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# Forward Modeling for IASI: Spectroscopic Issues and LBL\_CRA

**Tony Clough**

*Clough Radiation Associates, LLC*

*IASI, Sevrier, FR  
26 Jan 2010*

# Collaborators and IASI Cases

- **Collaborators:**

- M. Shephard, V. Payne, K. Cady-Pereira and J. Delamere      AER, Inc.
- W. Smith and S. Kireev      Hampton U.
- Extension of

**Performance of the line-by-line radiative transfer model (LBLRTM) for temperature and species retrievals: IASI case studies from JAIVEx:** M. W. Shephard, S. A. Clough, V. H. Payne, W. L. Smith, S. Kireev, and K. E. Cady-Pereira, Atmos. Chem. Phys., 9, 7397-7417, 2009

- **IASI Cases from JAIVEx**

- **2007\_04\_19**

**Case Study**

- » Over SGP site (surface **emissivity retrieved**)
    - » Atmosphere
      - Clear and Homogeneous (h<sub>2</sub>O)
      - ‘Well Characterized’

- **2007\_04\_20**

**‘Control’**

- » Over Gulf of Mexico ”
    - » Atmosphere
      - Broken Clouds and Highly Inhomogeneous (h<sub>2</sub>O)
      - Not So Well Characterized

e.g. Matricardi ACP, 2009

- **Temperature**

## – Carbon Dioxide

- » Line Parameters: CDDb (2008), Tashkun et al. JQSRT, 2009
- » Line Coupling: Niro et al., JQSRT, 2005 J.M.Hartmann
- ✓ Agreement between CO<sub>2</sub>  $\nu_2$  and CO<sub>2</sub>  $\nu_3$
- ✓ Q-Branch 667 cm<sup>-1</sup>
- ✓ Band Head 2385 cm<sup>-1</sup>

- Nitrous Oxide

- ? Agreement between CO<sub>2</sub> v<sub>2</sub> and N<sub>2</sub>O v<sub>3</sub>
- » N<sub>2</sub>O profile scaling required:
- |                |      |
|----------------|------|
| 19 April case: | 1.04 |
| 20 April case: | 1.02 |

- **Methane**

- ✓ Line Coupling: Tran et al., JQSRT, 2006 J.M.Hartmann

# Water Vapor

- A slide of its own
- Significant improvements but ...

# Introduction

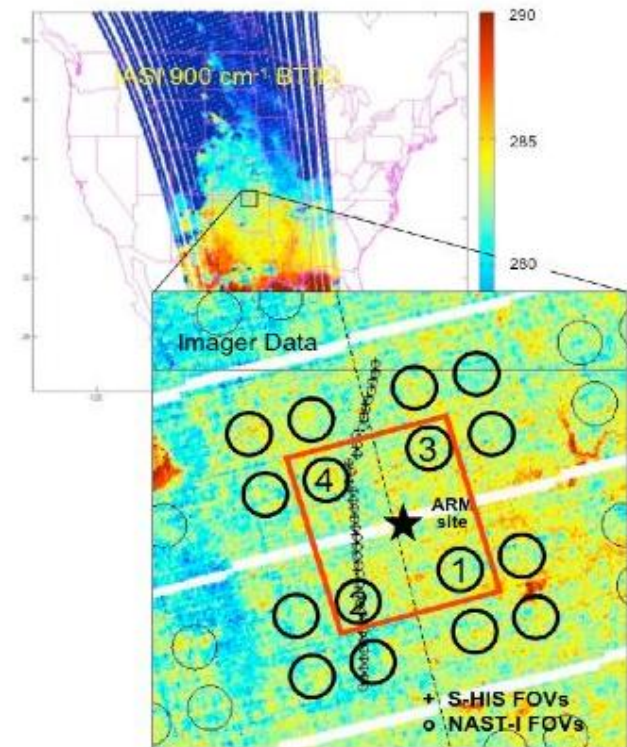
## IASI

- 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  $\pm 48.98^\circ$
  - Swath  $\pm 1066$  km
  - Spectral Range 645 to 2760  $\text{cm}^{-1}$
  - **Resolution (hw/hh)** **0.25  $\text{cm}^{-1}$**
  - 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.

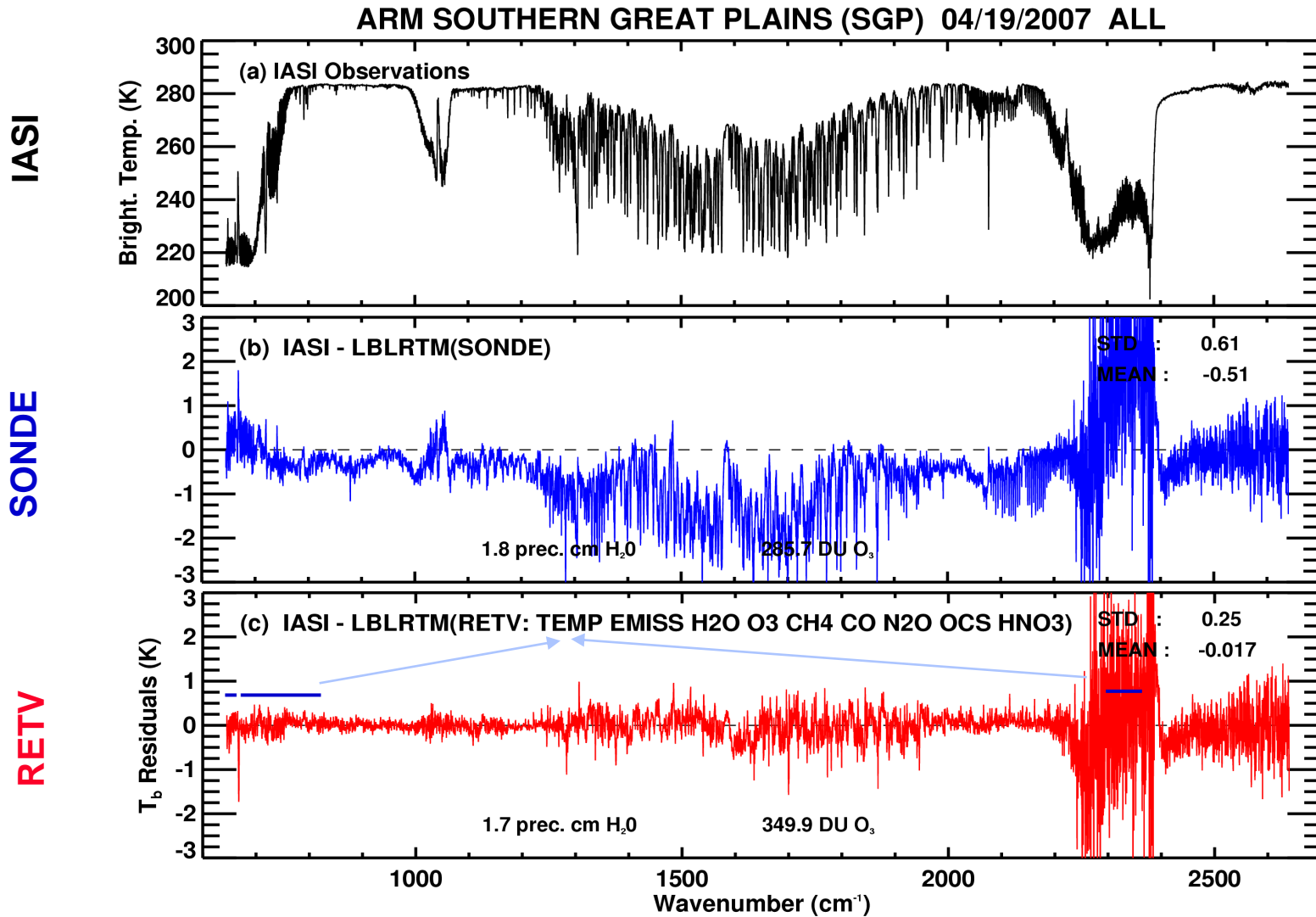
## Joint Airborne IASI Validation Experiment

**JAIVEx 19 Apr 2007**

**CART-site (03:35 UTC)**



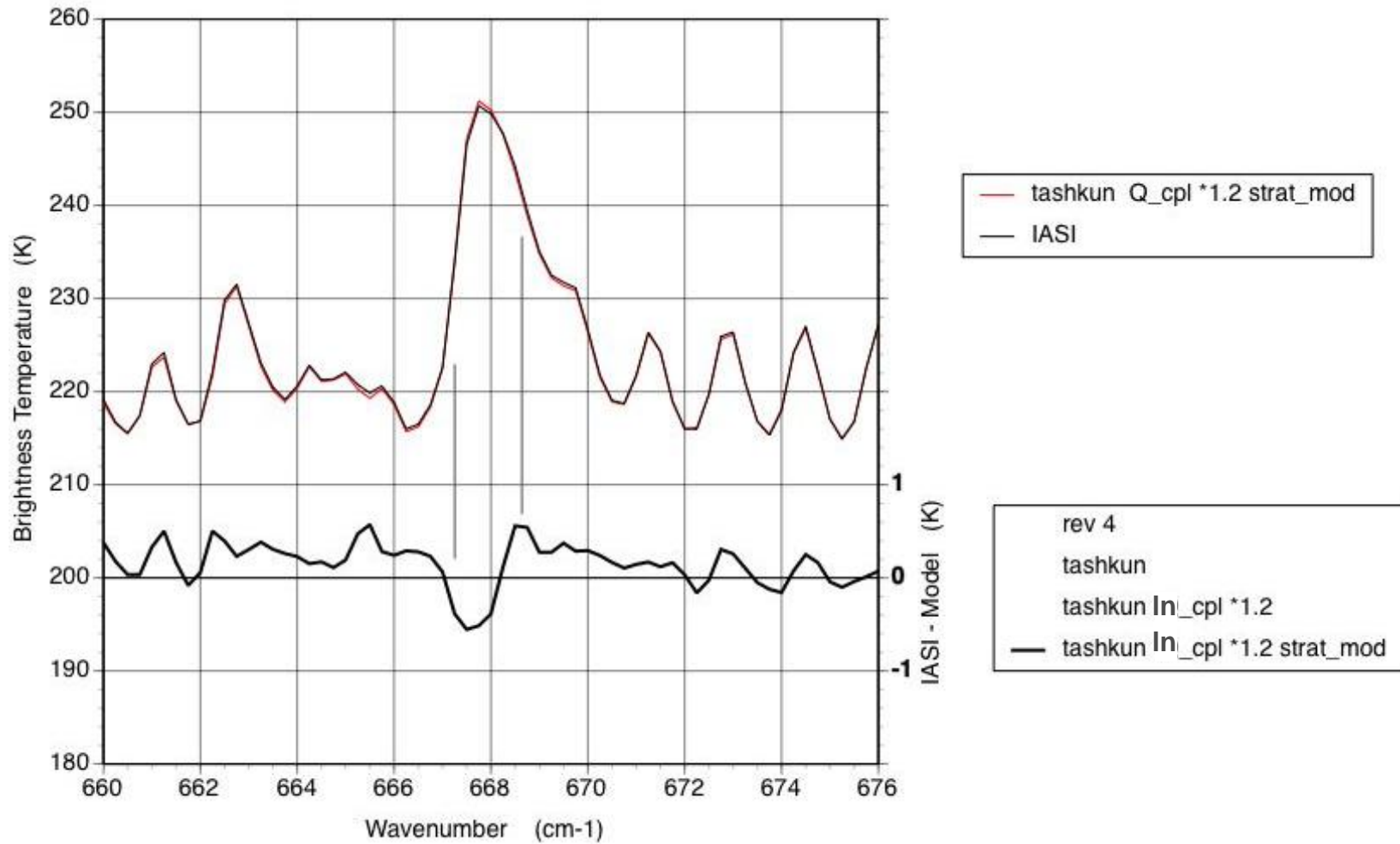
# IASI/LBLRTM Validation



**Strategy: to analyze the spectroscopy in the context of these red residuals**

# IASI 19 Apr 2007 CO<sub>2</sub> Q-Branch

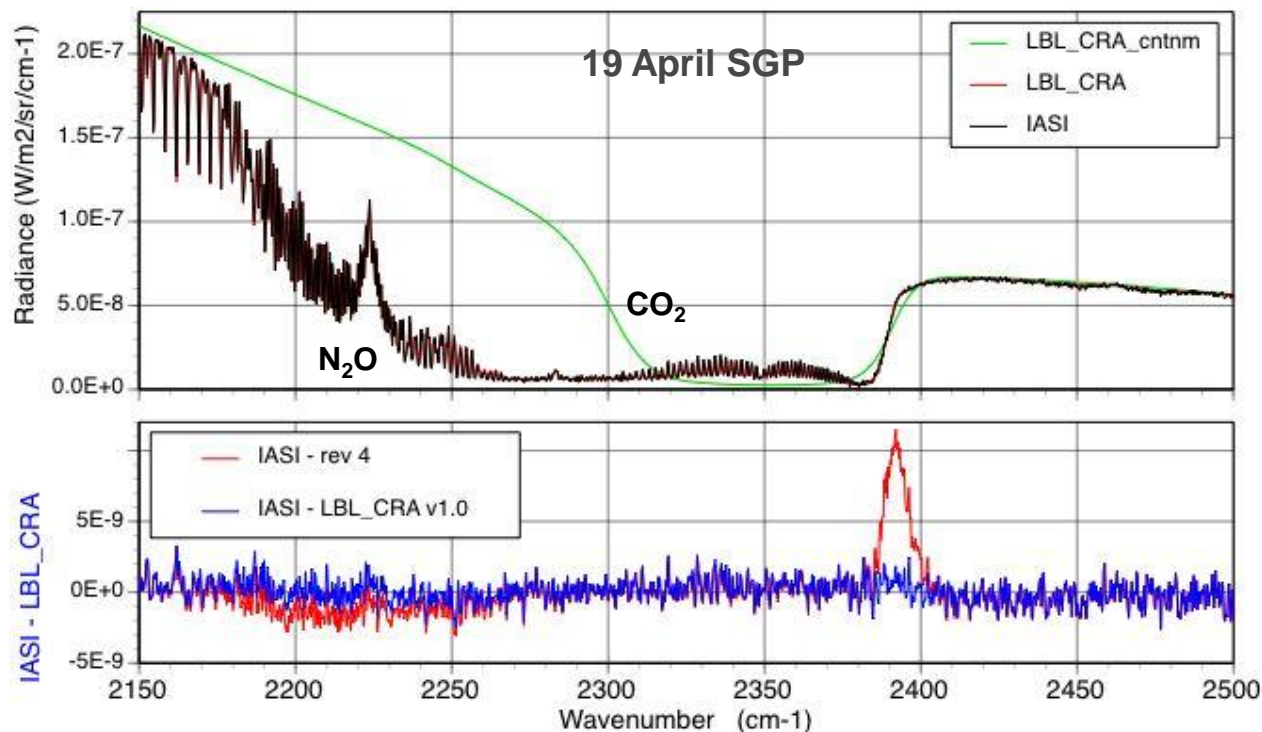
## Sensitivity to Upper Stratosphere



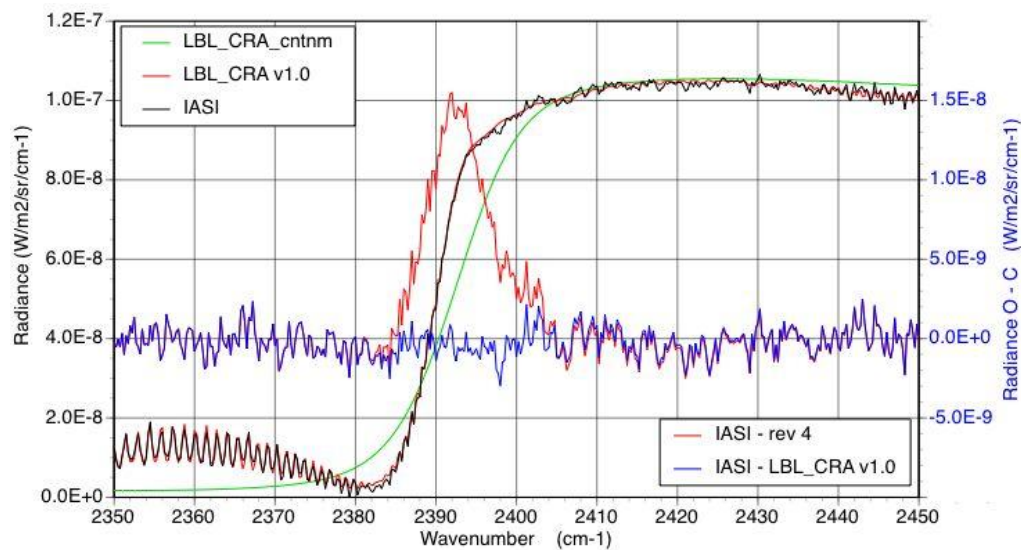
$\nu_3$  Bands of  
 $\text{N}_2\text{O}$  and  $\text{CO}_2$   
2150 - 2500  $\text{cm}^{-1}$

1

LBL\_CRA:  $\text{N}_2\text{O}$   
increased by 1.04



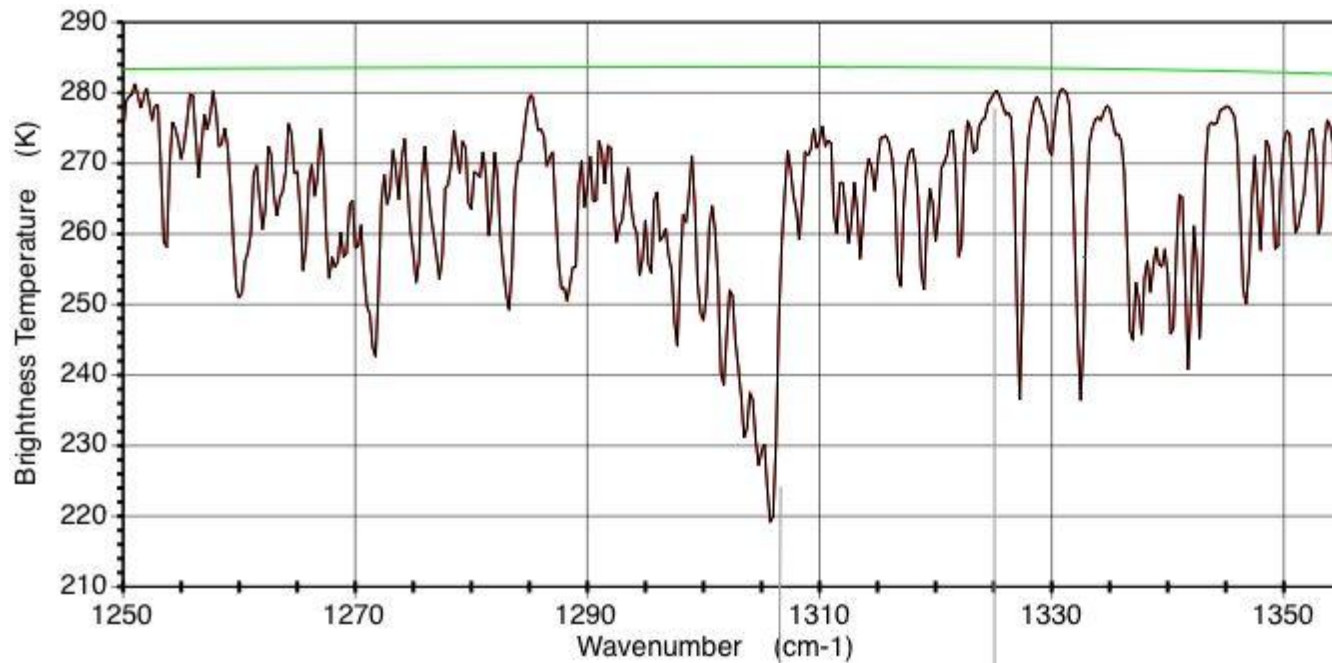
20 April GoM



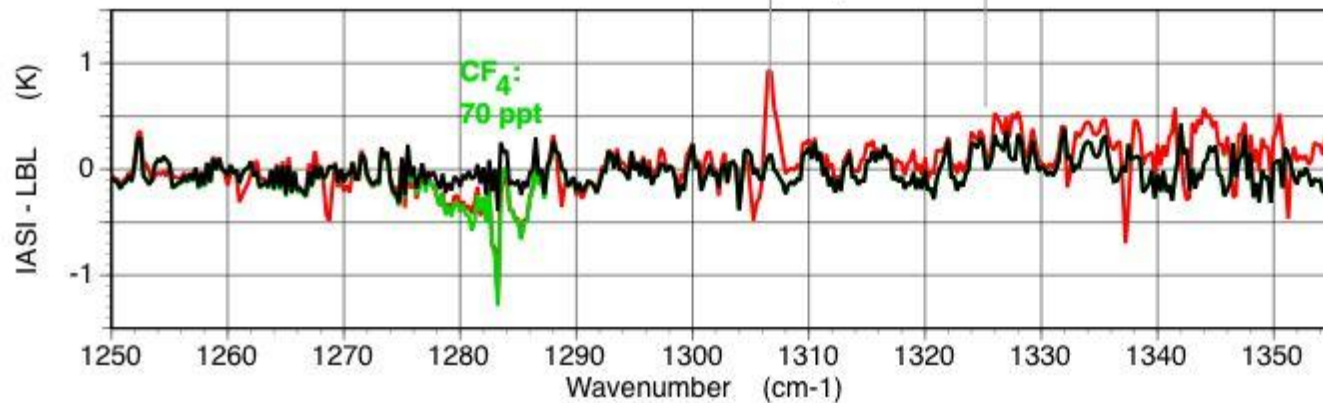


# Line Coupling in Methane

Tran et al., JQSRT, 2006



Ave: 0.035 K  
Std: 0.250 K  
Ave: -0.019 K  
Std: 0.145 K



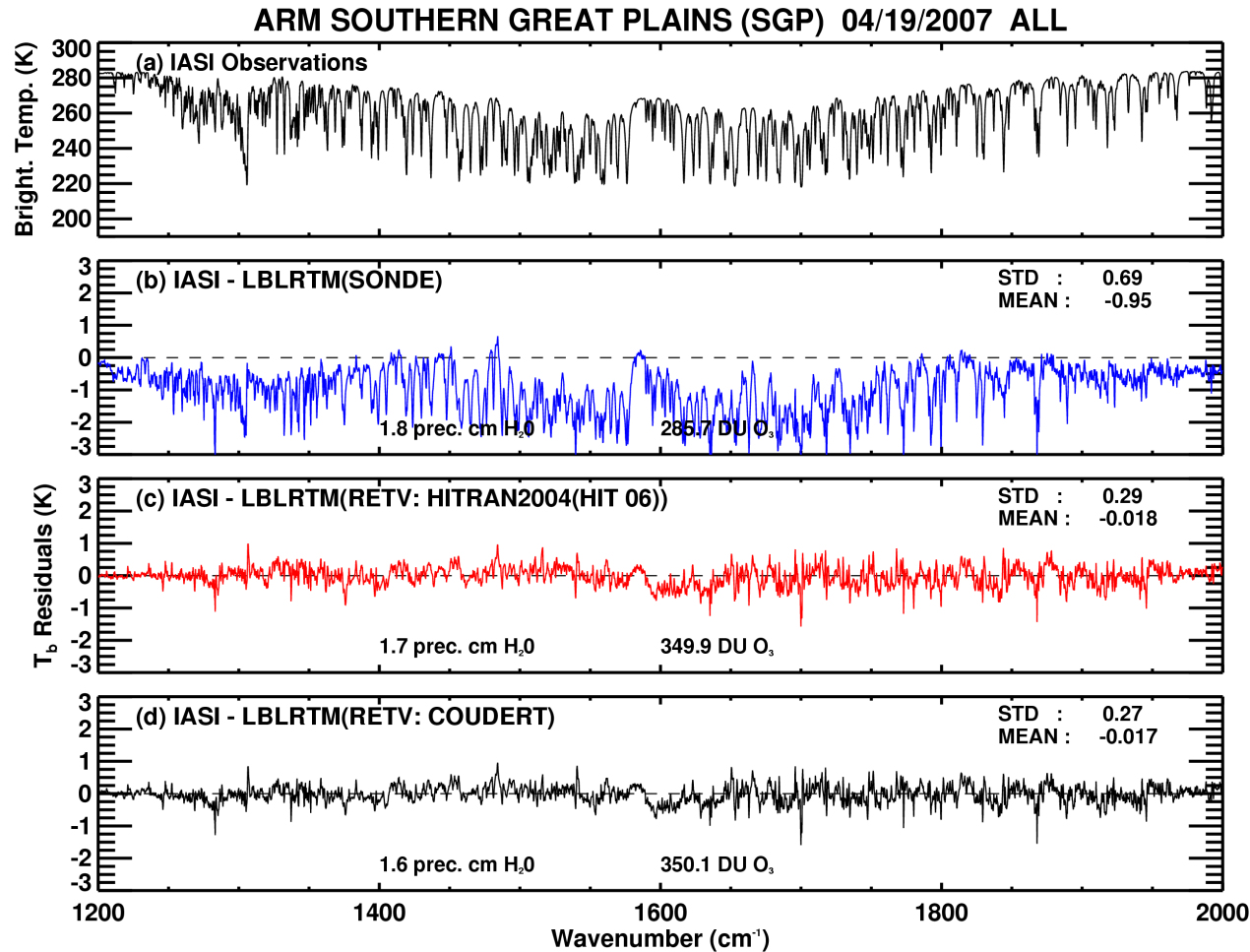


# Water Vapor: 'The Most Important Greenhouse Gas'

## Critical for NWP and Climate

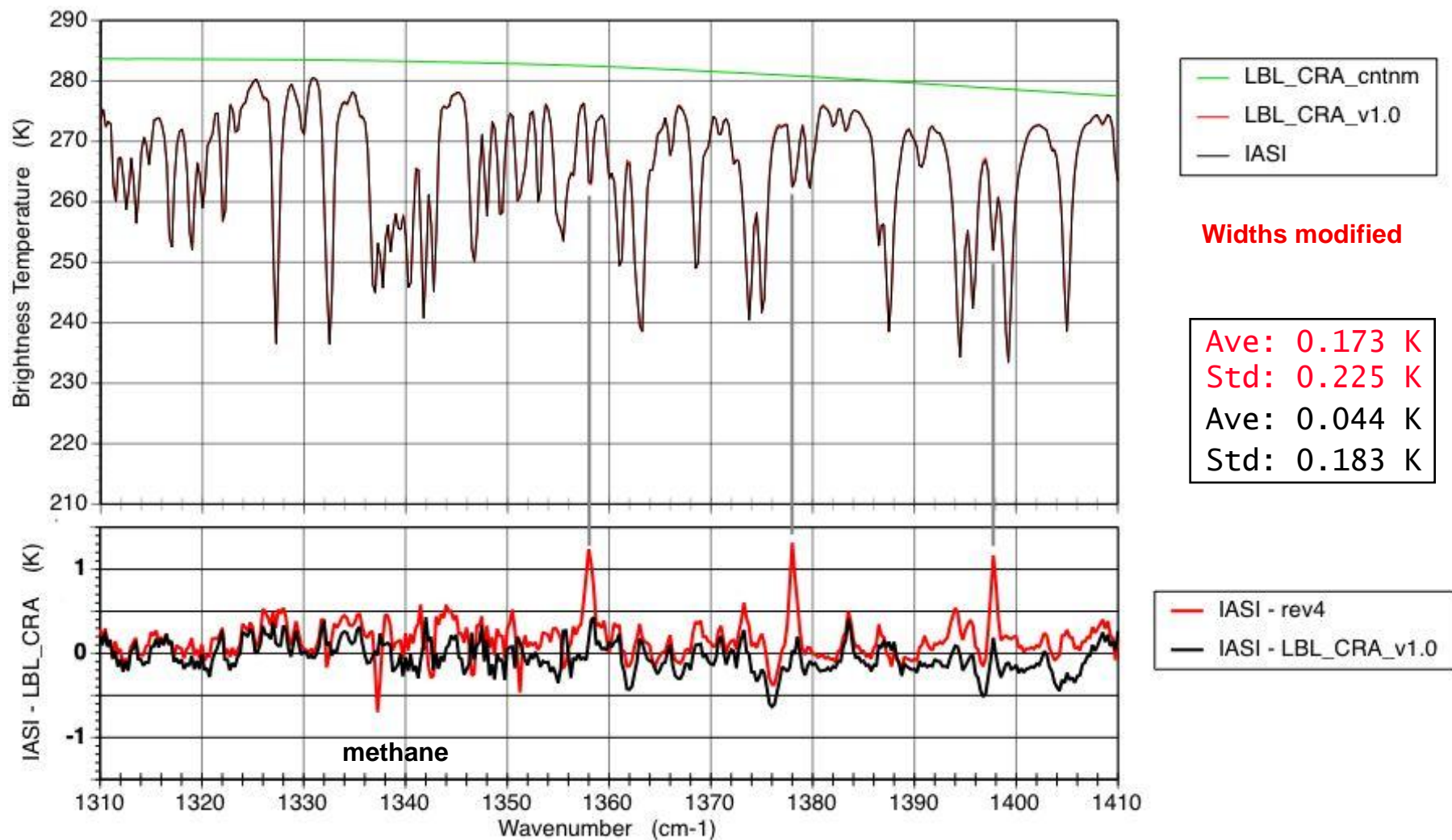
- **Line Parameters**
  - Laurent Coudert
    - » Strong Lines: Intensities increased by ~ 5 %
- **Line Widths and Shifts / Temperature Dependence**
  - Bob Gamache &
  - [this paper](#)
- **Line Coupling**
  - Linda Brown (accidental two line resonances)
  - [Revised relaxation rates](#)
  - First Order
- **Continuum**
  - Inextricably linked to the width
  - `mt_ckd_2.4`
  - [Scaled in selected regions of the water band by ~5%](#)

# Water Vapor $\nu_2$ Region : Impact of Coudert Intensities

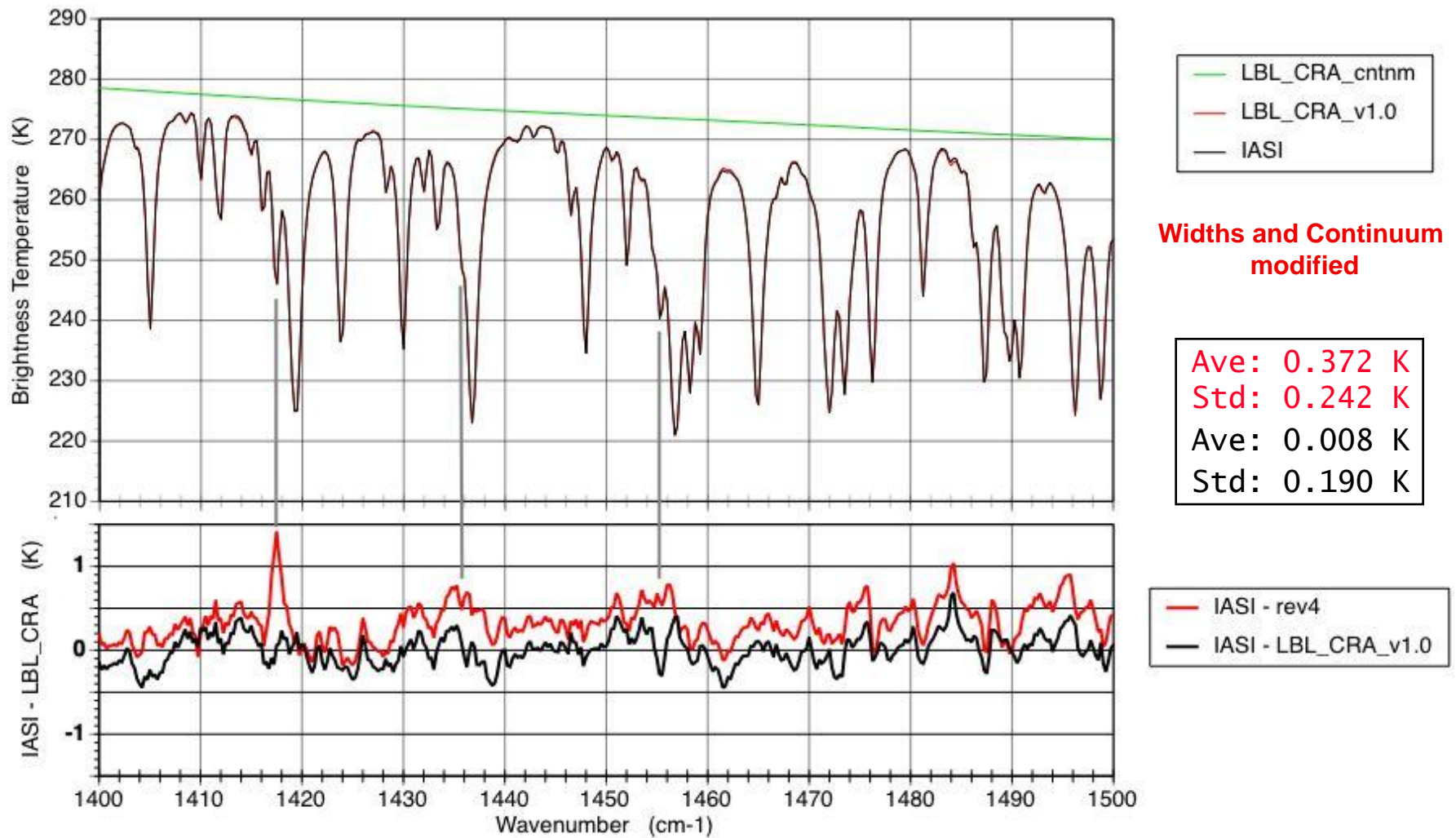


Scaled to  $\mu$ wave  
radiometer

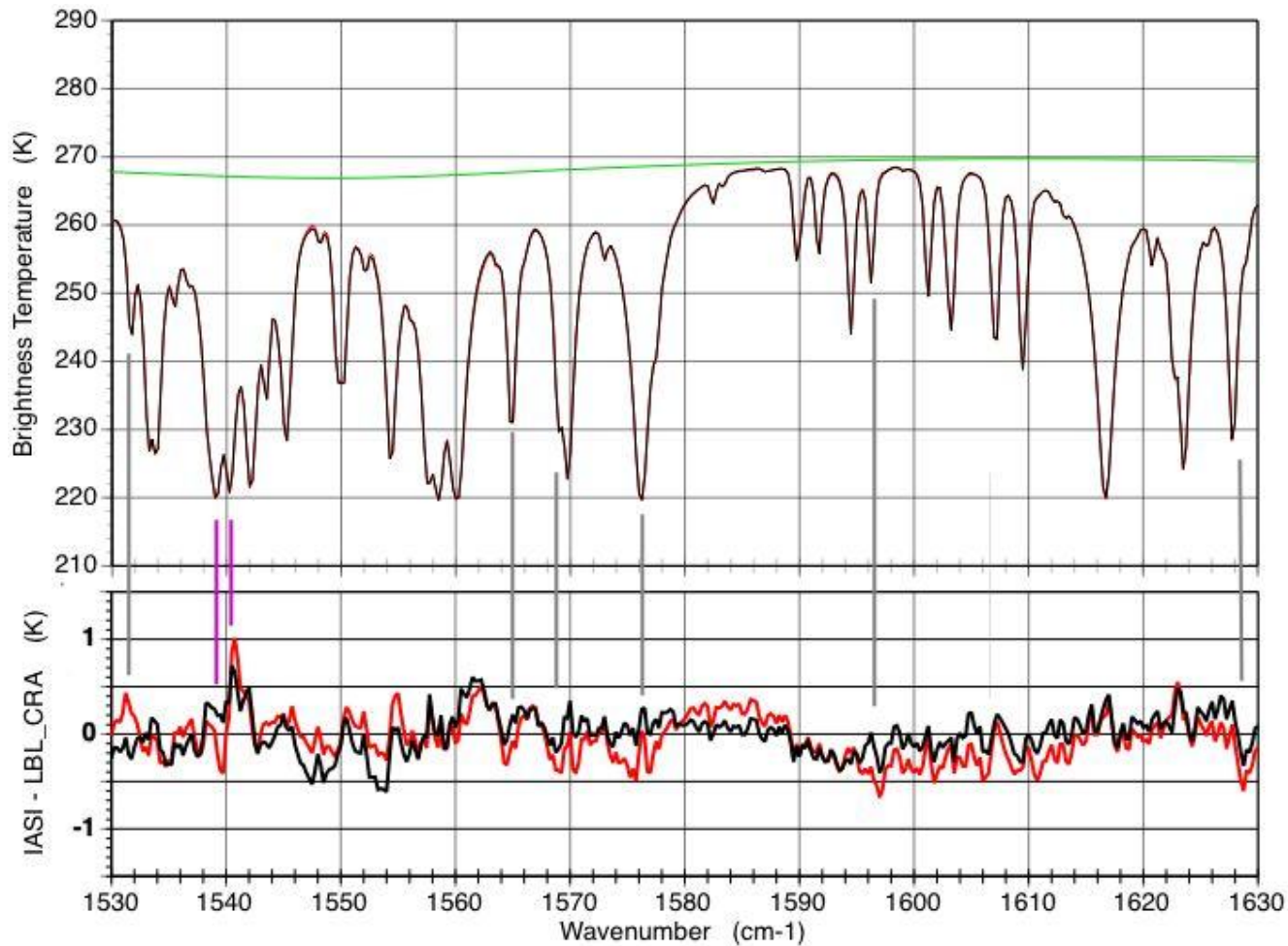
## Water Vapor P-Branch: 1310 -1410 cm<sup>-1</sup>



## Water Vapor P-Branch: 1400 -1500 cm<sup>-1</sup>



## Water Vapor Band Center: 1530 -1630 cm-1



Line Coupling  
1540 cm-1

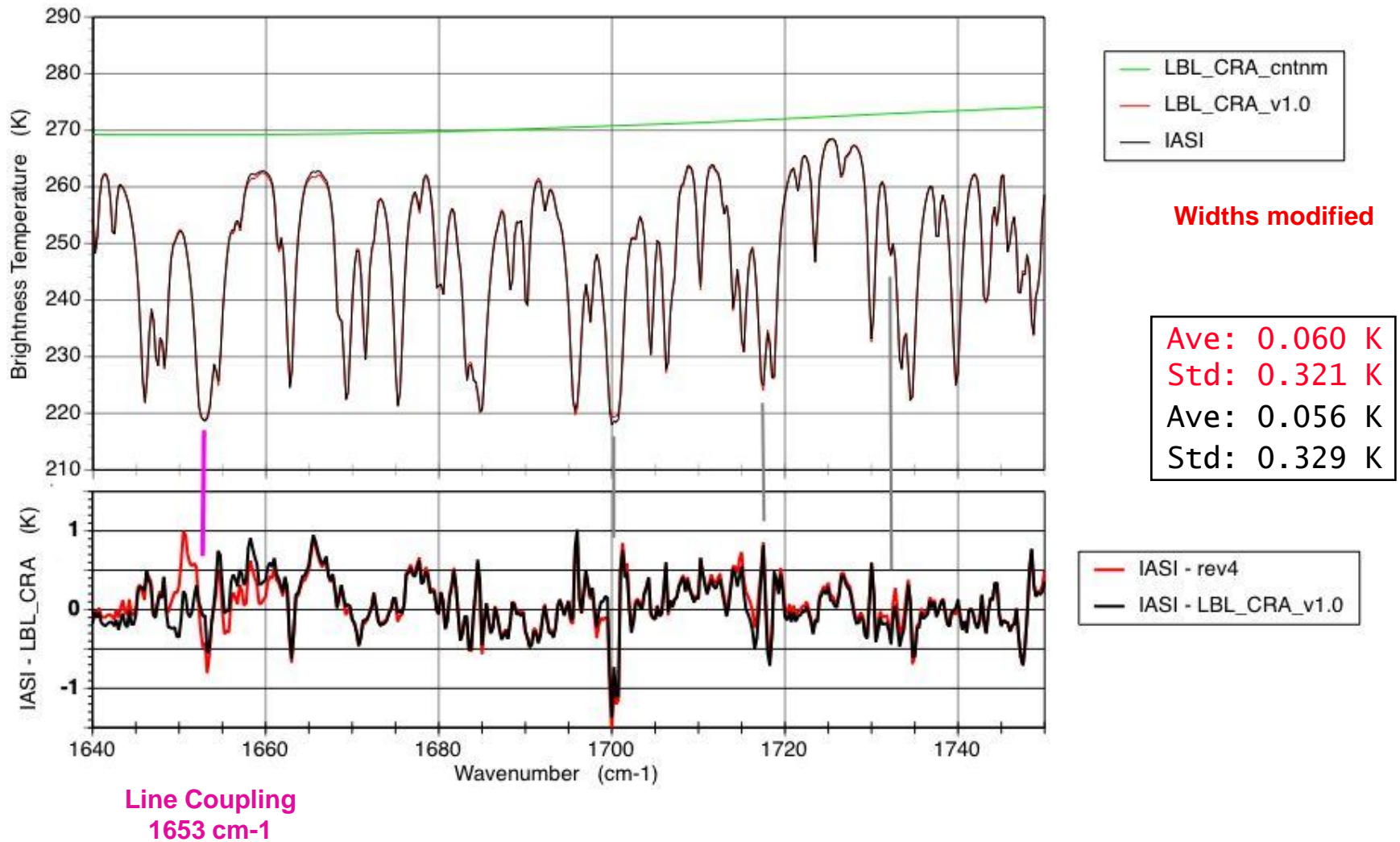
— LBL\_CRA\_cntnm  
— LBL\_CRA\_v1.0  
— IASI

**Widths and Continuum  
modified**

Ave: -0.047 K  
Std: 0.267 K  
Ave: 0.007 K  
Std: 0.219 K

— IASI - rev4  
— IASI - LBL\_CRA\_v1.0

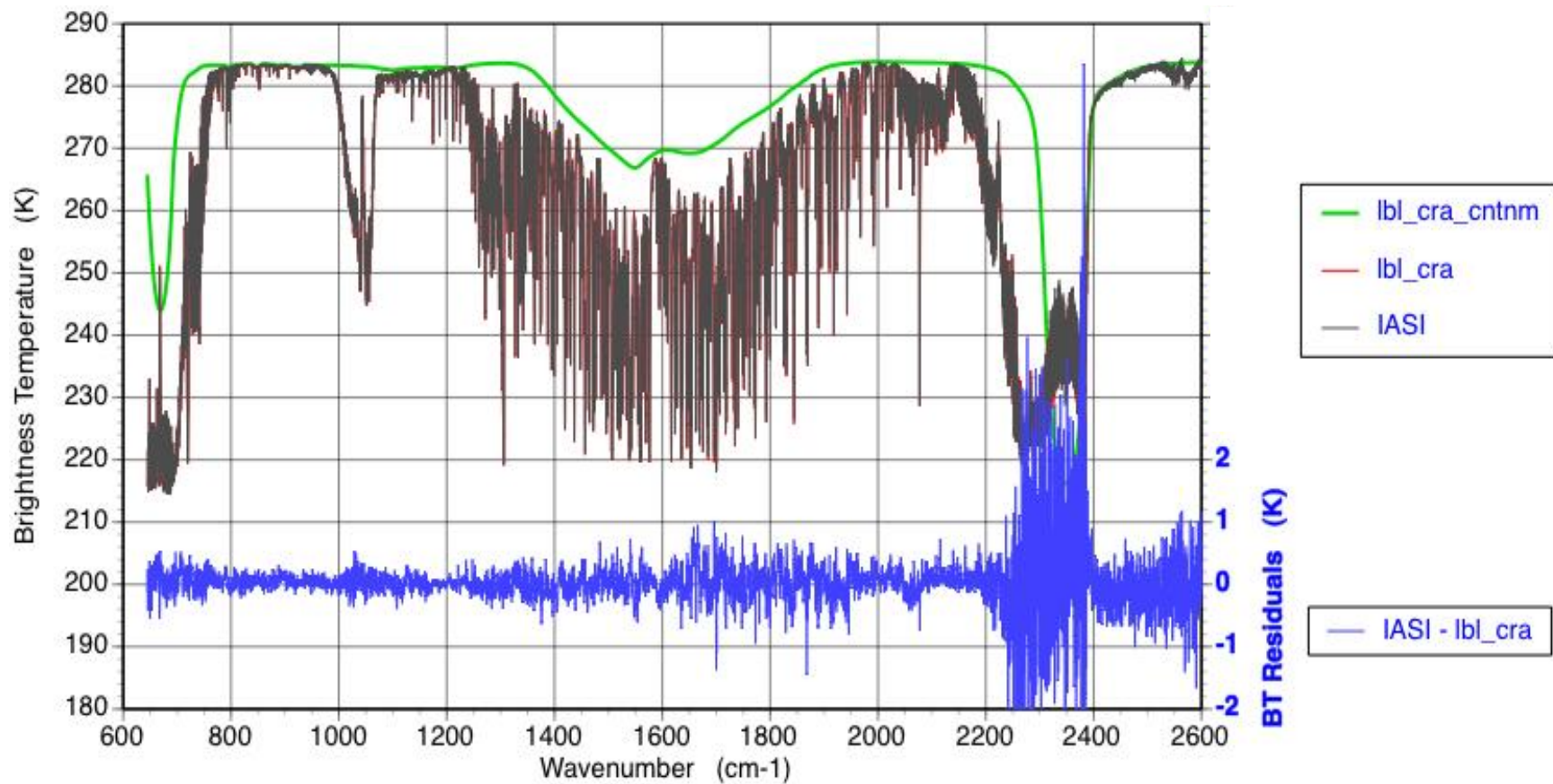
## Water Vapor R-Branch: 1640 -1750 cm<sup>-1</sup>





# Overall Comparison of LBL\_CRA with IASI

19 Apr 2007 SGP case





# Summary

- Temperature

- Carbon Dioxide

- » Line Parameters: CDDDB (2008), Tashkun et al. JQSRT, 2009
    - » Line Coupling: Niro et al., JQSRT, 2005 J.M.Hartmann
    - ✓ Agreement between  $\text{CO}_2 \nu_2$  and  $\text{CO}_2 \nu_3$
    - ✓ Q-Branch 667  $\text{cm}^{-1}$  line coupling resolve: \* 1.2
    - ✓ Band Head 2385  $\text{cm}^{-1}$  robust for both cases

- Nitrous Oxide

- ? Agreement between  $\text{CO}_2 \nu_2$  and  $\text{N}_2\text{O} \nu_3$
    - »  $\text{N}_2\text{O}$  profile scaling required: 19 April case: 1.04  
20 April case: 1.02

- Methane

- ✓ Line Coupling: Tran et al., JQSRT, 2006 J.M.Hartmann
  - ✓ \* 1.5

# Summary

- Water Vapor
  - Coudert strengths
    - Is it possible that there are errors in R lines?
  - Widths are the current major issue
  - Widths and continuum are inextricably linked
  - Line shape may be an issue as refinements proceed
  - P-Branch has much lower residuals in LBL\_CRA than R-Branch
  - **Sondes provide an excellent first guess / structure**
  - 19 April 2007 case is superb for FM improvement
  - Due to the resolution of IASI there is a limit to the extent spectroscopic improvements can be made

# Summary

- **Next Steps**
  - **Resolve R-Branch Issues**
  - **More Cases**
    - **Night time IASI preferred (we have some AIRS cases)**
    - **High Water**

## **Model Availability:**

- **unfortunate situation**
- **Mark Shephard > Environment Canada**
- **contact me for the package- return 20 February**
- **clough.associates@gmail.com**

```

c      if (vj.ge.1300. .and. vj.lt.1590.) fact = 0.9
c      if (vj.gt.1590. .and. vj.lt.1900.) fact = 1.1
c      fh2o(j) = fact*fh2o(j)

```

```

fscal_sav = fscal

```

```

i_fac = (vj-v1_h2o)/dv_h2o + 1.0001

```

```

c      if (i_fac.eq.29) fscal = 0.95*fscal ! 1530
c      if (i_fac.eq.30) fscal = 0.95 *fscal ! 1540
c      if (i_fac.eq.31) fscal = 0.95 *fscal ! 1550
c      if (i_fac.eq.32) fscal = 0.95 *fscal ! 1560
if (i_fac.eq.33) fscal = 0.90 *fscal ! 1570
if (i_fac.eq.34) fscal = 0.90 *fscal ! 1580
if (i_fac.eq.35) fscal = 0.98 *fscal ! 1590
if (i_fac.eq.36) fscal = 1.07 *fscal ! 1600
if (i_fac.eq.37) fscal = 1.10 *fscal ! 1610
if (i_fac.eq.38) fscal = 1.08 *fscal ! 1620
c      if (i_fac.eq.39) fscal = 1.092*fscal ! 1630
if (i_fac.eq.39) fscal = 1.06 *fscal ! 1630
c      if (i_fac.eq.40) fscal = 1.084*fscal ! 1640
if (i_fac.eq.40) fscal = 1.04 *fscal ! 1640
c      if (i_fac.eq.41) fscal = 1.076*fscal ! 1650
if (i_fac.eq.41) fscal = 1.02 *fscal ! 1650
c      if (i_fac.eq.42) fscal = 1.068*fscal ! 1660
if (i_fac.eq.42) fscal = 0.98 *fscal ! 1660
c      if (i_fac.eq.43) fscal = 1.060*fscal ! 1670
if (i_fac.eq.43) fscal = 0.98*fscal ! 1670
c      if (i_fac.eq.44) fscal = 1.052*fscal ! 1680
if (i_fac.eq.44) fscal = 0.98*fscal ! 1680
c      if (i_fac.eq.45) fscal = 1.044*fscal ! 1690
if (i_fac.eq.45) fscal = 0.98*fscal ! 1690
c      if (i_fac.eq.46) fscal = 1.036*fscal ! 1700
if (i_fac.eq.46) fscal = 0.98*fscal ! 1700
c      if (i_fac.eq.47) fscal = 1.028*fscal ! 1710
if (i_fac.eq.47) fscal = 0.99*fscal ! 1710
c      if (i_fac.eq.48) fscal = 1.020*fscal ! 1720
if (i_fac.eq.48) fscal = 0.98*fscal ! 1720

```

# What is 'Truth'?

- **Spectral Residuals are Key!**

- **Consistency within a band system**

- $\nu_2$  band to investigate consistency for H<sub>2</sub>O

- **Consistency between bands**

- IASI  $\nu_2$  and  $\nu_3$  bands to investigate consistency for CO<sub>2</sub>

- **Consistency between species**

- TES: temperature from O<sub>3</sub> and H<sub>2</sub>O consistent with CO<sub>2</sub> ; N<sub>2</sub>O

- **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**
- **Duration of collision effects- chi factor**
- **Line intensities- MIPAS line strengths**
  - **Tashkun, Teffo, Flaud et al.**
- **H<sub>2</sub>O broadening of CO<sub>2</sub>**

# CO<sub>2</sub> Line Coupling : Effect on Spectra

- **Line Parameters:**

- Niro, F., K. Jucks, J.-M. Hartmann, Spectra calculations in central and wing regions of CO<sub>2</sub> 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

Chi Factor

- **Line Shape:**

- Impact Approximation
- Duration of collision effects under study

- **Continuum:**

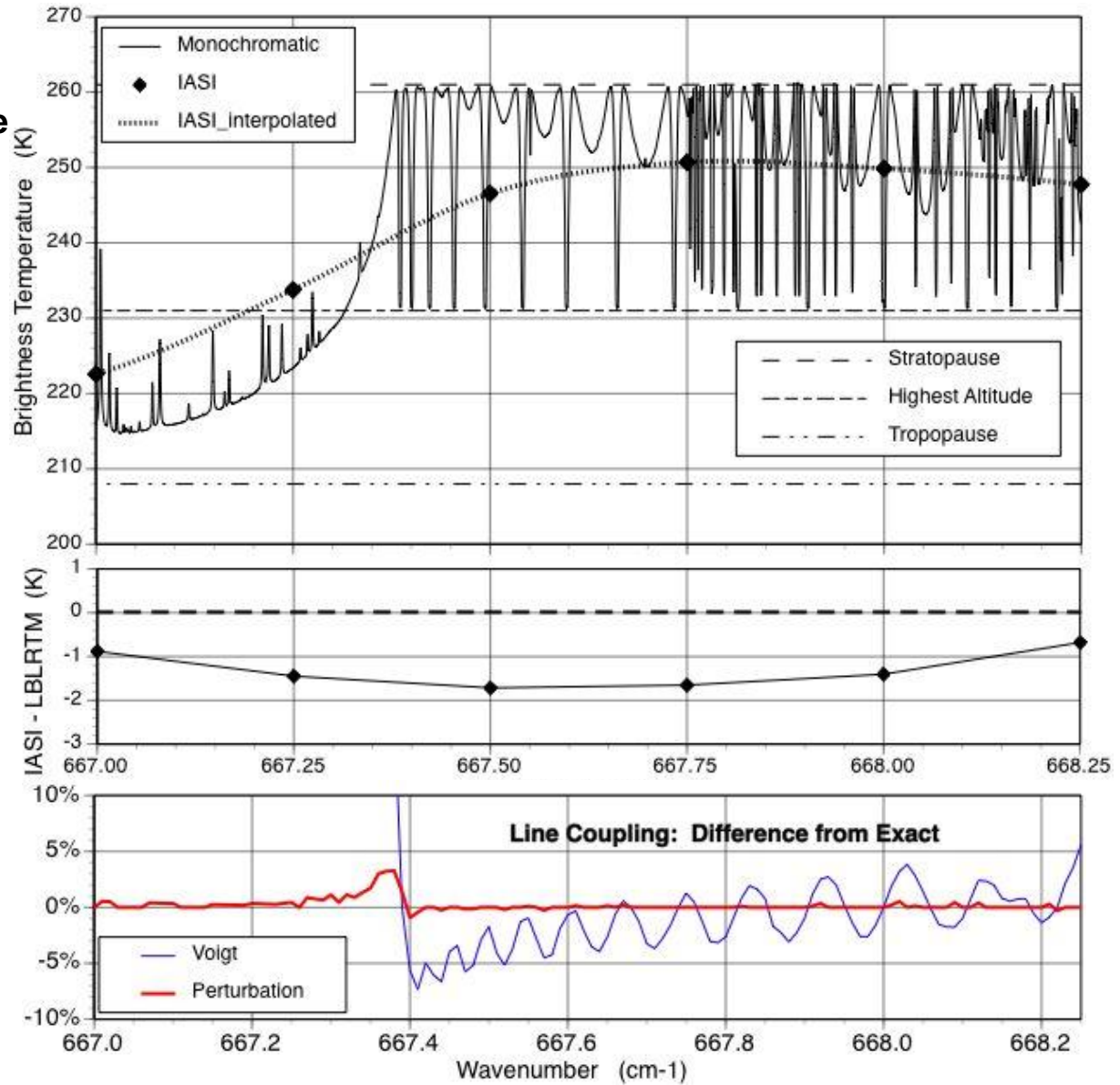
- X Factor
- Sampled 2 cm<sup>-1</sup>
- New definition required
- Temperature dependence ??



## CO2 Q-Branch: 667 cm-1

IASI

Monochromatic Radiance



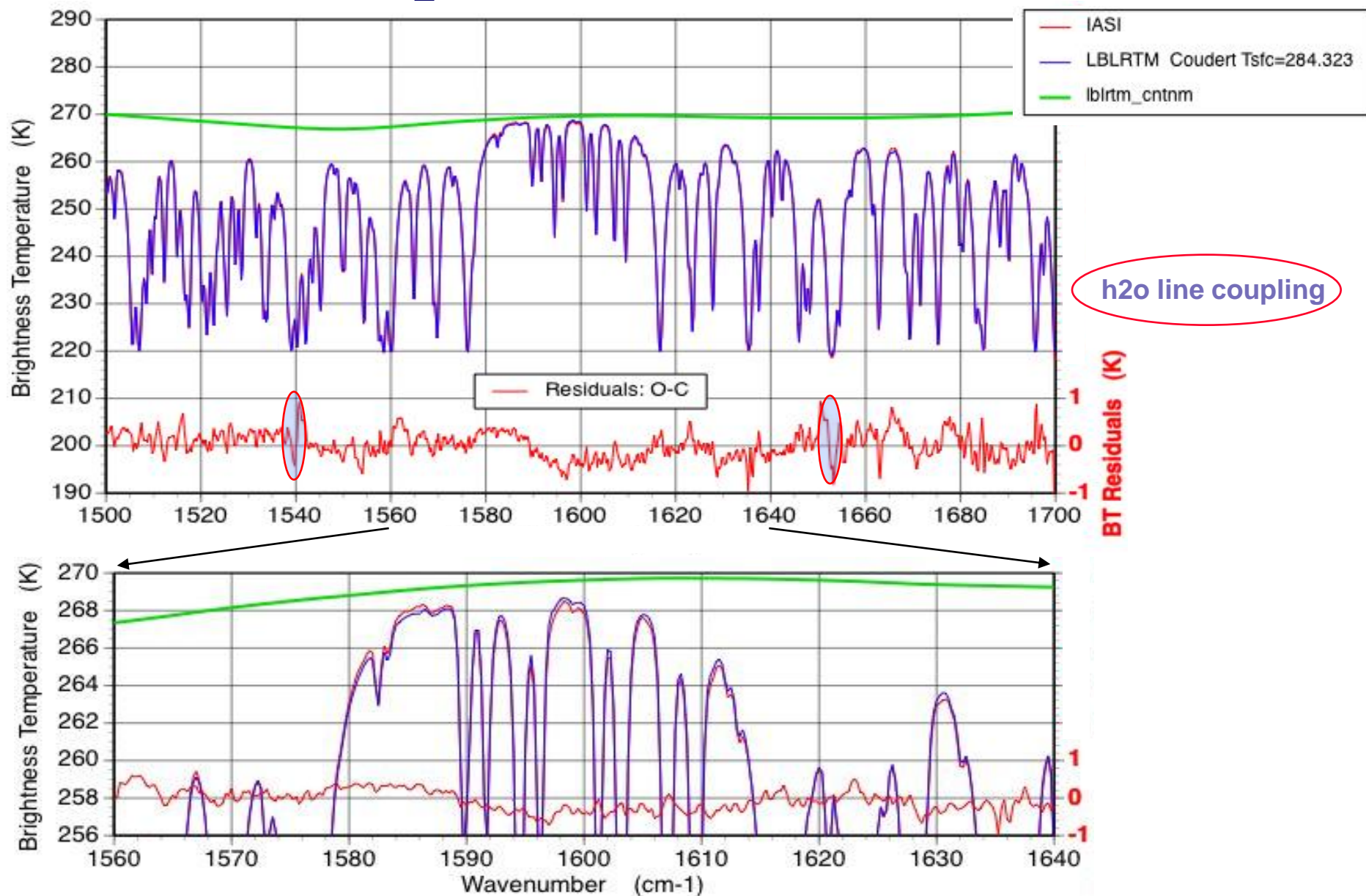
Residuals

Line Coupling:  
% difference from exact

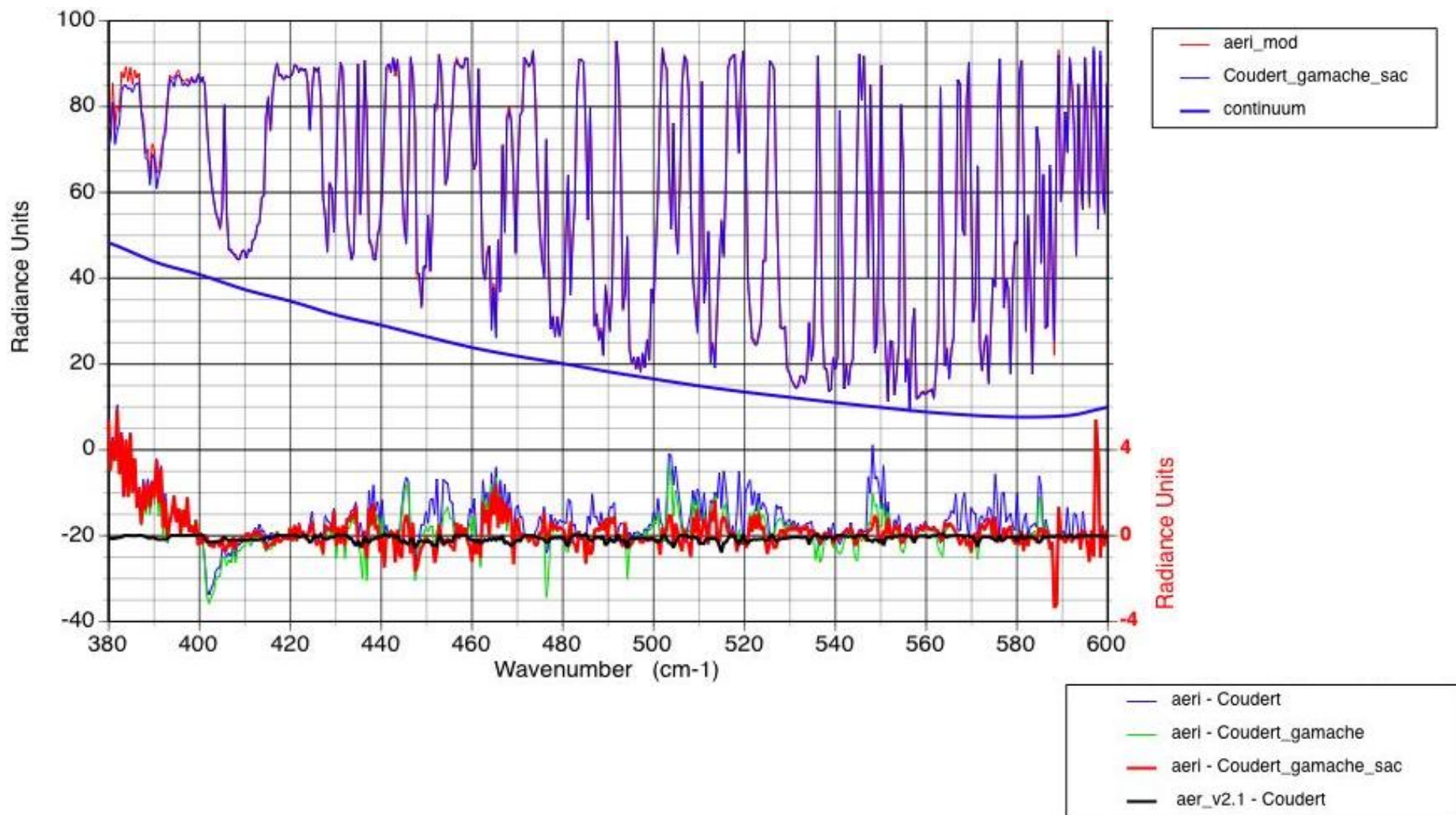
# Water Vapor Retrievals

- **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  $\sim 50 \text{ cm}^{-1}$**
    - **Same line shape is used for every line from the Microwave to UV**
  - **Implications from downwelling spectra at the ARM NSA site.**

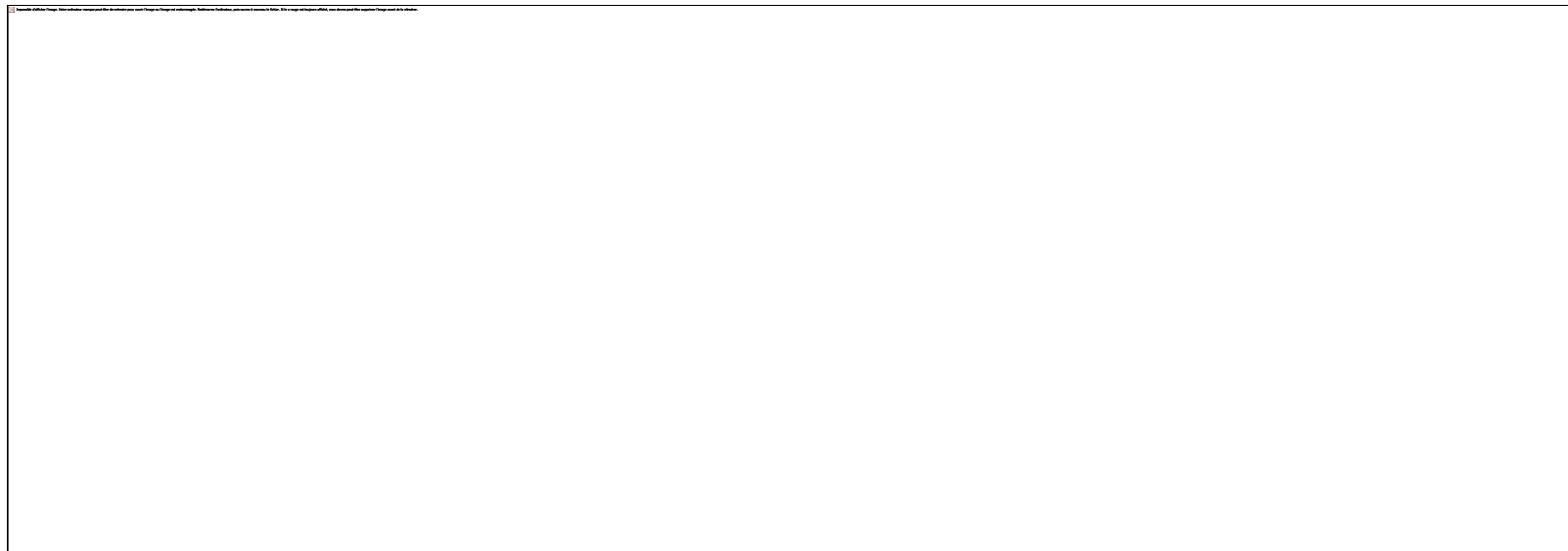
# H<sub>2</sub>O: Detail of Band Center



# AERI Downwelling Radiances ARM NSA Site



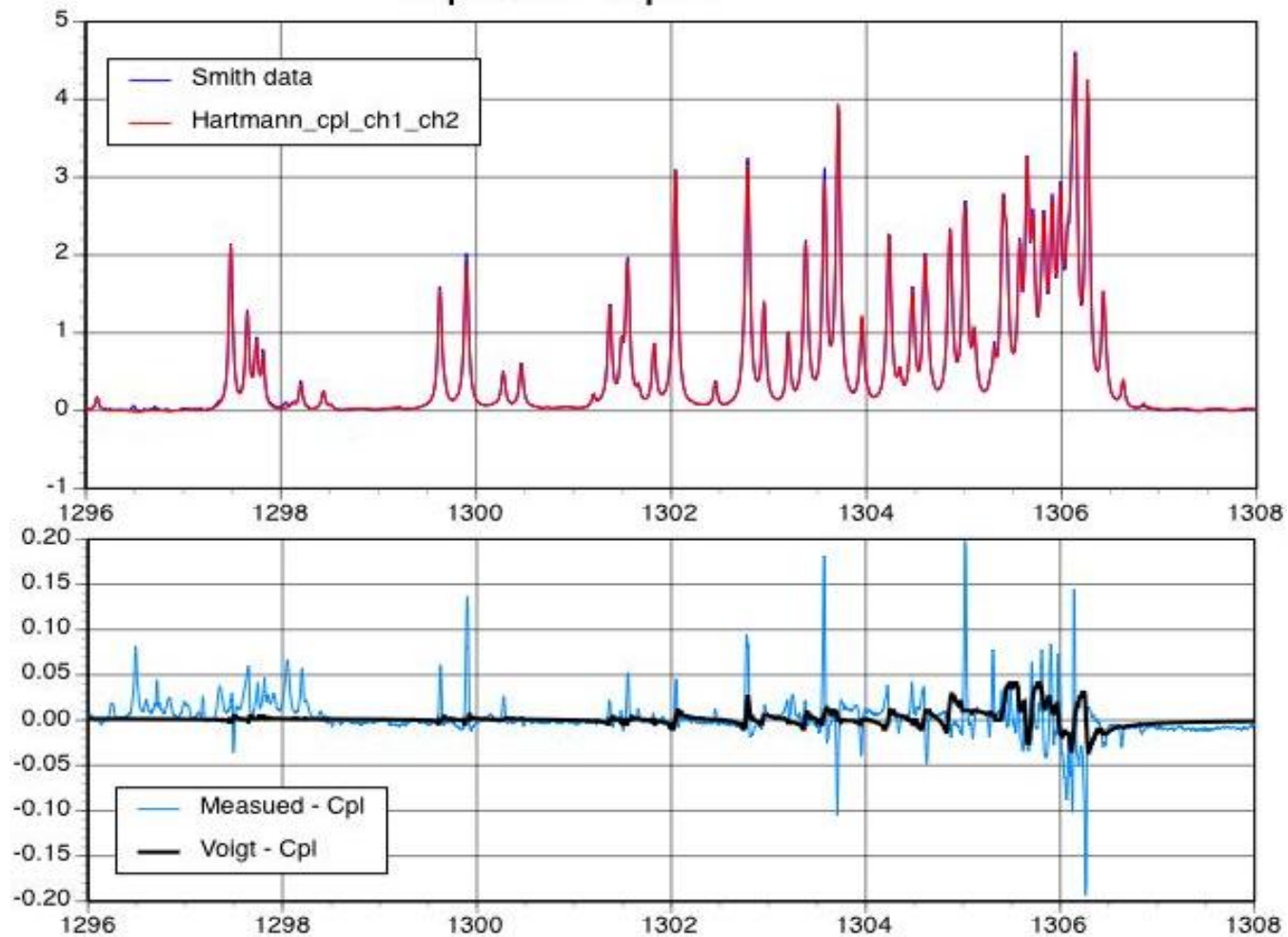
# AERI Downwelling Radiances: 408 cm<sup>-1</sup> ARM NSA Site



							Transition Frequency		Strength	E"	Gamache Width	% Change	"Clough Width"
10	4	6		9	3	7	400.221819	0.259221	1.053E-20	1216.2313	0.0791	-25.0	0.0593
10	6	4		9	5	5	400.481040		1.051E-20	1474.9810	0.0510	-25.0	0.0383



## Optical Depth



# Summary

- **Carbon Dioxide:**
  - Line Coupling is critical!
  - Relaxation Matrix needs adjustment  
and/or
  - Duration of Collision Effects need to be included
  - $\nu_2$  and  $\nu_3$  approaching consistency  $\nu_2$  and  $\nu_3$  approaching consistency
  - $\nu_2$  Q-Branch not yet understood
- **Water Vapor:**
  - Line Intensity Issue  
Coudert Line Parameters have been adopted  
Internal consistency is not necessarily conclusive
  - Residuals are too large (much larger than IASI noise)
  - Line Coupling, Widths, Shifts, Speed Dependent Voigt ?
- **Retrievals for other species are generally very good**
- **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 !***

# Summary

- **Carbon Dioxide:**
  - **Line Coupling is critical!**
  - **Relaxation Matrix needs adjustment  
and/or**
  - **Duration of Collision Effects need to be included**
  - **CO<sub>2</sub> Continuum requires modification**
  - **$\nu_2$  and  $\nu_3$  approaching consistency**
    - Tashkun  $\nu_3$  line parameters to be evaluated**
  - **$\nu_2$  Q-Branch not yet understood**

# Summary

- **Water Vapor:**
  - **Line Intensity Issue**
    - Coudert Line Parameters have been 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**

# More Spectroscopy Than You Ever Hoped to Hear About

**Tony Clough**

**Advanced High Spectral Resolution Infrared Observations  
EUMETSAT**

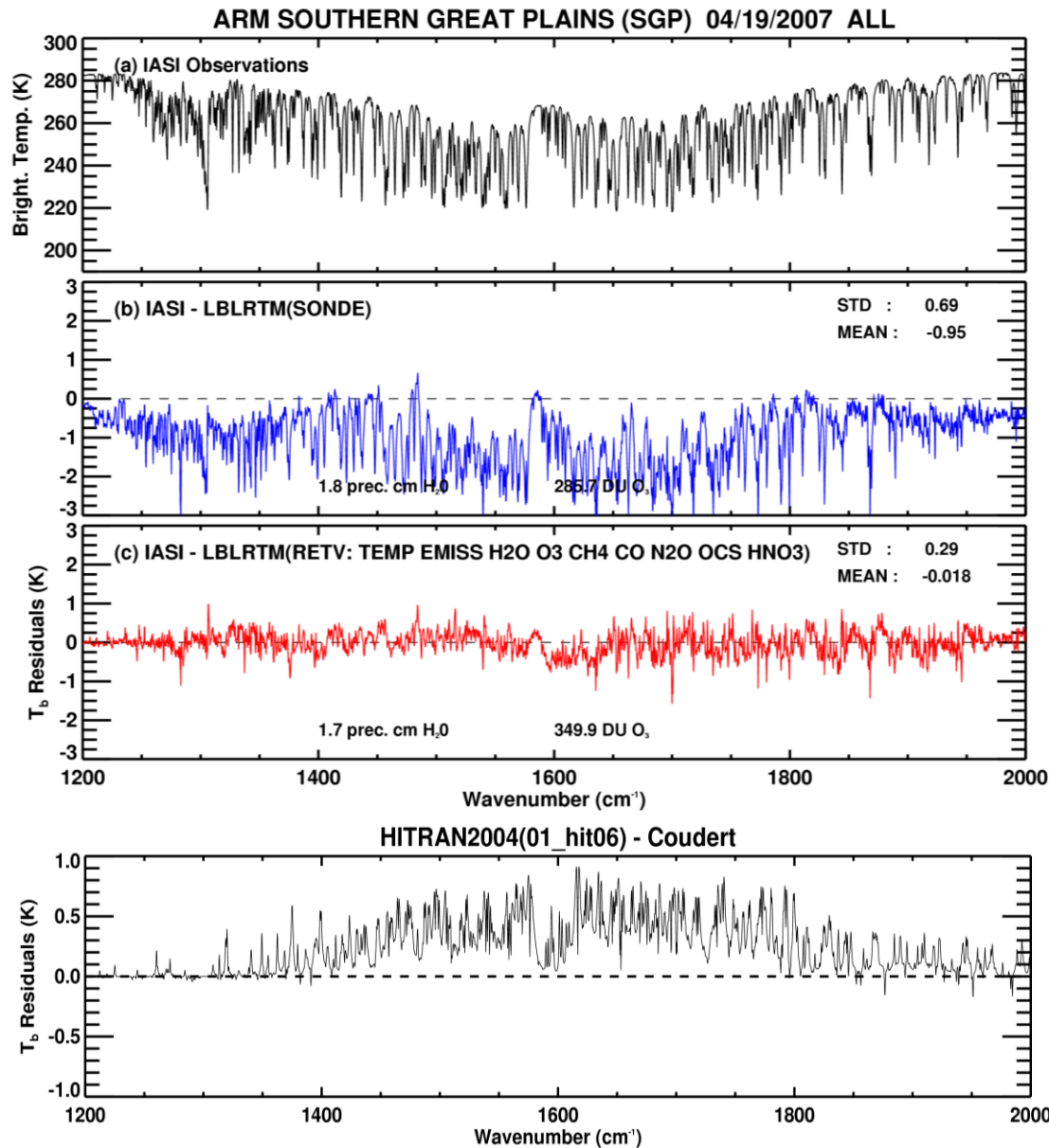
**16 September 2008**

# 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

# Water Vapor $\nu_2$ Region



Larger residuals remain:

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

Coudert water vapor intensities?

# AERI Downwelling Radiances

## ARM NSA Site



Transition Frequency								Strength	Gamache Width	% Change	"Clough Width"	Self Width
396.432560	8	2	6	7	1	7		2.396E-20	0.0807	-7.5	0.0746	0.384
397.318923	9	3	6	8	2	7		5.811E-20	0.0804	-7.5	0.0743	0.328
397.675624	10	6	5	9	5	4		3.104E-20	0.0565	-7.5	0.0522	0.301
398.941390	9	7	3	8	6	2		1.825E-20	0.0415	-20.5	0.0330	0.328
398.976486	9	7	2	8	6	3		5.476E-20	0.0414	-20.5	0.0329	0.328
400.221819	10	4	6	9	3	7		1.053E-20	0.0791	-25.0	0.0593	0.301
400.481040	10	6	4	9	5	5		1.051E-20	0.0510	-25.0	0.0383	0.301



# SRF file: srftables\_031115v3.hdf

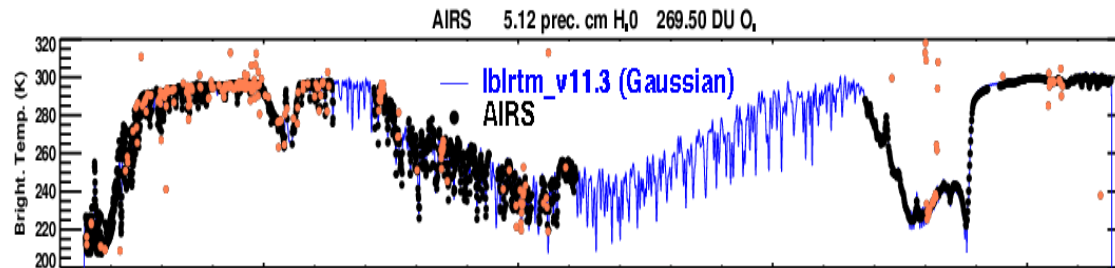
AIRS - sarta (v4,tuned)

AIRS - sarta (v4,untuned)

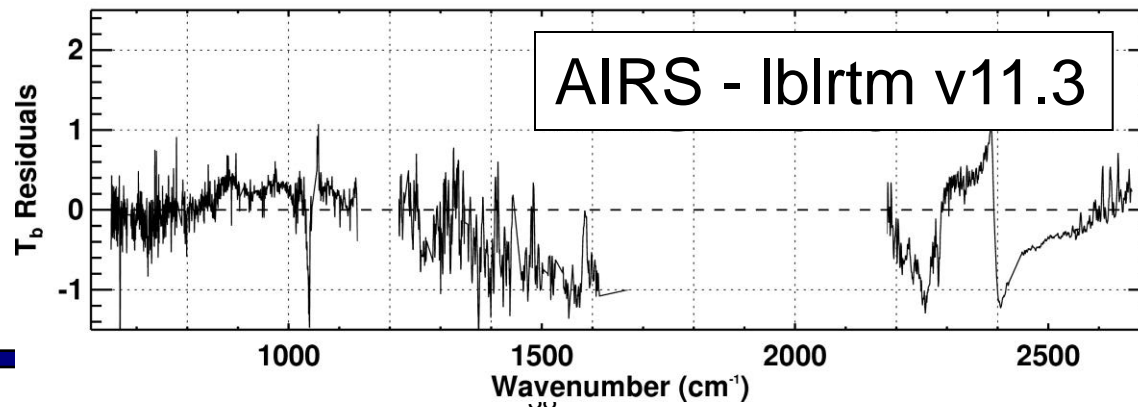
AIRS - lbrtm v11.3

# 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

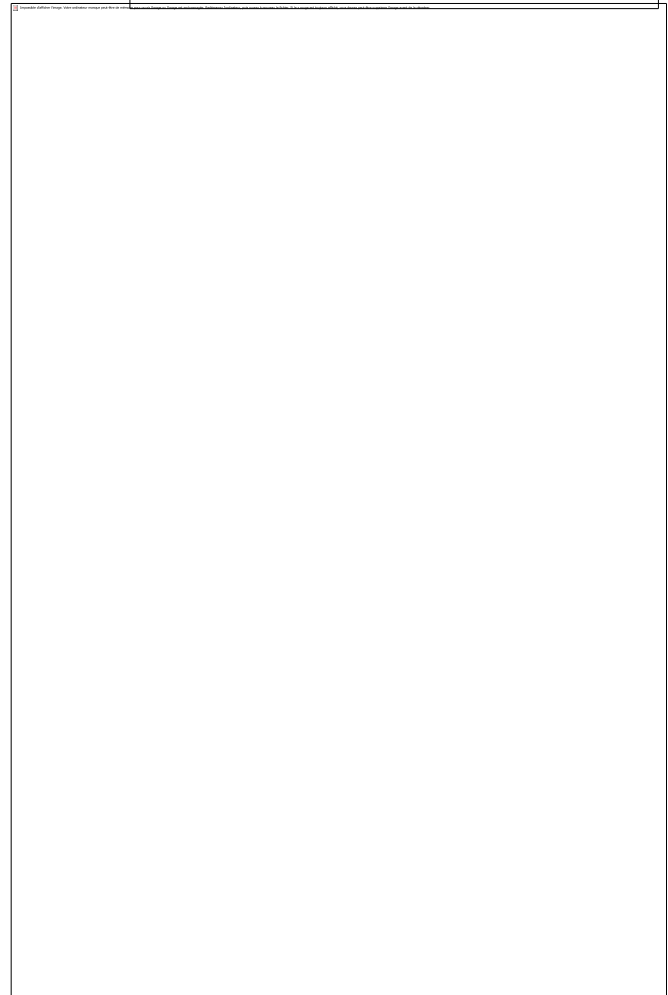
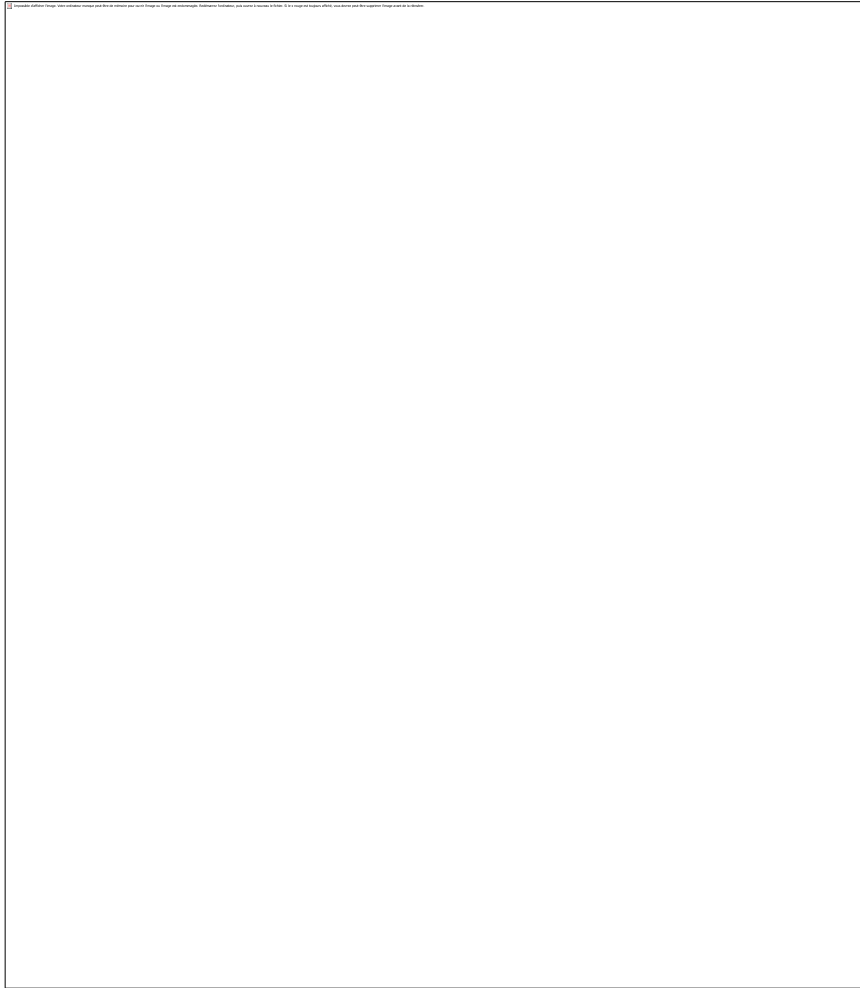


Mean residuals  
for all “clear-  
sky” cases

# Temperature

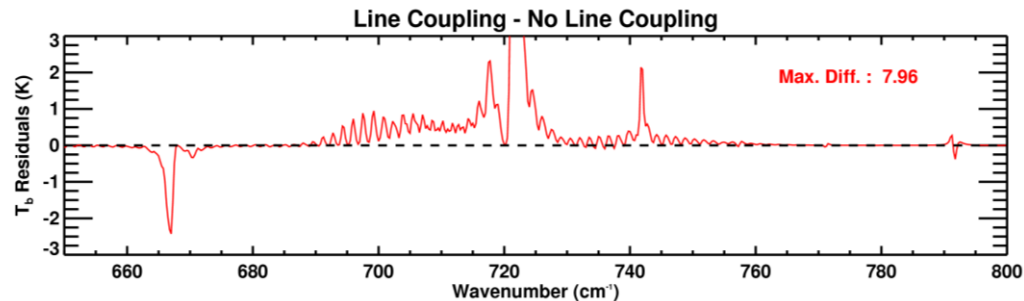
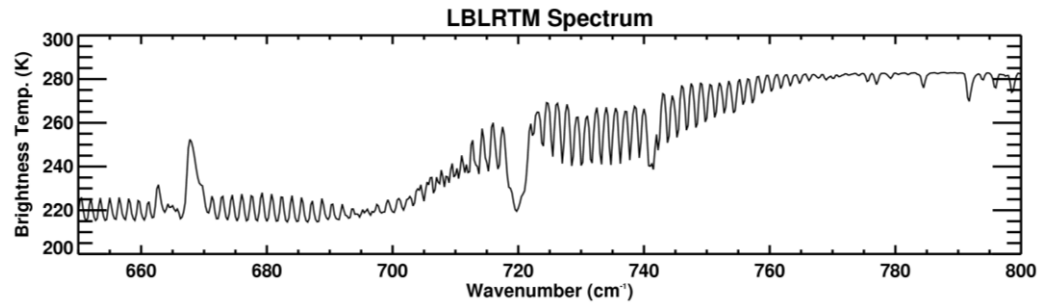
1. Temperature is the degree of hotness or coldness of a body. It is a scalar quantity. It is measured in degrees Celsius (°C) or Kelvin (K). The SI unit of temperature is Kelvin (K). The Celsius scale is based on the freezing and boiling points of water. The Kelvin scale is based on absolute zero, the lowest possible temperature.

2. Temperature is a measure of the average kinetic energy of the particles in a substance. The higher the temperature, the more kinetic energy the particles have. Temperature is a scalar quantity. It is measured in degrees Celsius (°C) or Kelvin (K). The SI unit of temperature is Kelvin (K). The Celsius scale is based on the freezing and boiling points of water. The Kelvin scale is based on absolute zero, the lowest possible temperature.

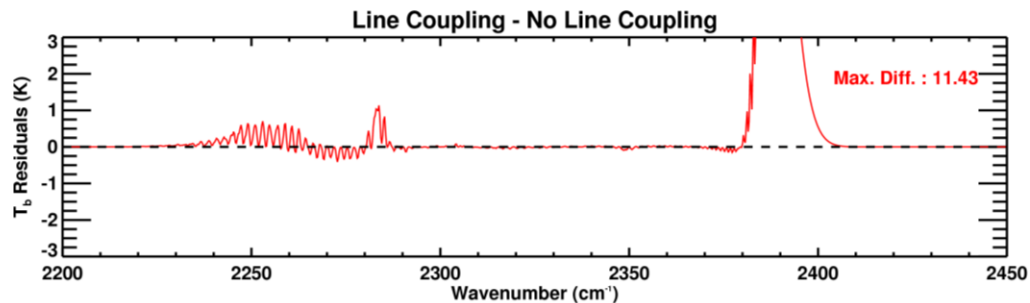
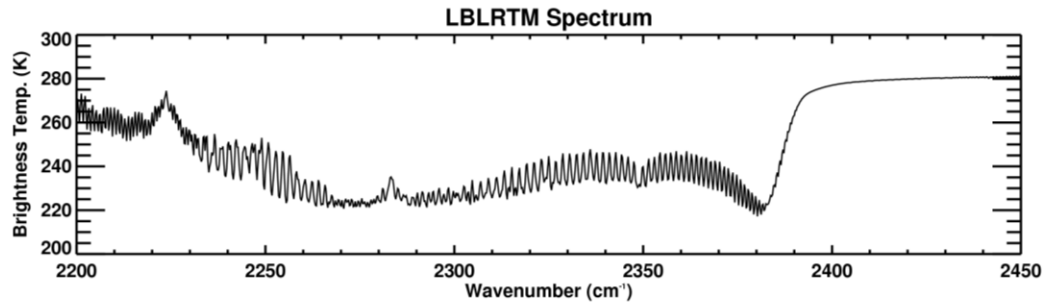


# Impact of CO<sub>2</sub> Line Coupling in the Infrared

CO<sub>2</sub> v<sub>2</sub>



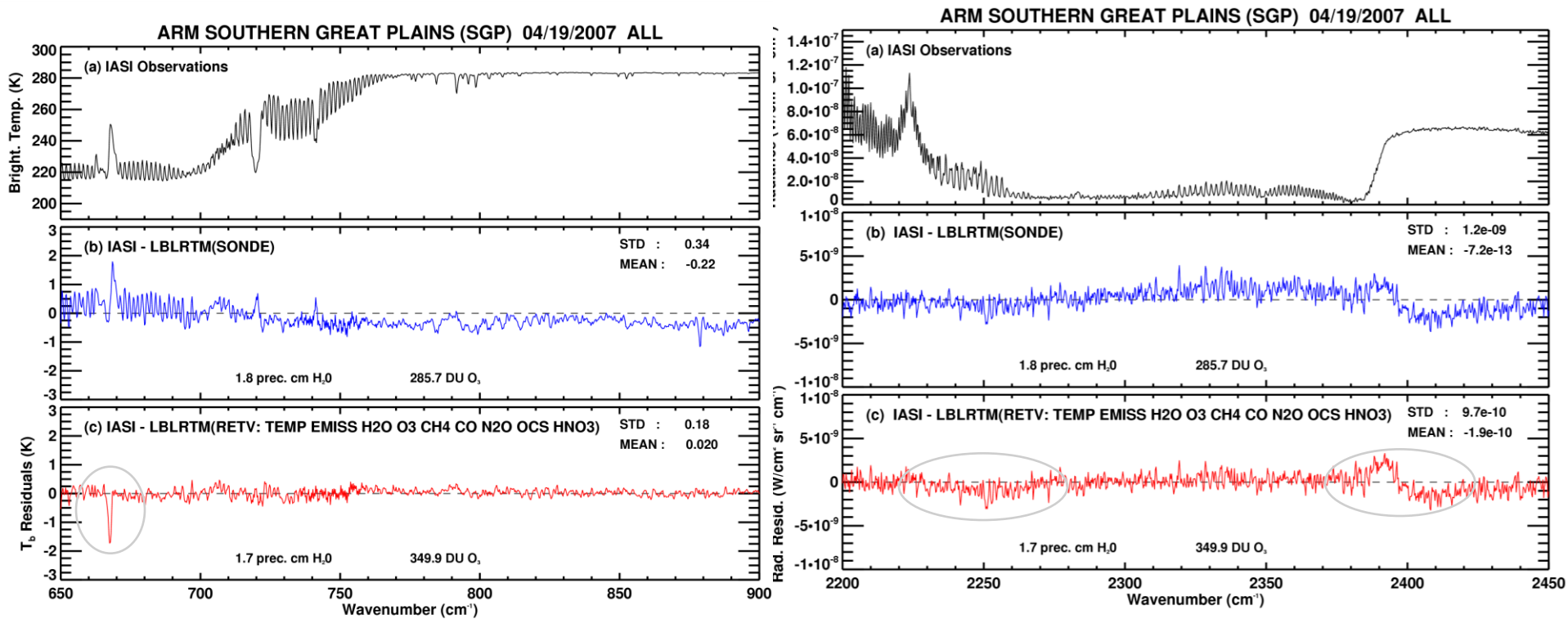
CO<sub>2</sub> v<sub>3</sub>



# Temperature: CO<sub>2</sub> Spectral Regions

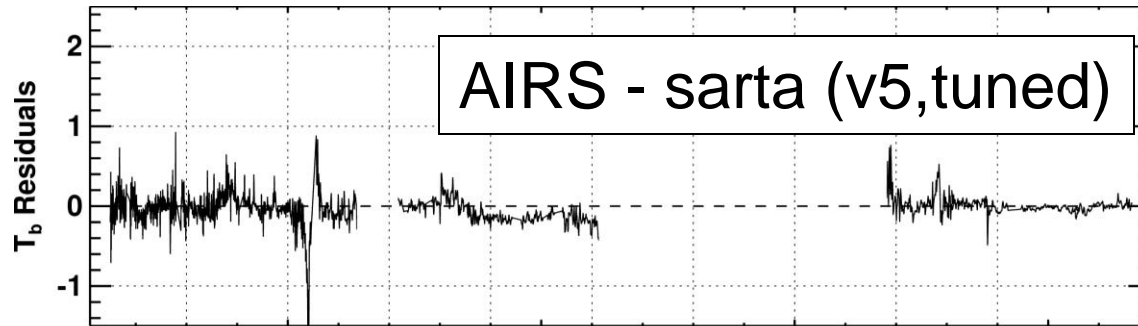
CO<sub>2</sub> v<sub>2</sub>

CO<sub>2</sub> v<sub>3</sub>

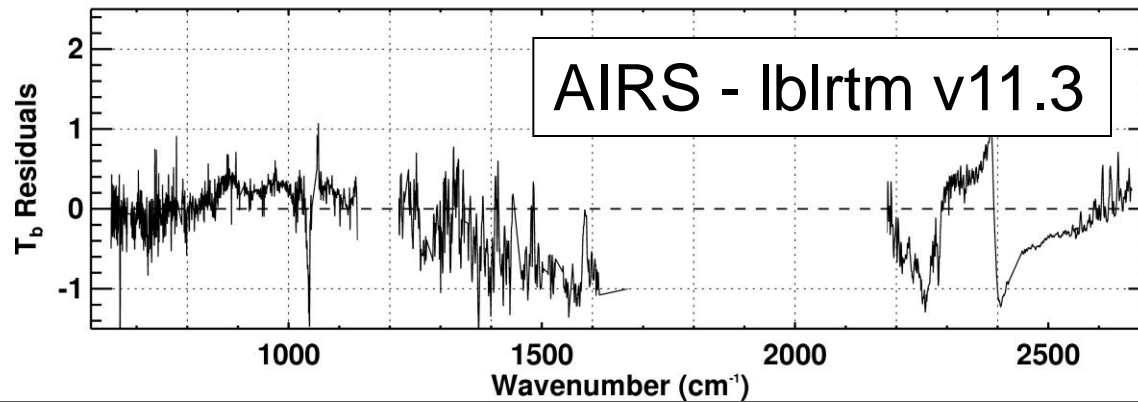


# SRF file: srftables\_051118v4.hdf

(d)



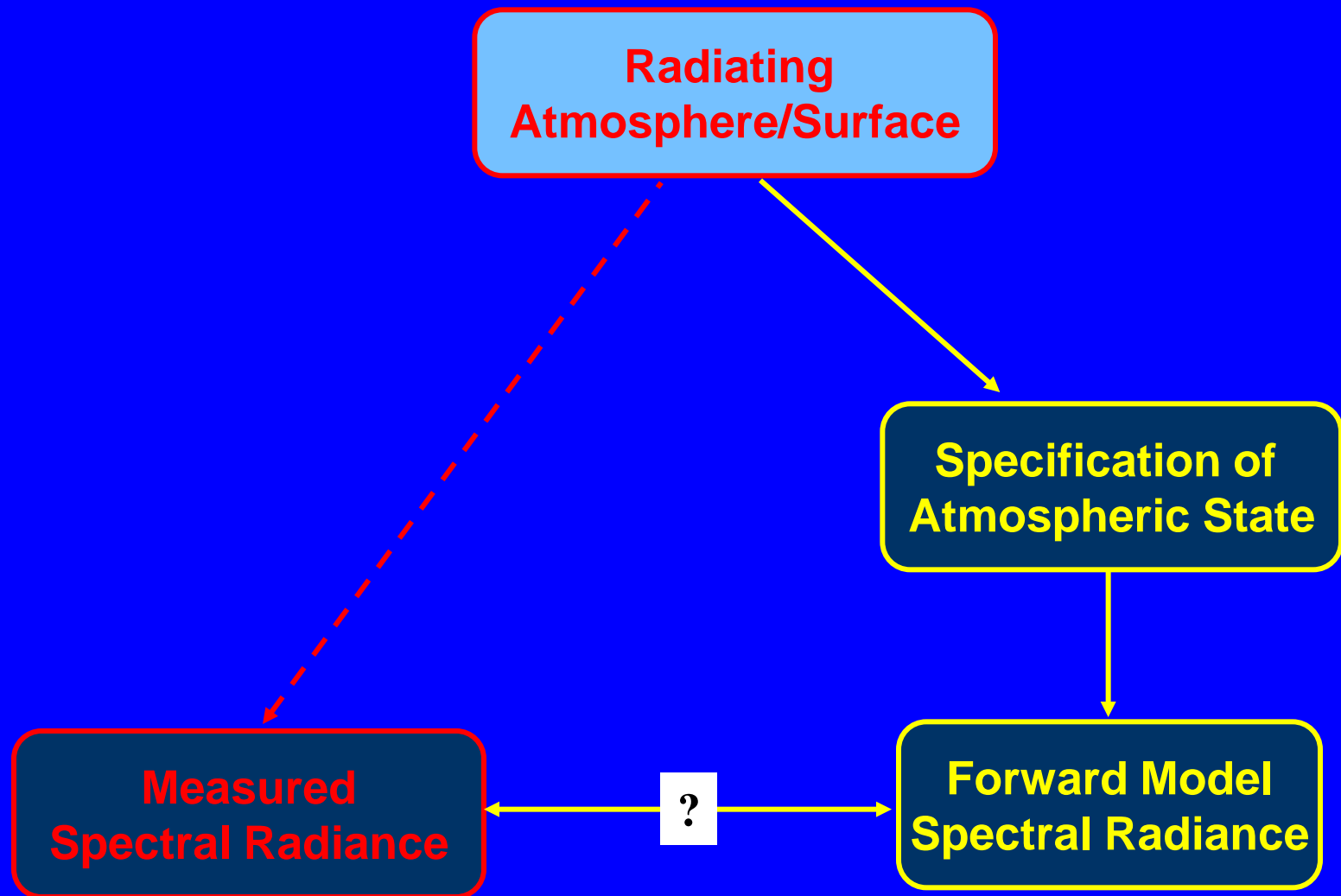
(e)



## Water Vapor

Impression d'effectuer l'image, toute information manque peut être de mémoire pour votre image ou l'image est endommagée. Habituellement l'ordinateur, est connecté à l'écran. Si le message est toujours affiché, vous devez peut-être supprimer l'image avant de la réinstaller.

 Example: If you have 100% of the supply, you can put the supply on the market for 100% of the time. If you have 50% of the supply, you can put the supply on the market for 50% of the time. If you have 25% of the supply, you can put the supply on the market for 25% of the time. If you have 10% of the supply, you can put the supply on the market for 10% of the time. If you have 5% of the supply, you can put the supply on the market for 5% of the time. If you have 1% of the supply, you can put the supply on the market for 1% of the time. If you have 0% of the supply, you can put the supply on the market for 0% of the time.

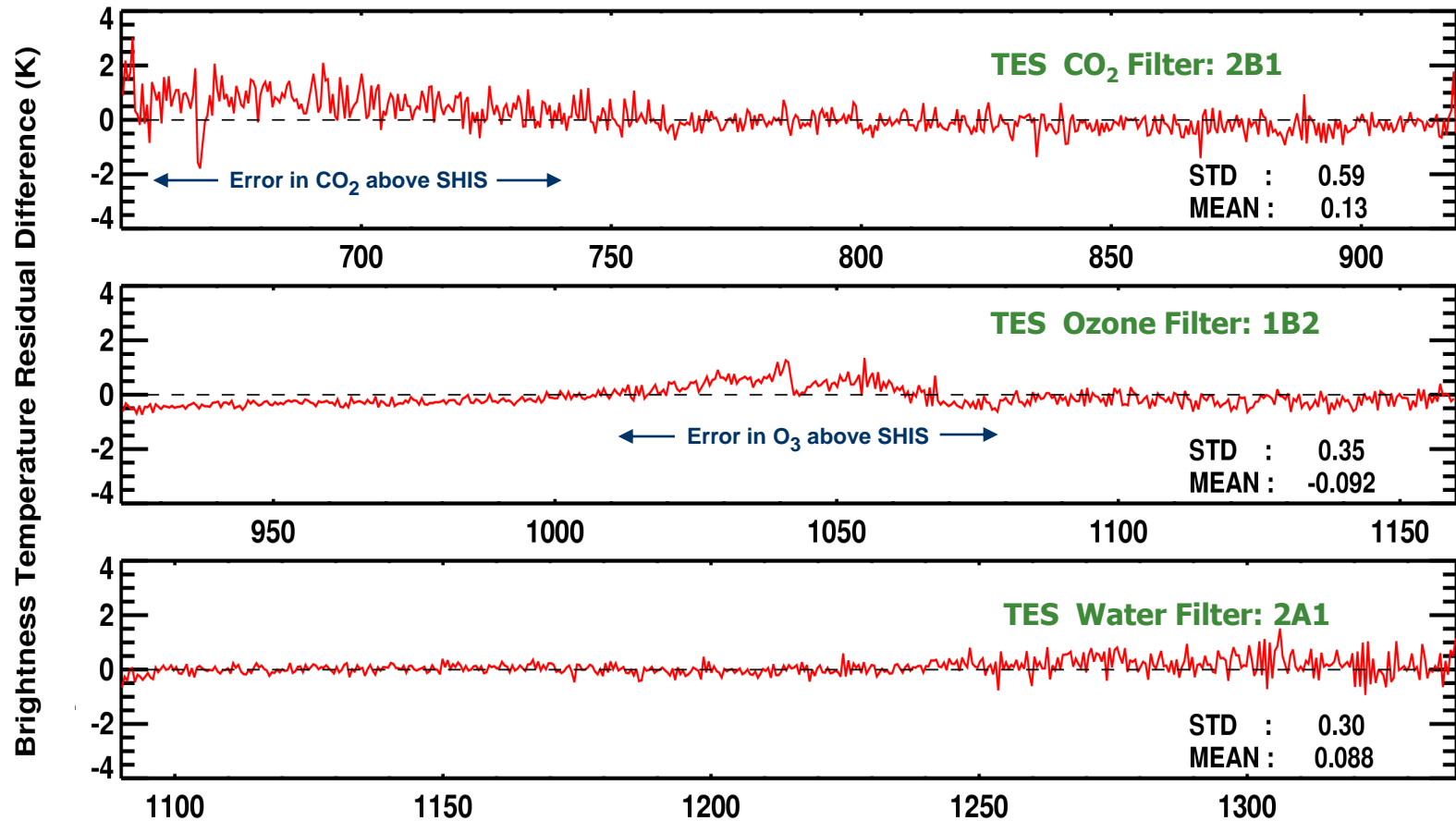




## TES - SHIS Radiance Comparison

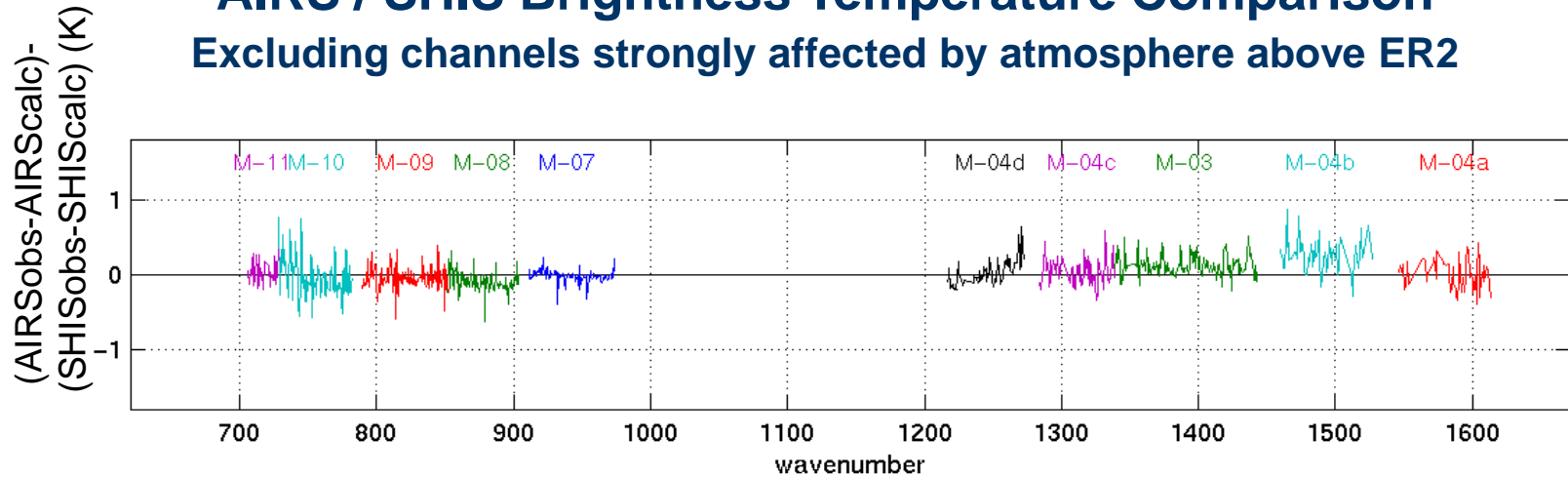
- TES Convolved to SHIS ILS
- $\{\text{TES} - \text{LBLRTM}(\text{TES Geometry})\} - \{\text{SHIS} - \text{LBLRTM}(\text{SHIS Geometry})\}$

Aura Validation Experiment (AVE) 11/07/04 2298\_0003\_10

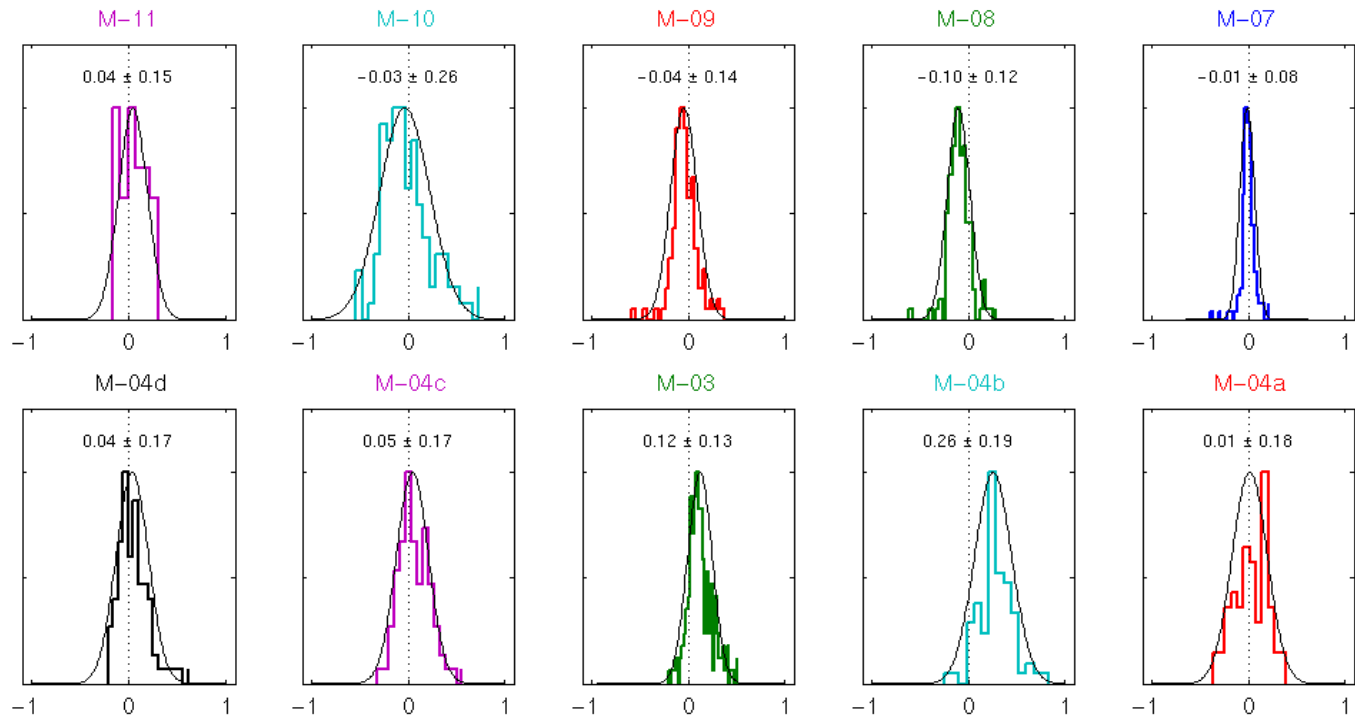


# AIRS / SHIS Brightness Temperature Comparison

## Excluding channels strongly affected by atmosphere above ER2

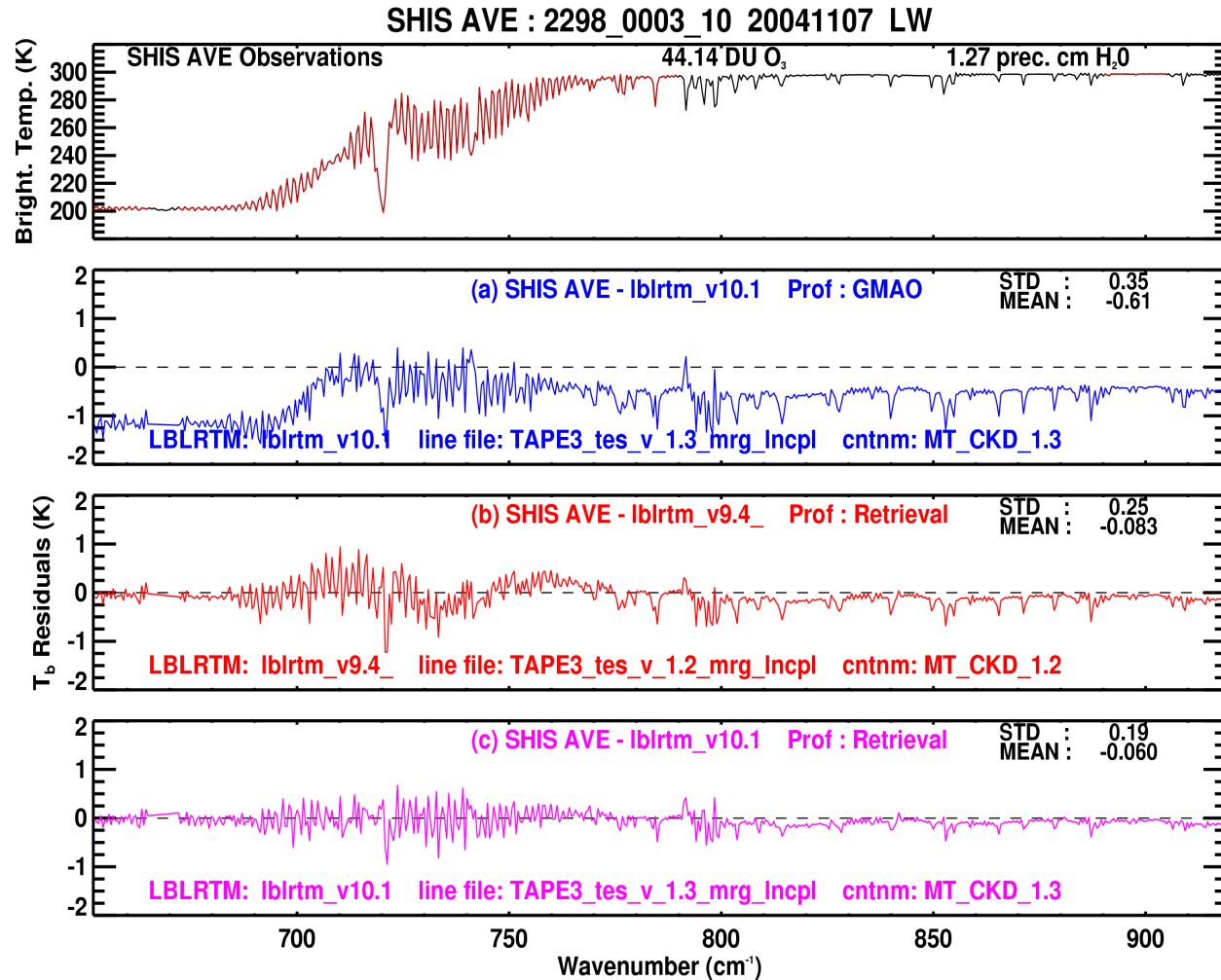


Histograms



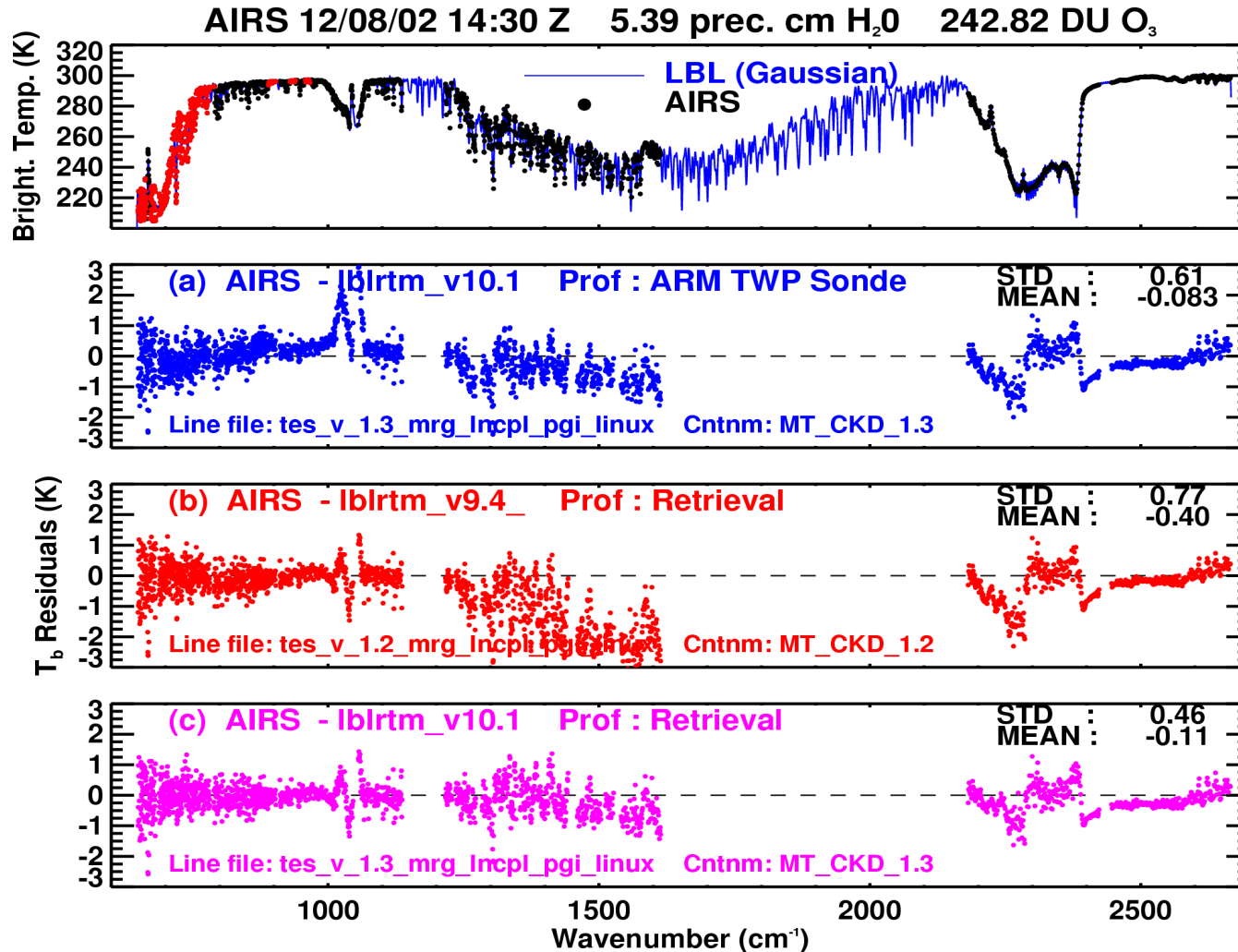
# SHIS Analysis from AURA Validation Experiment Gulf of Mexico - no sonde

M. W. Shephard and S. A. Clough, (AER) 12 Jun 06 18:57



# 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:**
  - **$\chi$  factor and continuum strongly influenced by line coupling**
  - **need to introduce small  $\chi$  factor for duration of collision effects**
  - **CO<sub>2</sub> Continuum has been reduced by 25% for best fit at bandhead**
- **$\nu_2$  and  $\nu_3$  are apparently not yet fully consistent**
- **Line Coupling for N<sub>2</sub>O**
- **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

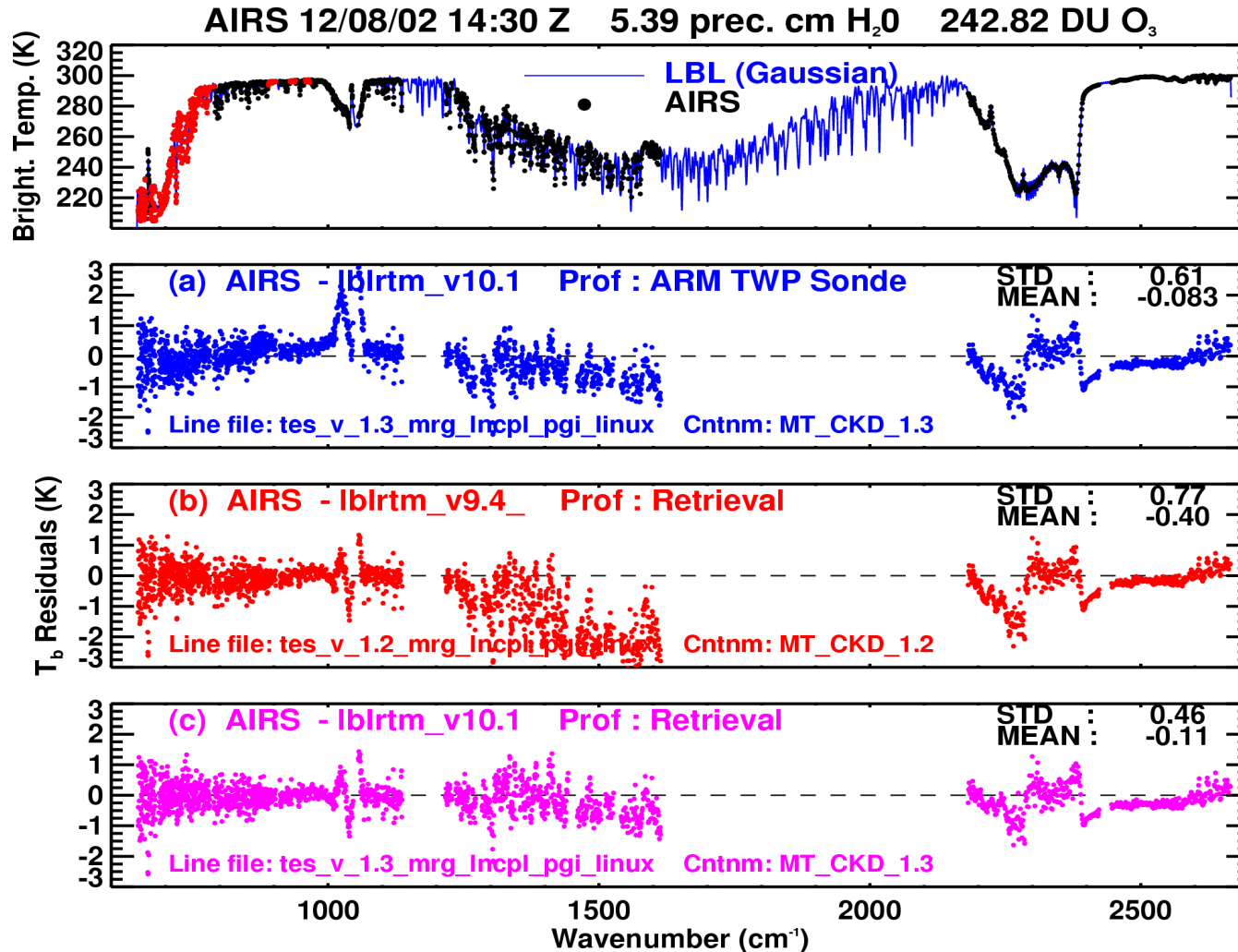
- Line wing formalism constrained by the known physics with relevant parameters ( $\sim 2$ ) determined from laboratory and **atmospheric** Measurements
- Same line shape is used for every line from the Microwave to 20,000  $\text{cm}^{-1}$

## 2. Collision-Induced contribution

- **Provides the extra absorption previously provided by the 'super Lorentzian' chi factor**
- **Based on dipole allowed transitions with widths  $\sim 50 \text{ cm}^{-1}$**
- **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  $\text{cm}^{-1}$

# 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  $\text{cm}^{-1}$  (microwave); 400-500  $\text{cm}^{-1}$ ; 800 -1300  $\text{cm}^{-1}$ ; and 2500-2700  $\text{cm}^{-1}$  (SST)
- Validations needed 10-400  $\text{cm}^{-1}$  and Shortwave
- Temperature Dependence! Laboratory Measurements (Lafferty)
- MT\_CKD Water Vapor Continuum is publicly available
  - <http://rtweb.aer.com>