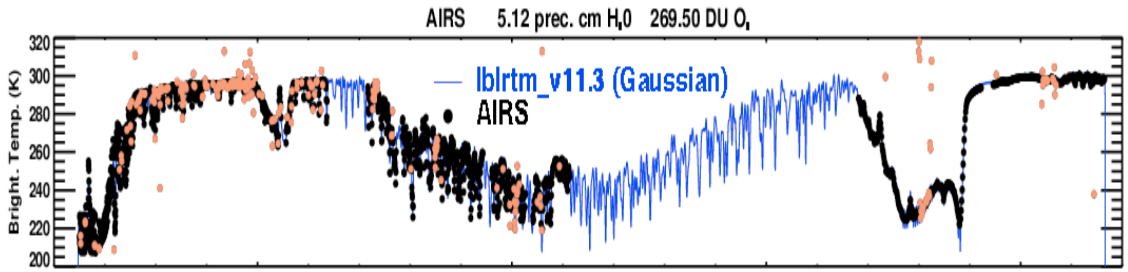
- Water Vapor:
  - Line Intensity Issue
    Coudert Line Parameters being adopted
    Internal consistency is not necessarily conclusive
  - Residuals are too large (much larger than IASI noise)
  - Line Coupling, Widths and Shifts ?
- xx Simultaneous retrieval of Temperature and Water Vapor xx
- Retrievals for other species are generally excellent
- Updated Code and Line Parameters are available
  - Separate Line Coupling file (Hartmann) available: aer_v2.1
- Spectral Residuals are a CRITICAL validation criterion

IASI

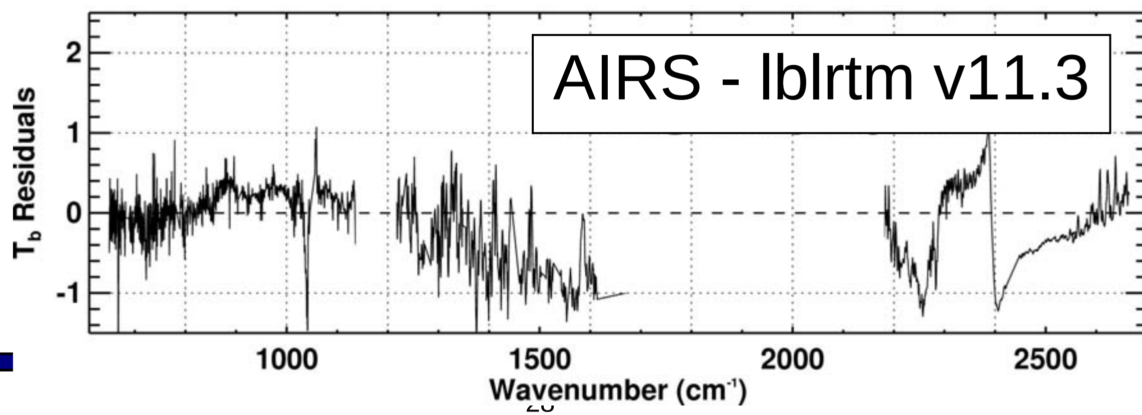
C’est Incroyable !

AIRS/model comparisons

- **Mean residuals for 36 "clear-sky" cases**
  - **ARM TWP Phase 1 AIRS validation**
  - **Layer profiles, AIRS and SARTA radiances supplied by L. Strow and S. Hannon**



Example case

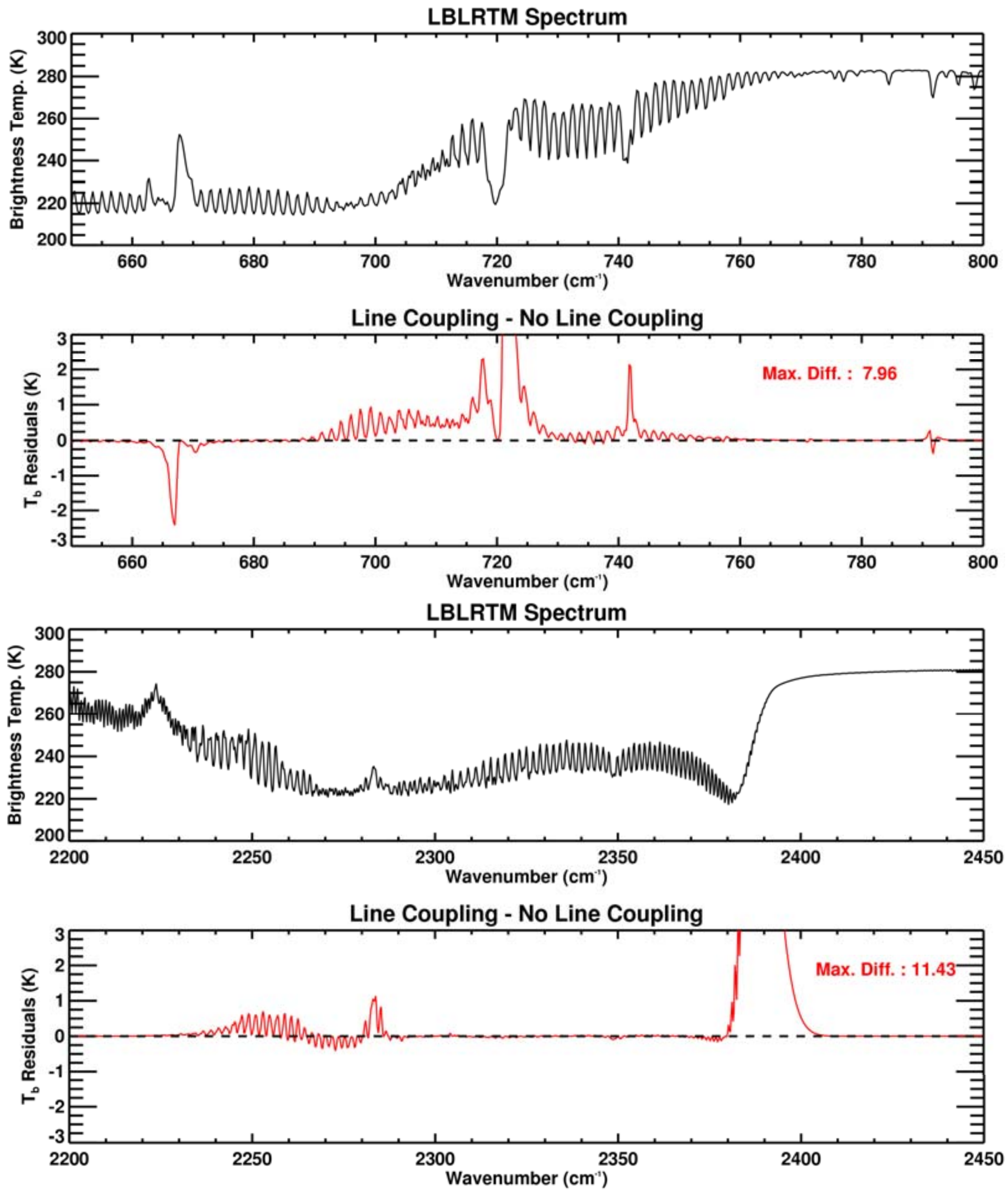


Mean residuals for all "clear-sky" cases

Impact of CO_2 Line Coupling in the Infrared

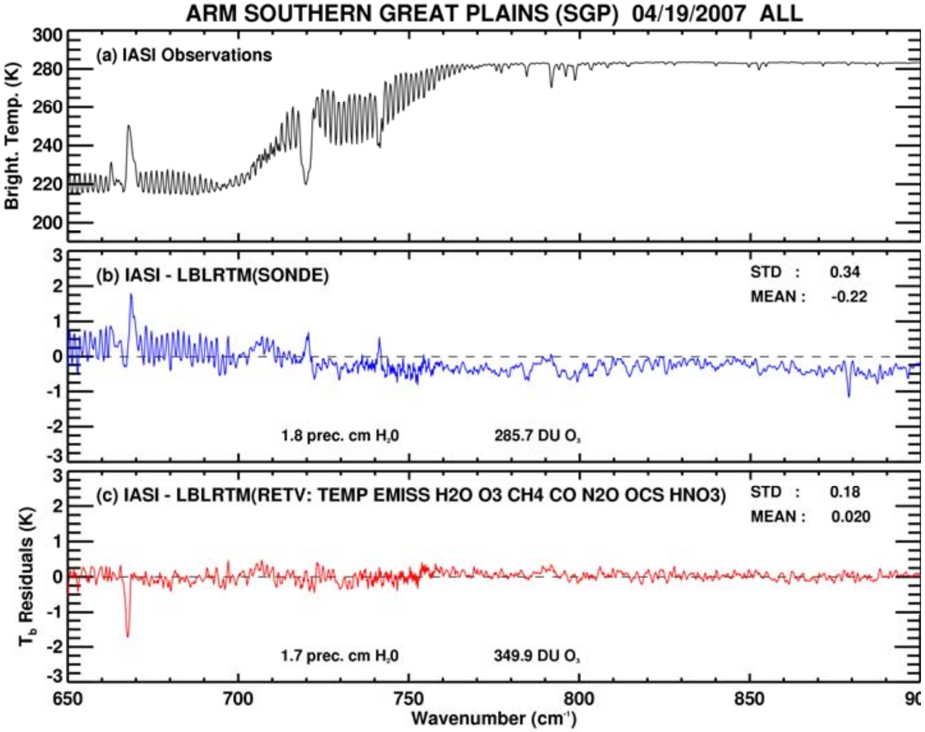
CO_2 v_2

CO_2 v_3

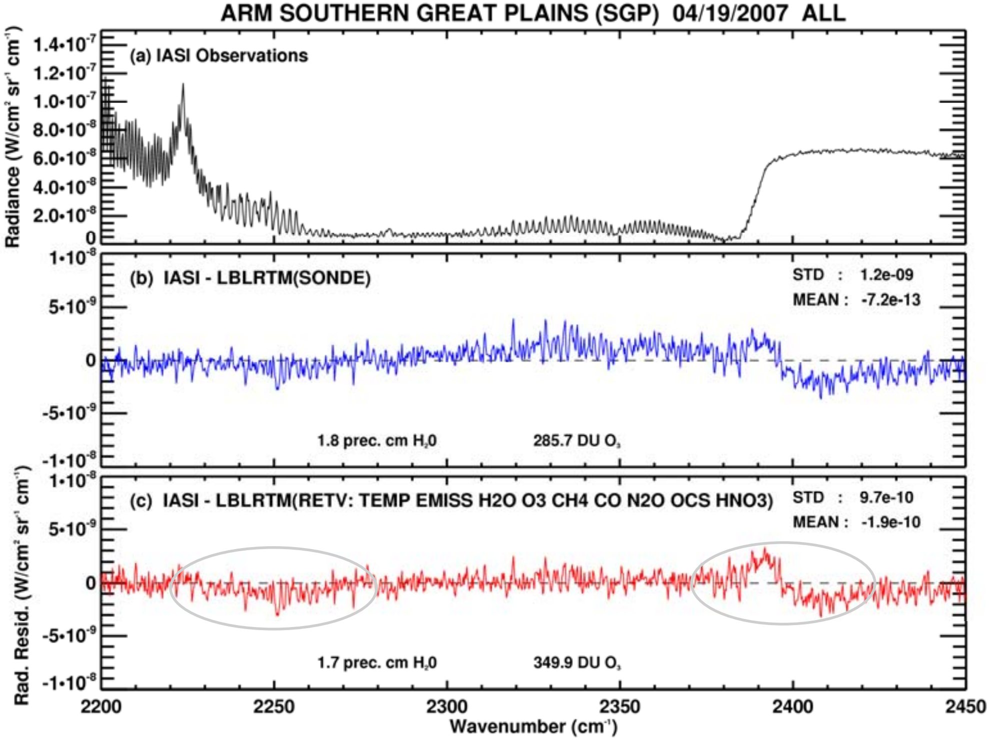


Temperature: CO_2 Spectral Regions

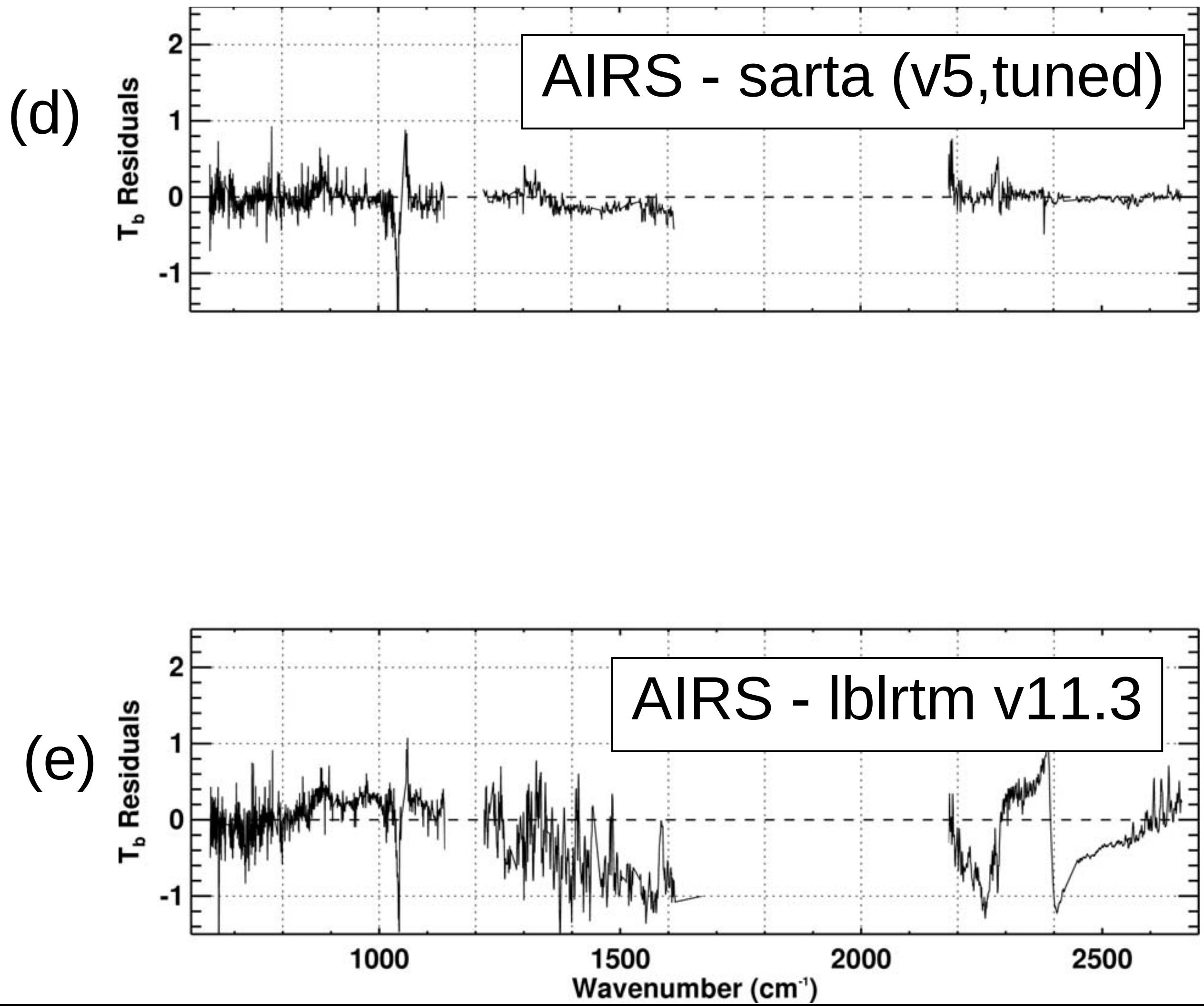
CO_2 v_2



CO_2 v_3

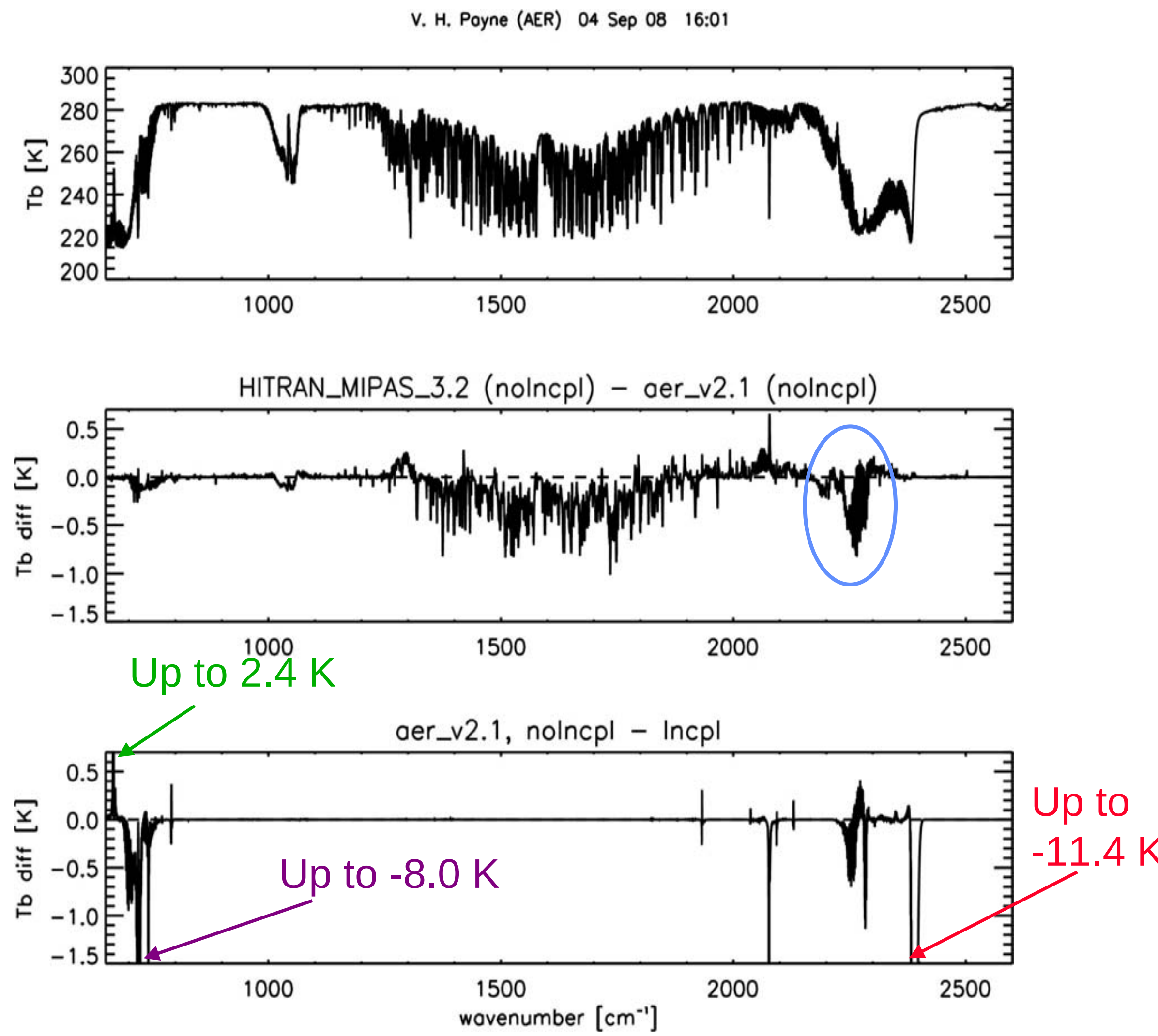


SRF file: srftables_051118v4.hdf



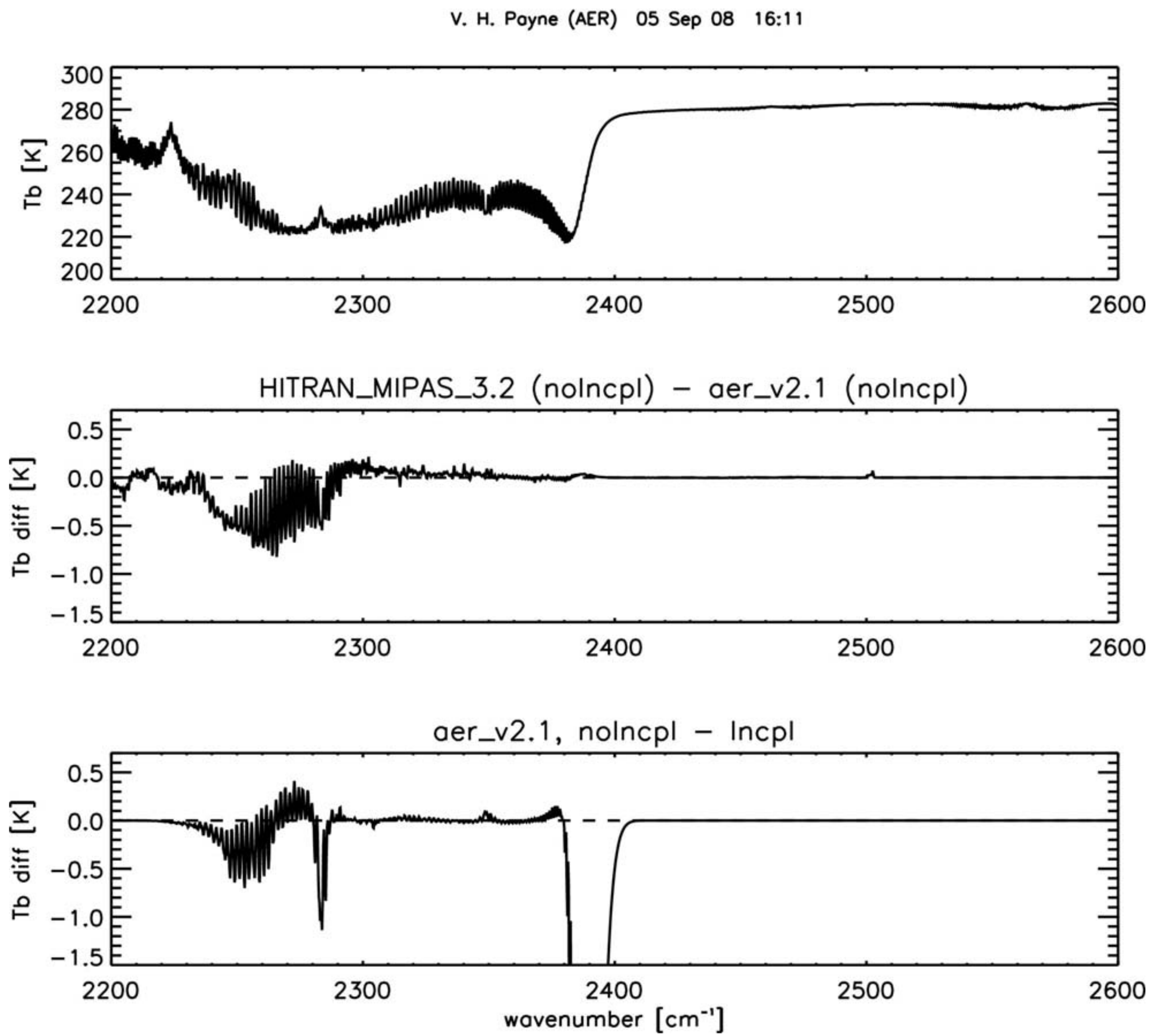
CO_2 ν3 line parameters

- aer_v2.1:
  - CO_2 line parameters from HITRAN 2K
- HITRAN_MIPAS_3.2:
  - CO_2 line parameters from Tashkun, Teffo, Flaud et al.
  - Validated by Flaud et al using MIPAS spectra.
- Line coupling coefficients in aer_v2.1 are for HITRAN 2K CO_2 line parameters
  - Niro et al., 2005
  - code supplied by J-M. Hartmann).
- Next: calculate line coupling coefficients for “HITRAN_MIPAS” CO2 line parameters, using same code.



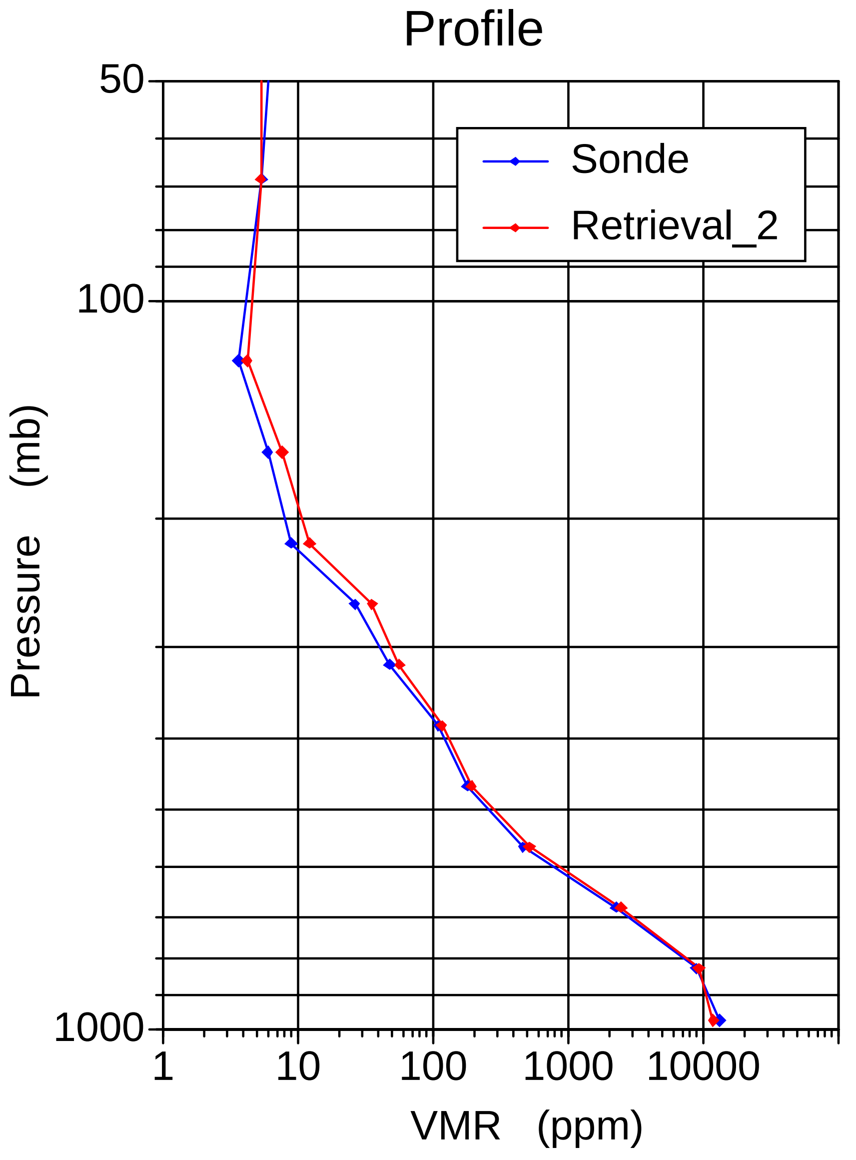
Profile from IASI JAIVEx case

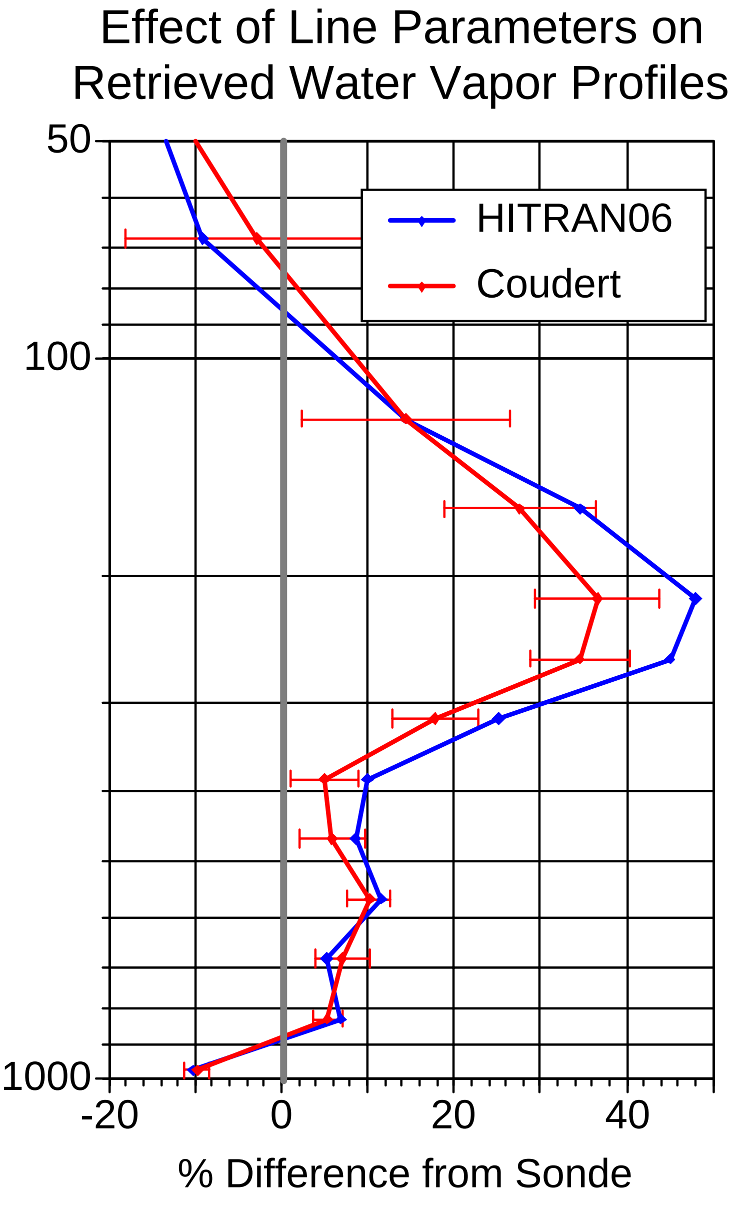
CO_2 ν3 line parameters



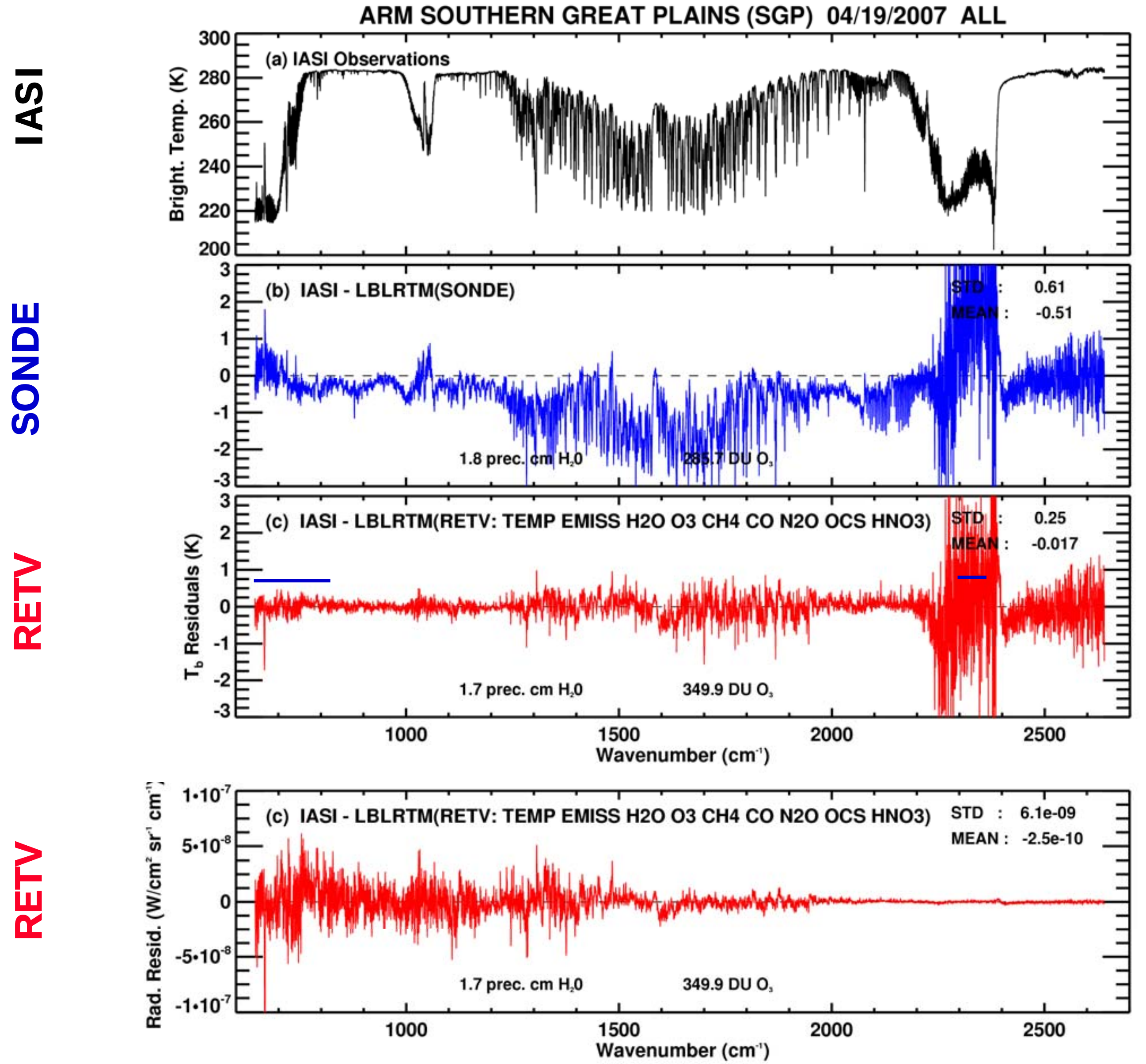
Profile from IASI JAIVEx case

Water Vapor


Profile
50
100
1000
1
10
100
1000
10000
VMR (ppm)
Pressure (mb)
Sonde
Retrieval_2


Effect of Line Parameters on
Retrieved Water Vapor Profiles
50
100
1000
-20
0
20
40
% Difference from Sonde
HITRAN06
Coudert

IASI/LBLRTM Validation



Status of Two Key Elements of the Forward Model in the Longwave: Carbon Dioxide Spectroscopy and the Water Vapor Continuum

Tony Clough

Atmospheric & Environmental Research, Inc.

EGU, Vienna

16 April 2007

Carbon Dioxide Spectroscopy

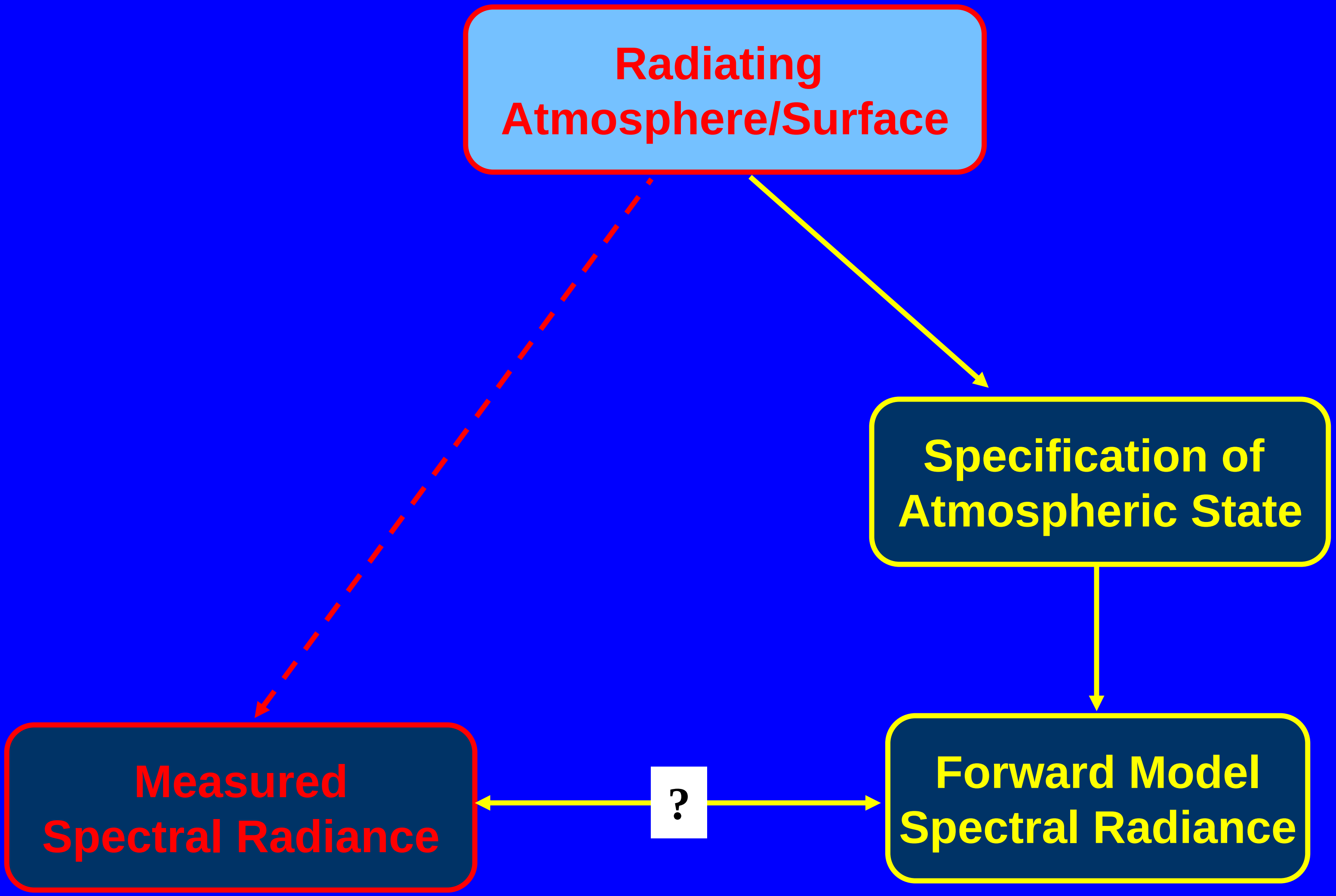
Mark Shephard and Vivian Payne

Observations

- Tropospheric Emission Spectrometer (TES)
- Scanning High Resolution Interferometric Sounder (SHIS)
- Atmospheric InfraRed Spectrometer (AIRS)

Acknowledgments

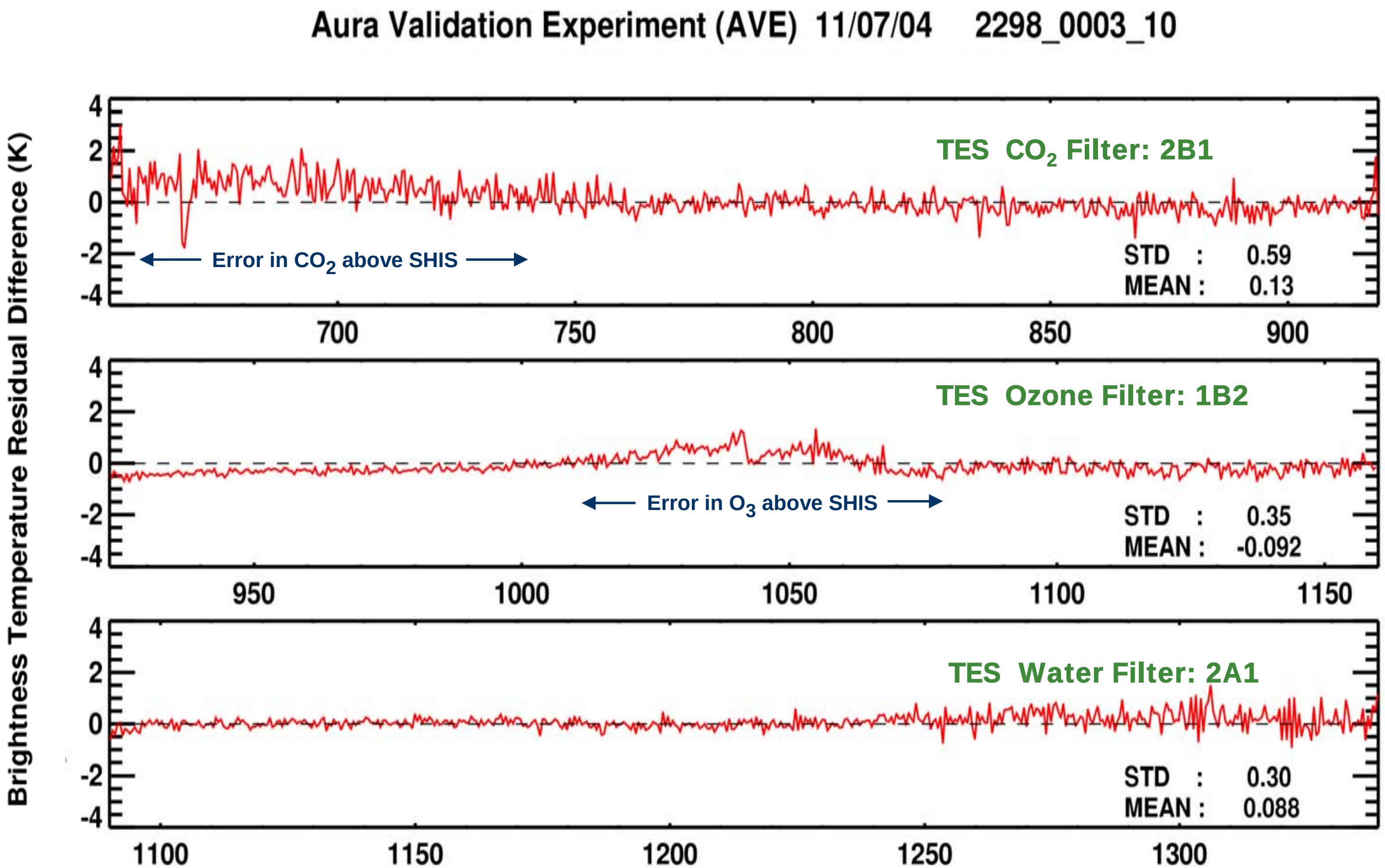
- **University of Wisconsin**
  Hank Revercomb, Bob Knuteson and Dave Tobin
- **TES Team**
  Linda Brown, Aaron Goldman, Curtis Rinsland, Helen Worden, etc., etc.
- **Creteill**
  Jean Michel Hartmann's Group



Radiating
Atmosphere/Surface
Specification of
Atmospheric State
Measured
Spectral Radiance
?
Forward Model
Spectral Radiance

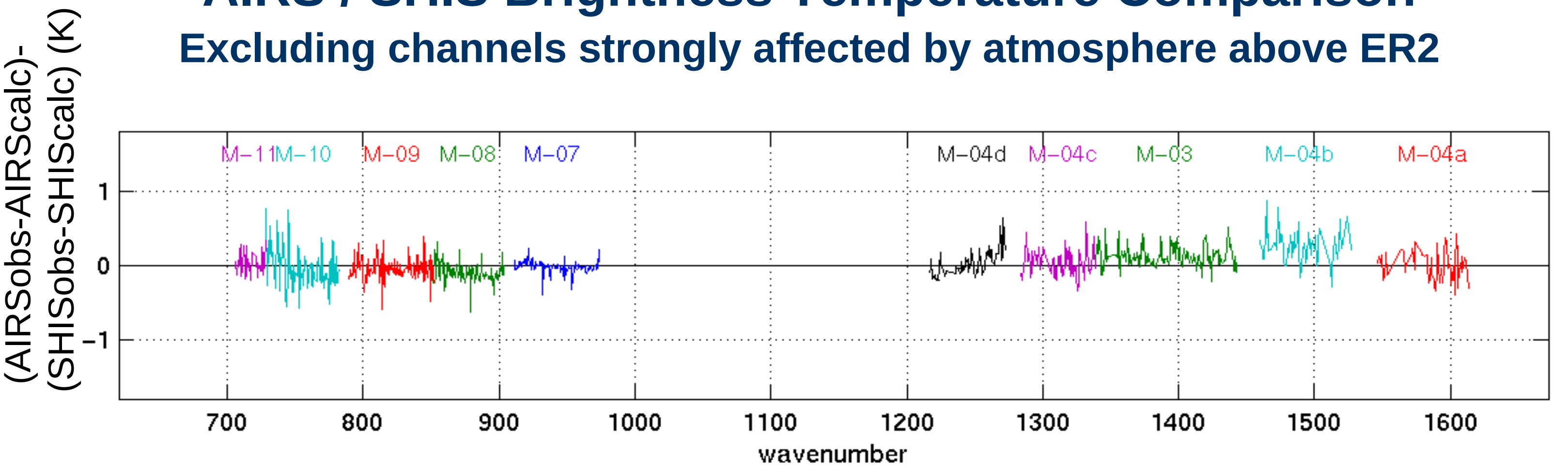
TES - SHIS Radiance Comparison

- **TES Convolved to SHIS ILS**
- **{TES - LBLRTM(TES Geometry)} - {SHIS - LBLRTM(SHIS Geometry)}**

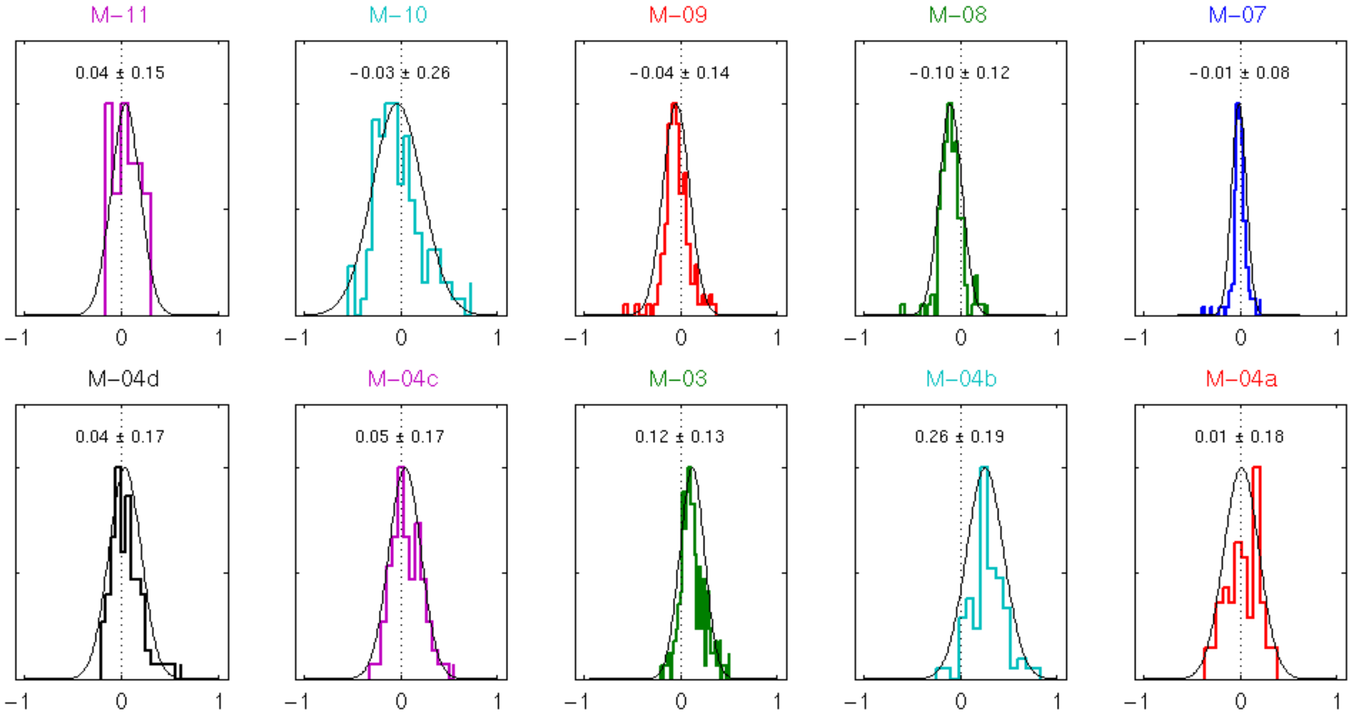


AIRS / SHIS Brightness Temperature Comparison

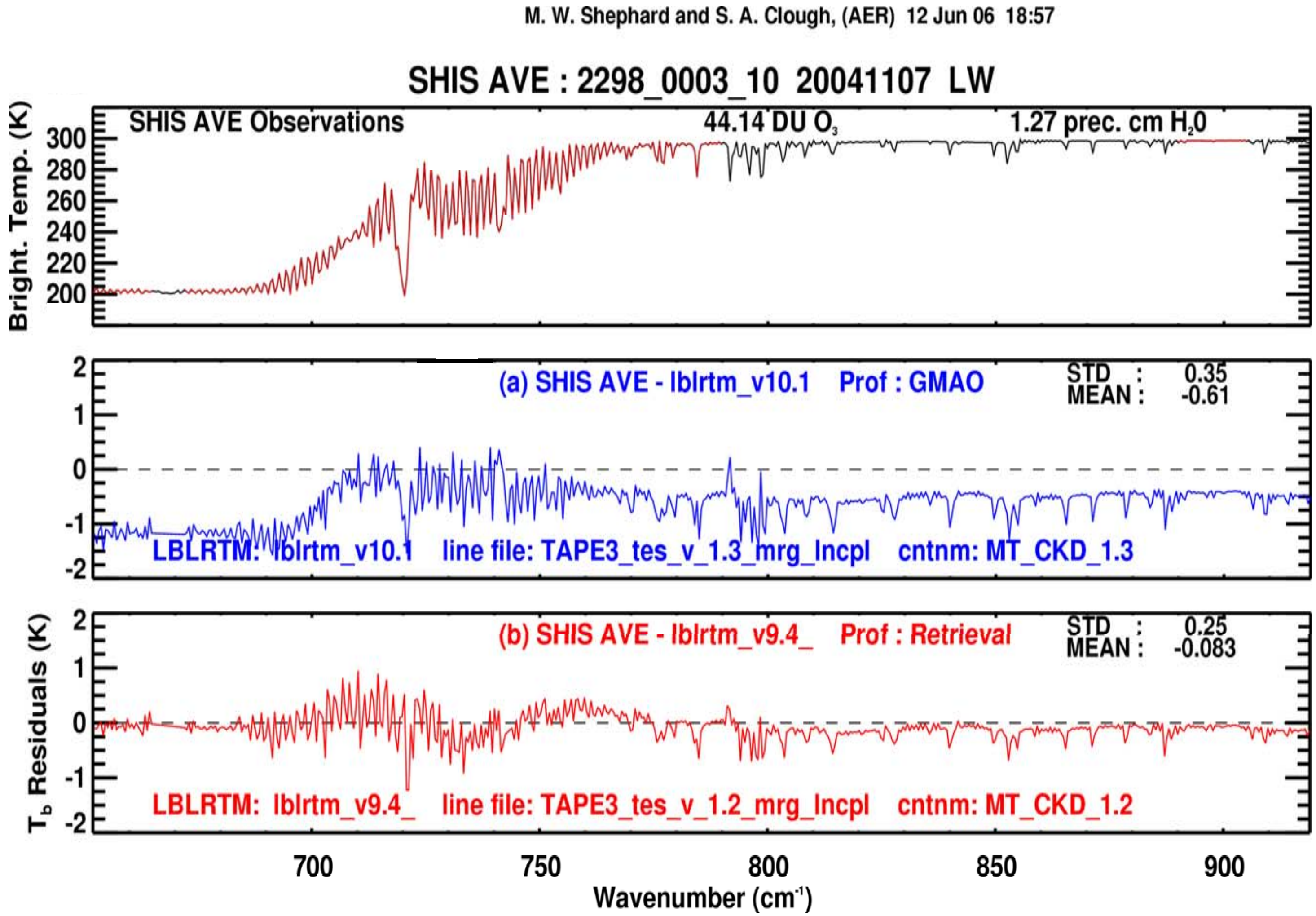
Excluding channels strongly affected by atmosphere above ER2



Histograms



SHIS Analysis from AURA Validation Experiment
Persistent Spectral Residuals



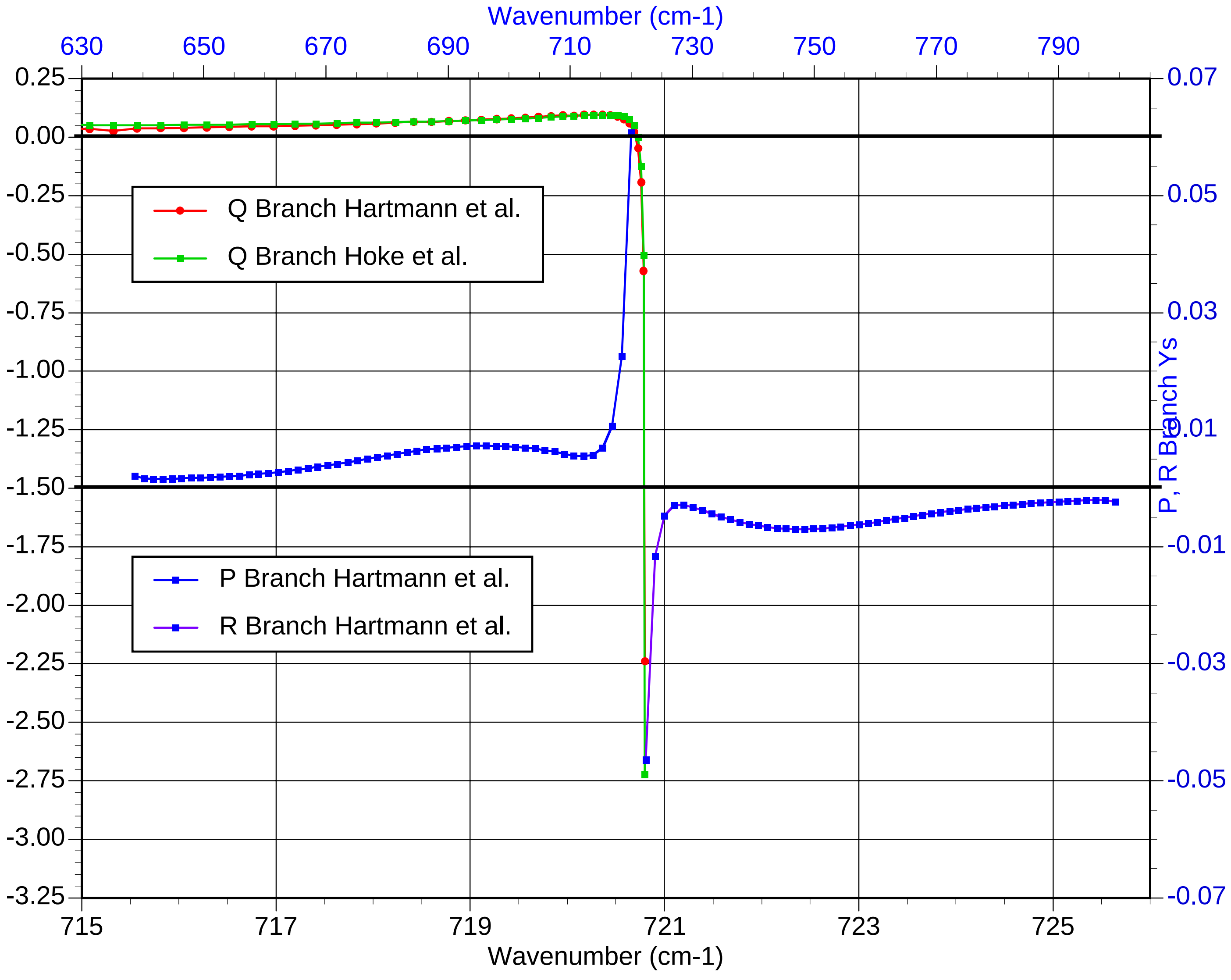
LBLRTM Approach for Carbon Dioxide (up to this point)

Lorentz Impact

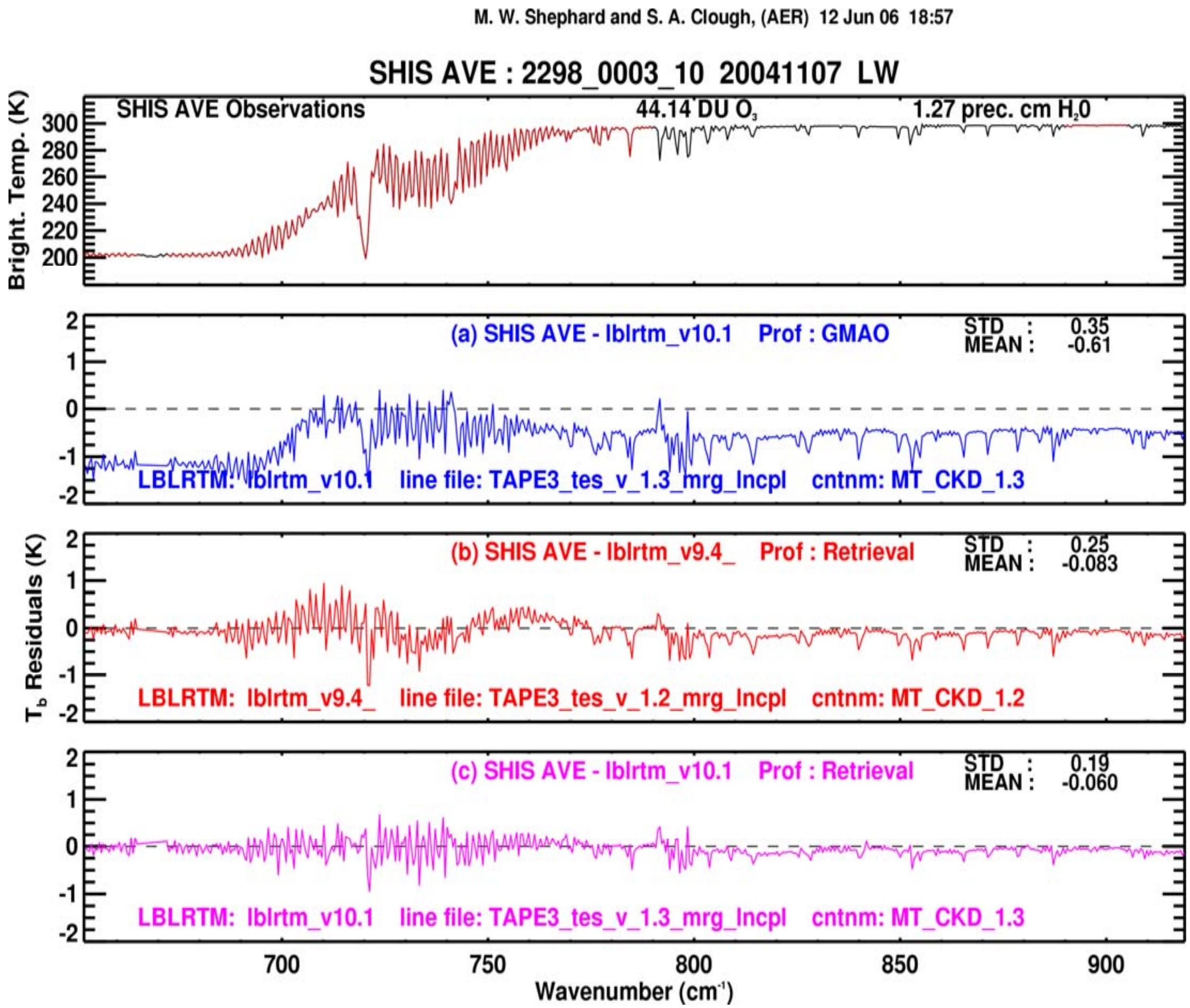
$$k_i(\nu) = \frac{1}{\pi} \frac{S_i}{(\nu - \nu_i)^2 + \alpha_i^2} \quad \left[\chi(\nu - \nu_i)\right]$$

χ_i: line coupling and duration of collision effects

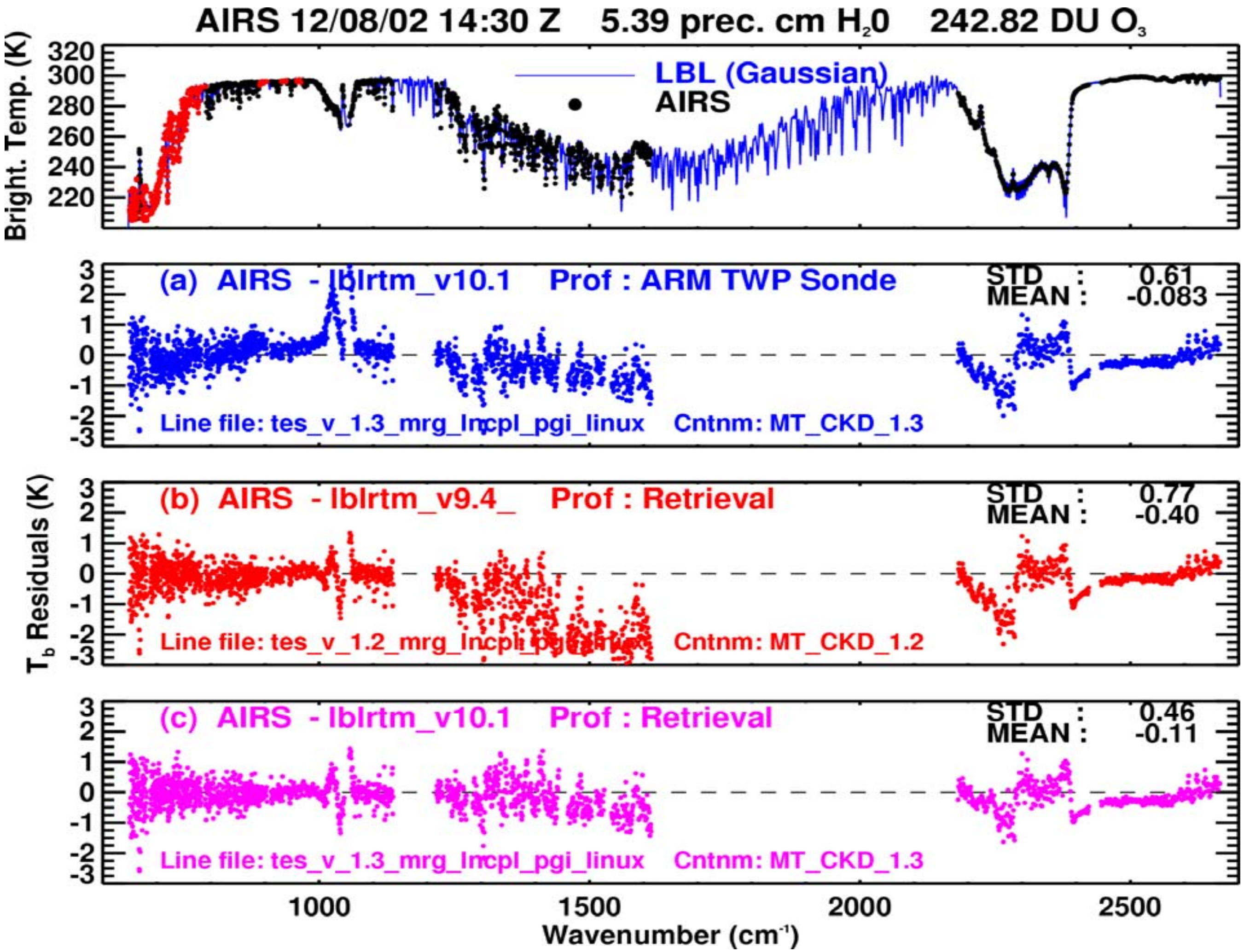
Line Coupling Parameters for the 5 < 2 Band



SHIS Analysis from AURA Validation Experiment
Gulf of Mexico - no sonde



AIRS Analysis
ARM Tropical Western Pacific site - sonde



Summary 1

- Forward Model for Temperature Retrievals significantly improved
  - P-R line coupling is a key element
- Carbon Dioxide:
  - χ factor and continuum strongly influenced by line coupling
  - need to introduce small χ factor for duration of collision effects
  - CO_2 Continuum has been reduced by 25% for best fit at bandhead
- ν_2 and ν_3 are apparently not yet fully consistent
- Line Coupling for N_2O
- Updated Code and Line Parameters to be made public
  - separate Line Coupling file (Hartmann) available: TAPE2
- Spectral Residuals will likely become the validation criterion

MT_CKD Water Vapor Continuum Model

- **Definition: Continuum is that absorption with slow spectral dependence which,**

  when added to the line by line absorption, provides agreement with measurement.
- **Scaling: Dependence on pressure, temperature and mixing ratio must be correct**
- **The model is based on contributions from two sources:**

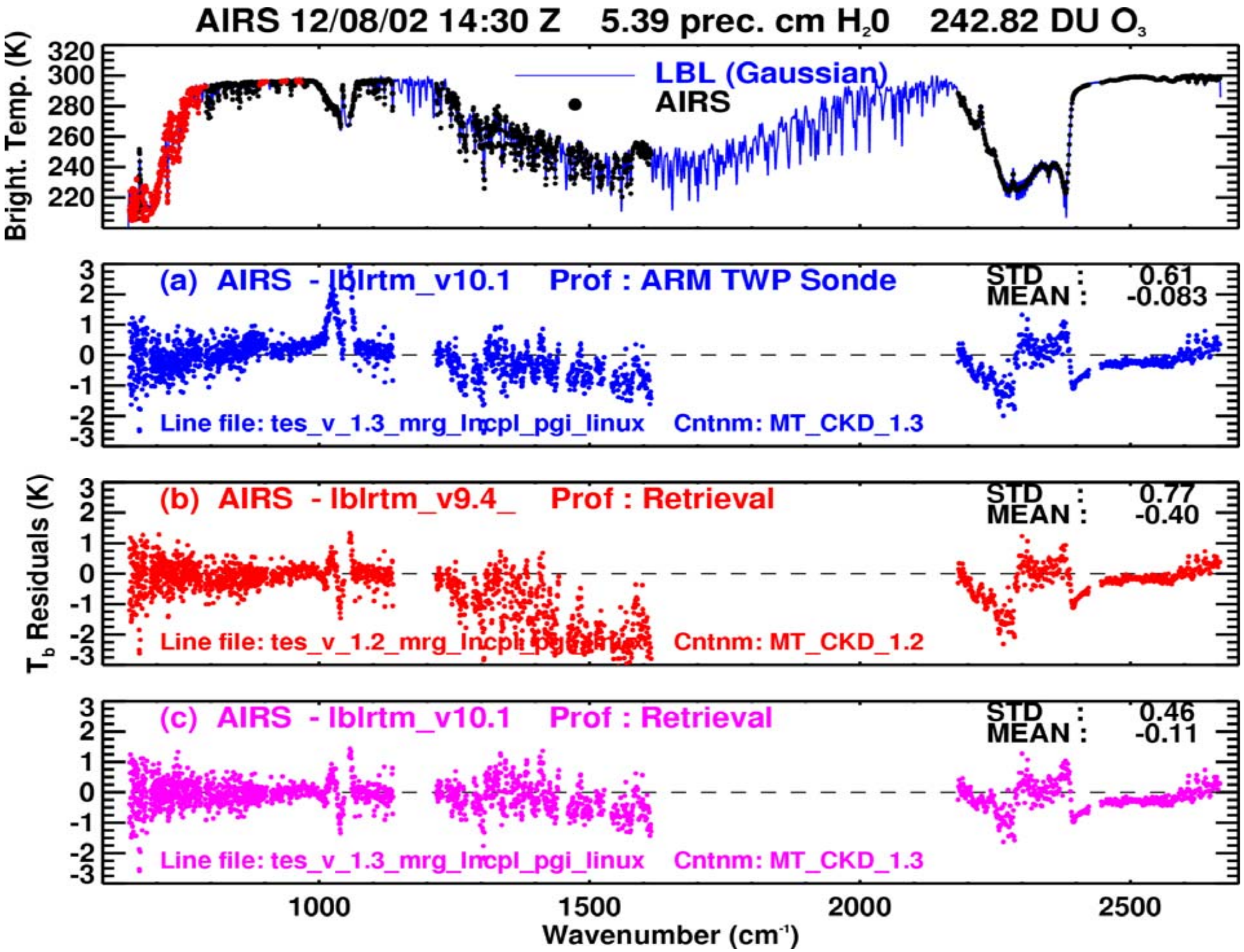
  1. Allowed line contribution

  - **Line wing formalism constrained by the known physics with relevant parameters (~2) determined from laboratory and atmospheric Measurements**
  - **Same line shape is used for every line from the Microwave to 20,000 cm-1**

  2. Collision-Induced contribution

  - **Provides the extra absorption previously provided by the 'super Lorentzian' chi factor**
  - **Based on dipole allowed transitions with widths ~ 50 cm-1**
  - **Same line shape is used for every line from the Microwave to UV**
- **The model includes both self and foreign continuum**
- **Spectral region: 0 - 20,000 cm^{-1}**

AIRS Analysis
ARM Tropical Western Pacific site - sonde



Summary 2

- Issues with water vapor continuum have become remarkably muted
- Collision induced component addresses measurement issues
  - No direct validation of mechanism is apparent
- Self and Foreign each use a single separate line shape for all lines to construct the respective continua over full frequency domain
- Self Continuum (line wing component) dominant between bands
- Foreign Continuum (collision induced) dominant within bands
- Well Validated in 0-10 cm-1 (microwave); 400-500 cm-1; 800 -1300 cm-1; and 2500-2700 cm-1 (SST)
- Validations needed 10-400 cm-1 and Shortwave
- Temperature Dependence! Laboratory Measurements (Lafferty)
- MT_CKD Water Vapor Continuum is publicly available
  - http://rtweb.aer.com