CRA

Forward Modeling for
Microwave and Infrared Remote Sensing:
Spectroscopic Issues and Line-by-Line Modeling

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and a host of colleagues

Joint Center, Camp Springs, MD

15 Sep 2010

LBL Heritage and Presentation Outline

FASCODE	**AFGL**	**F**ast **A**tmospheric **S**ignature **CODE**	*1977*
LBLRTM	**AER**	**L**ine **B**y **L**ine **R**adiative **T**ransfer **M**odel	*1983*
LBL_CRA	**CRA**		*2010*

Outline

- **Emphasis on Physics**
- **Background and Intellectual Underpinnings**
- **Line Shape**
- **Line Coupling**
- **Validation Issues**
- **Validation Cases**
  - **AERI**
  - **IASI**
- **To Do List**
- **Summary**

Related Models

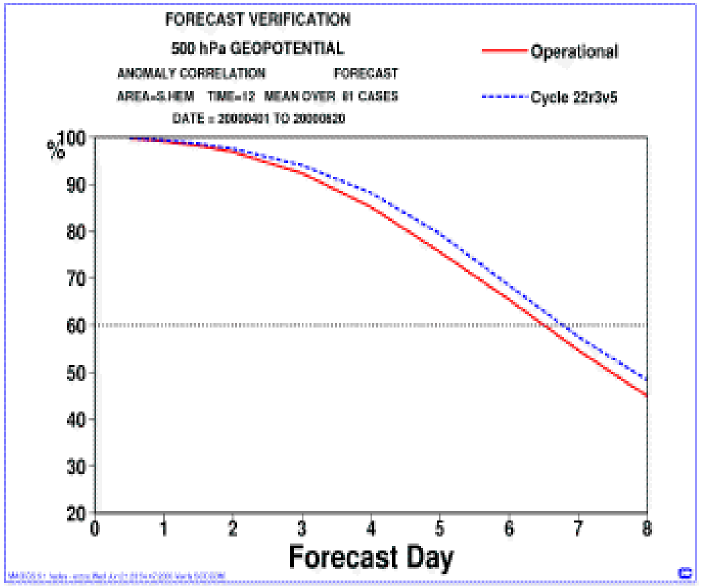
LBLxxx		Clough et. al.
CHARTS	Multiple scattering Adding Doubling Method	Moncet and Clough
• **MonoRTM**	MonochromRTM for limited # of frequencies e.g. microwave	Boukabara, Cady-Pereira and Clough
DISORT	Multiple Scattering Discrete Ordinate Method	Stamnes and Wiscombe
• **RRTM***	Rapid RTM General Circulation Models	Mlawer and Clough
• **OSS**	Optimal Spectral Sampling	Moncet
• **MT_CKD**	Continuum	Mlawer, Payne and Clough

* adjoint easily developed due to coding attributes (next slide)

Physics consistent with LBLxxx in these models !

Example of Code Utilization

Acceptance of RRTM by the GCM community is a direct consequence of the acknowledged accuracy of LBLRTM



Main features of the McRad radiation package

The main features of the McRad radiation package are summarised in the table

	$RRTM_{LW}$	$RRTM_{SW}$
Solution of Radiation Transfer Equation	Two-stream method	Two-stream method
Number of spectral intervals	16 (140 g-points)	14 (112 g-points)
Absorbers	H_2O, CO_2, O_3, CH_4, N_2O, CFC_{11}, CFC_{12}, aerosols	H_2O, CO_2, O_3, CH_4, N_2O, CFC_{11}, CFC_{12}, aerosols
Spectroscopic database	HITRAN, 1996	HITRAN, 1996
Absorption coefficients	From LBLRTM line-by-line model	From LBLRTM line-by-line model
Cloud handling	True cloud fraction	True cloud fraction
Cloud optical properties method	16-band spectral emissivity	14-band τ, g, ω
Data: ice clouds	Ebert & Curry, 1992 Fu et al., 1998*	Ebert & Curry, 1992 Fu, 1996*
Data: water clouds	Smith & Shi, 1992 Lindner & Li, 2000*	Fouquart, 1987 Slingo, 1989*
Cloud overlap assumption set up in cloud generator	Maximum-random or generalised*	Maximum-random or generalised*
References	Mlawer et al., 1997 Morcrette et al., 2001	Mlawer & Clough, 1997

LBL Model Attributes

- **Computational Accuracy**

Voigt Line Shape	Planck Fn	Layer Merging	Optical Depth	Radiance
0.1%	0.05%	0.1%	0.1%	0.1%

- **Computational Gain**

Optimal Sampling	Voigt Line Shape	Line Coupling^{2nd}	Planck Fn
10x	10x	10x	2x

Computational gain can be utilized to do more complicated problems in the same amount of time

- **Attributes**
  - Linear Algebra wherever possible
  - Piecewise continuous wherever possible
  - Planck Fn ‘linear in tau’ across inhomogeneous layer
  - Voigt Fn obtained as a linear combination of precalculated functions
  - Units: cgs
  - Line Coupling (second order)
  - NonLTE
  - Analytic Derivatives
  - Logical structure of high order
  - Modular and proven very flexible
  - Coding: **Horrendous**

Formalism for LBL Calculations

- Validity from Microwave through Solar UV
- Detail Balance across entire extent of the line
  - Radiance = Planck_Fn * [1 - Transmittance]

A Bit of History: With a nod to heroes of the profession!

Problem: (~1972)

Incoherent understanding of line shape associated with binary collisions

What is the validity of the impact line shape ?

What is the line shape far from line center that satisfies the physical constraints?

Development of a Water Vapor Continuum Model (Clough and Kneizys 1975)

- Phillip Anderson thesis (student of Van Vleck) (1950)
- Huber and Van Vleck I (1966)
- Huber and Van Vleck II (1972)
- John Van Vleck (Rev Mod Phys; 1978)

Formalism for LBL Calculations II

$$k(\nu) = \nu \left\{ \frac{1-e^{-hc\nu/kT}}{1+e^{-hc\nu/kT}} \right\} \qquad \mathrm{Im} < \phi(\nu) + \phi(-\nu) >$$

$$k(\nu) = \nu \ \tanh\left(hc\nu/2kT\right) \qquad \mathrm{Im} < \phi(\nu) + \phi(-\nu) >$$

radiation field

molecular system ⇔ radiation interaction

(line shape)

<symmetrized spectral density function>

- Radiation balance is satisfied over the full extent of the spectral line irrespective of accuracy of $\phi(\nu)$!
- F-sum rule rigorously satisfied: integral over ν ? value of the band strength
- Led to the development of the CKD continuum model

Impact Result:

$$\approx \nu \left\{ \frac{1-e^{-hc\nu/kT}}{1+e^{-hc\nu/kT}} \right\} < S_i(T) \frac{1}{\pi} \left[\frac{\alpha_i P}{(\nu_i+\nu)^2 + (\alpha_i P)^2} + \frac{\alpha_i P}{(\nu_i-\nu)^2 + (\alpha_i P)^2} \right] >$$

Microwave:

$$\approx \frac{hc\nu^2}{2kT} < S_i(T) \frac{1}{\pi} \left[\frac{\alpha_i P}{(\nu_i+\nu)^2 + (\alpha_i P)^2} + \frac{\alpha_i P}{(\nu_i-\nu)^2 + (\alpha_i P)^2} \right] >$$

Van Vleck - Weisskopf
Gross, etc. xxx

Infrared:

$$\approx \nu \quad < S_i(T) \frac{1}{\pi} \left[\frac{\alpha_i P}{(\nu_i-\nu)^2 + (\alpha_i P)^2} \right] >$$

Lorentz

LBL Model

Atmosphere (lblatm)

Loop over Layers (xlayer)

Opt_Dpth (hirac)

Radiance (xmerge)

Postprocessing (e.g. fftscan)

Databases

Prestored Atmospheres

- Line parameters
- Partition Function
- Continuum
- NonLTE State Populations
- Cross Sections
- Aerosols and Clouds (absorbers)

HiRAC $\Leftrightarrow \langle \phi(\nu) + \phi(-\nu) \rangle$

High **R**esolution **A**bsorption **C**oefficient

Formalism for LBL Calculations III

Impact Approximation »» Duration of Collision »» $\chi(\nu_i - \nu)$ factor

$$k(\nu) \approx \nu \left\{ \frac{1 - e^{-hc\nu/kT}}{1 + e^{-hc\nu/kT}} \right\} < \tilde{S}_i(T) \frac{1}{\pi} \left[\frac{\alpha_i P}{(\nu_i + \nu)^2 + (\alpha_i P)^2} \chi(\nu_i + \nu) + \frac{\alpha_i P}{(\nu_i - \nu)^2 + (\alpha_i P)^2} \chi(\nu_i - \nu) \right] >$$

		grade		grade
$\tilde{S}_i(T)$	Strength	A+		
$\nu_i \Rightarrow \nu_i + \delta_i(P, T)$	Line Position	A++	Pressure Shift	C/D
$\alpha_i \Rightarrow \alpha_i \gamma_i^{T/T_0}$	Width	B	T Dependence	C
$\chi(\nu_i - \nu)$	χ Fn	?		

Line Coupling

The task is to evaluate the collision operator in Liouville (line) space: $[\nu - \nu_0 - i\, \mathrm{P} \bullet \mathrm{W}]^{-1}$

$$k(\nu) = \nu \tanh(\beta\nu/2) \;\; \mathrm{Im}[\phi(\nu) + \phi(-\nu)]$$

$$\phi(\nu) = \frac{1}{\Pi} \sum_{jk} \mu_j < j \left| \frac{1}{(\nu - \nu_o) - iPW} \right| k > \mu_k \rho_k$$

μ_k

ρ_k

transition rate operator

diagonalize: $(\nu_o + iPW)$

$$X^{-1}(\nu_o + iPW) X = \lambda' + i\lambda''$$

$$\nu - \nu_o - iPW = X\,(\nu - \lambda' - i\lambda'')\, X^{-1}$$

$$(\nu - \nu_o - iPW)^{-1} = X^{-1}(\nu - \lambda' - i\lambda'')^{-1} X$$

$S_l = \rho_l\, \mu_l^{\,2}$

$$\phi(\nu) = \frac{1}{\Pi} \sum_{jkl} \mu_j\, X_{jl}\, (\nu - \lambda_l' - i\lambda_l'')^{-1}\, X_{lk}^{-1}\, \mu_k\, \rho_k$$

$$= \frac{1}{\Pi} \sum_{l} \frac{(\nu - \lambda_l') + i\lambda_l''}{(\nu - \lambda_l')^2 + (\lambda_l'')^2} \sum_{jk} X_{lh}^{-1} \mu_k \rho_k \mu_{jl}$$

$$\mathrm{Im}\{\phi(\nu)\} = \frac{1}{\Pi} \sum_{l} \frac{\lambda_l'' S_l' + S_l''(\nu - \lambda_l')}{(\nu - \lambda_l')^2 + (\lambda_l'')^2}$$

$S', S'', \lambda', \lambda''$

$$S' = S_l \left(1 + g_l \left(\frac{P}{P_o}\right)^2\right)$$

$$S'' = S_l\, y_l \left(\frac{P}{P_o}\right)$$

$$\lambda'' = \alpha_l \left(\frac{P}{P_o}\right)$$

$$\lambda' = \nu_l + \delta_l \left(\frac{P}{P_o}\right)$$

Line Shape

Line Shape including widths, shifts and line coupling coefficients is the dominant source of error in current radiance calculations

- Doppler — Gaussian
- Collisional — Lorentzian — *frequency of collision: (P/T)*
- Voigt — Convolution of Gaussian with Lorentzian
- Duration of collision — Impact approximation is just that: *line wings must decay exponentially*
- Speed Dependent Voigt — Doppler and Collisional processes are not independent
- Line Coupling — Collisional relaxation matrix between lines required

Thoughts on Forward Model Validation and Spectroscopy

- The atmospheric conditions for which spectroscopic parameters are required are difficult to obtain in the laboratory- for water vapor, essentially impossible (long paths-cold temperatures)
- Spectroscopy error, though small, is the dominant error in most retrievals
- Spectroscopists have been making significant progress
- The OCO experiment has been a great motivator
- A strong commitment to study line shapes was articulated at the HITRAN meeting June 2010
- Nevertheless, improved spectroscopy is needed now!

In situ measurements are simply not adequate

- Spatial and temporal sampling issues
- Accuracy of the measurements themselves is not adequate
- *In situ* measurements are useful: e.g. vertical structure

My perspective is that the atmosphere will have to function as our laboratory

- Focus on a small number of cases (10) spanning a range of atmospheric conditions
- Initial cases: night time over ocean quiet atmosphere

  Progressing to day time cases, land cases always with as quiet an atmosphere as possible
- Spectral residuals to follow are based on *ad hoc* changes in line parameters

  Progressing to retrieval of line parameters from atmospheric spectra (tuning?)

What is Truth?

- **Spectral Residuals are Key!**

?

- **Consistency within a band system**
  - ν_2 band to investigate consistency for H_2O
- **Consistency between bands**
  - 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

Collaborators for IASI Case

- **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 (h2o)**
      - **'Well Characterized'**
  - **2007_04_20** **'Control'**
    - » **Over Gulf of Mexico "**
    - » **Atmosphere**
      - **Broken Clouds and Highly Inhomogeneous (h2o)**
      - **Not So Well Characterized**

Topics / Issues

- **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_2 ν_2 and CO_2 ν_3
    - ✓ Q-Branch 667 cm-1
    - ✓ Band Head 2385 cm-1
  - **Nitrous Oxide**
    - ? Agreement between CO_2 ν_2 and N_2O ν_3
    - » N_2O 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

- **Deserves a slide of its own**
- **Significant improvements but …**

Introduction

IASI

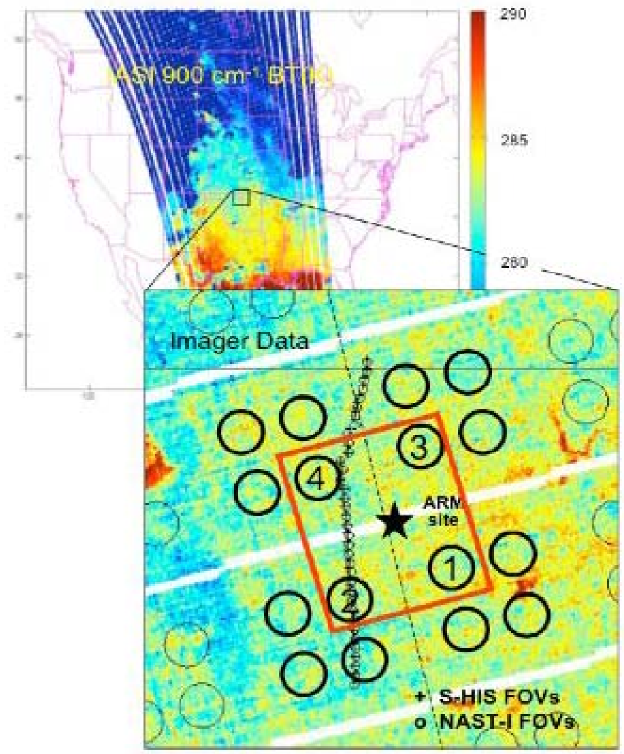
Scan Rate	8 secs
Scan Type	Step and dwell
Pixel IFOV	0.8225°
IFOV size at Nadir	**12 km**
Sampling at Nadir	18 km
Earth View Pixels / Scan	2 rows of 60 pixels each
Swath	± 48.98°
Swath	± 1066 km
Spectral Range	645 to 2760 cm-1
Resolution (hw/hh)	**0.25 cm-1**
Lifetime	5 years
Power	210 W
Size	1.2 m x 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.**

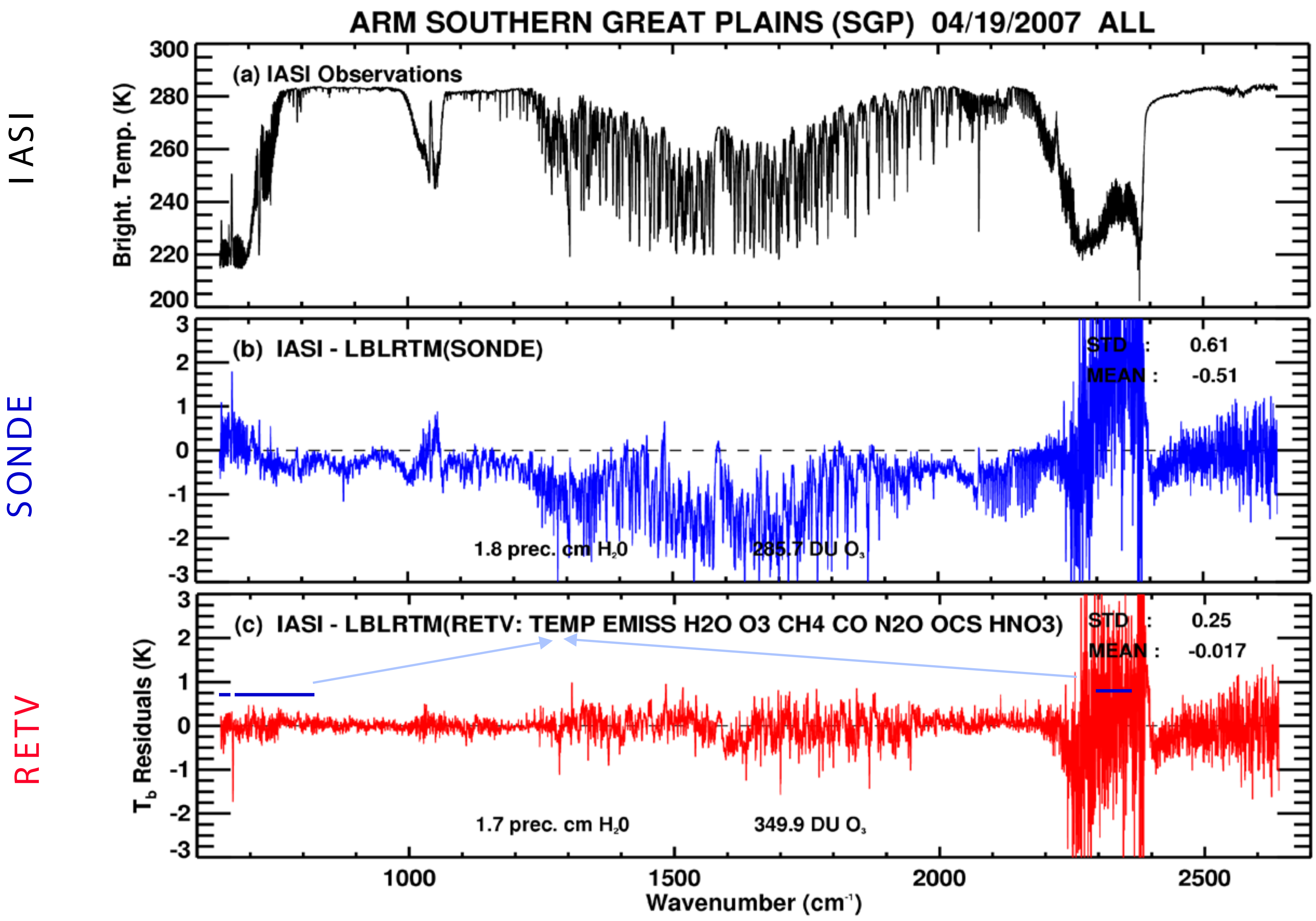
Joint Airborne IASI Validation Experiment

JAIVEx 19 Apr 2007

CART-site (03:35 UTC)



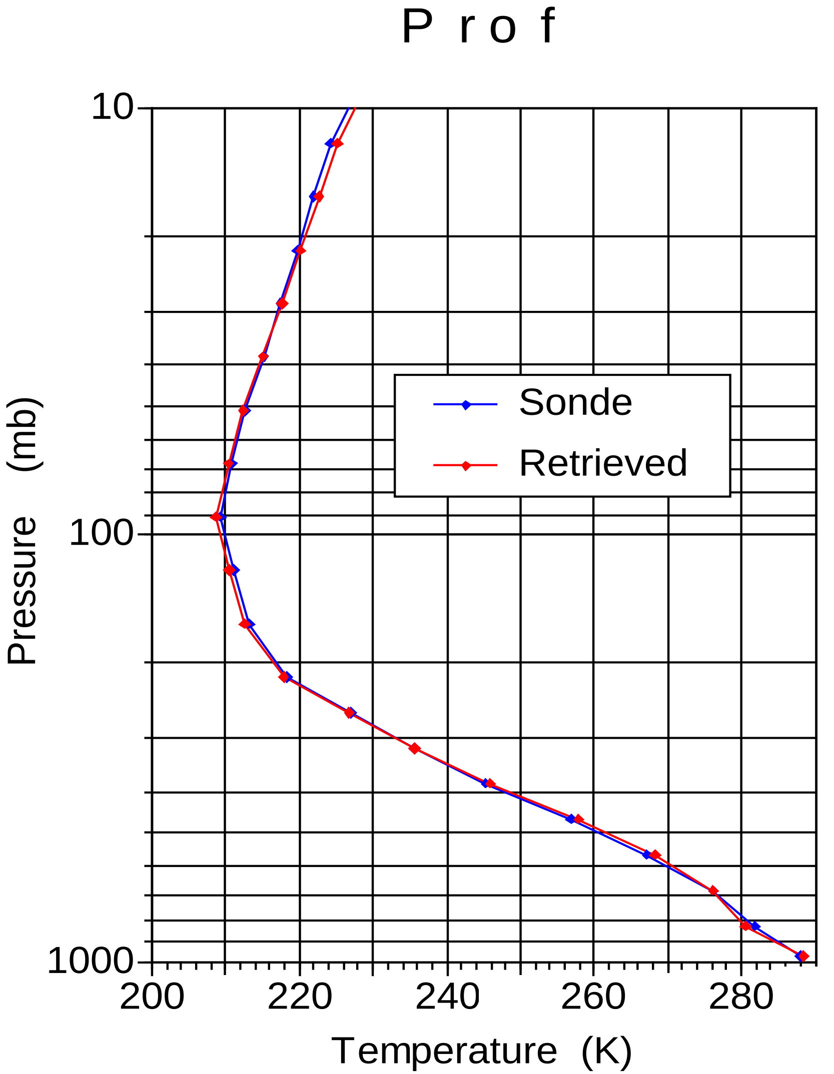
IASI/LBLRTM Validation

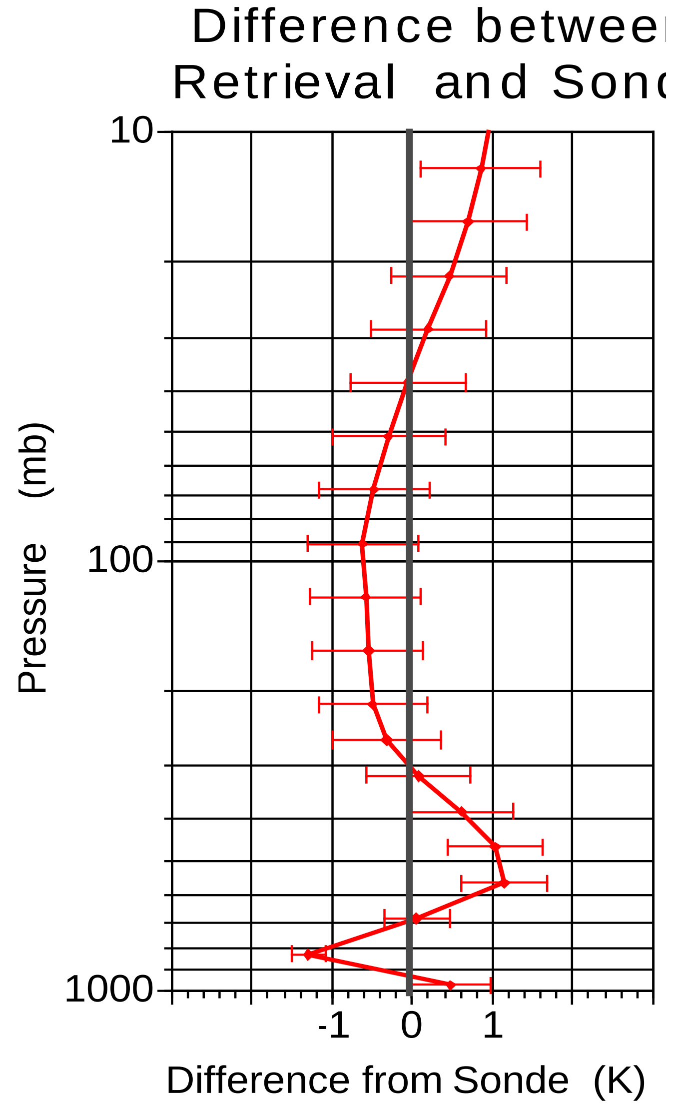


Tsfc: 284.323 K

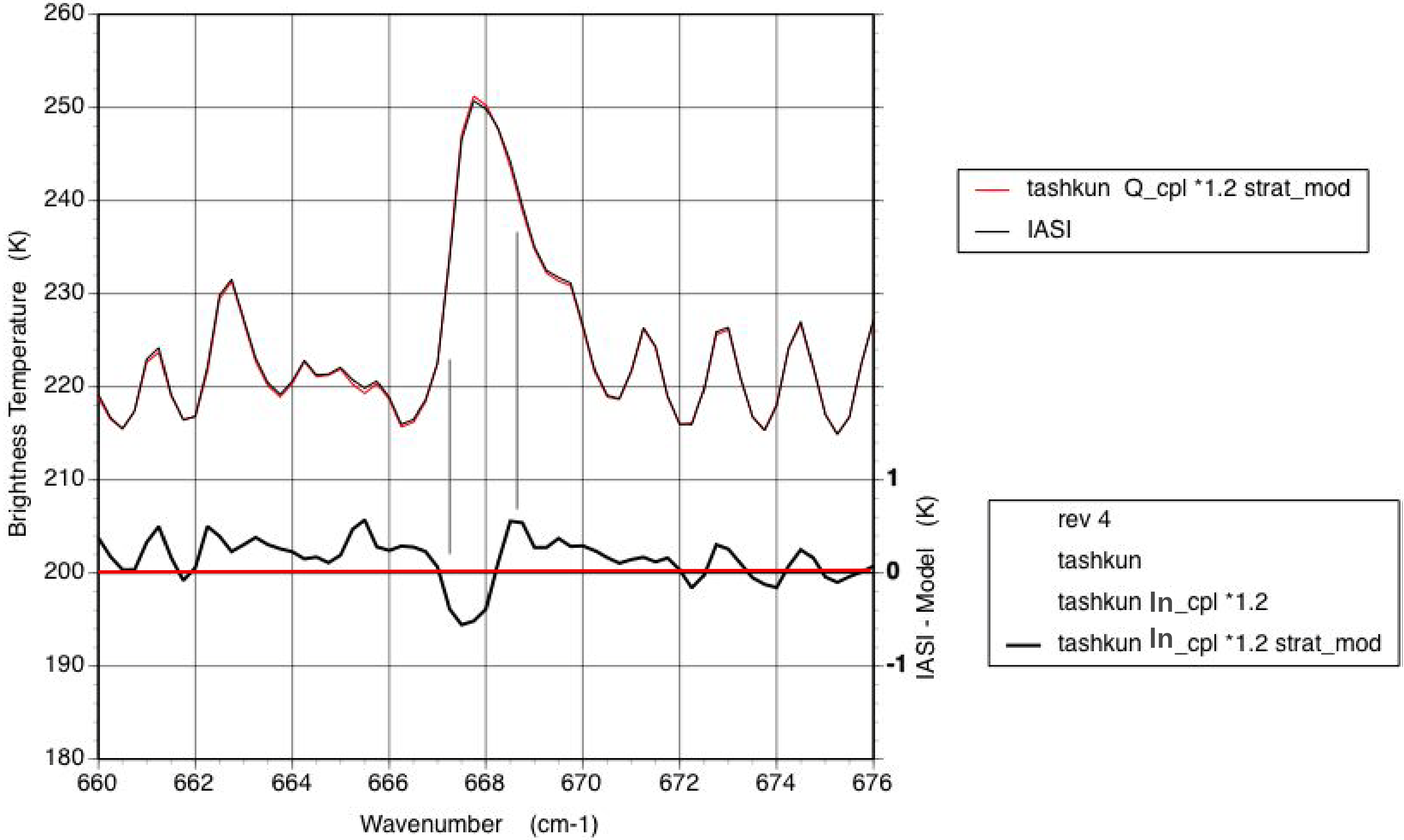
Strategy: to analyze the spectroscopy in the context of these red residuals

Temperature

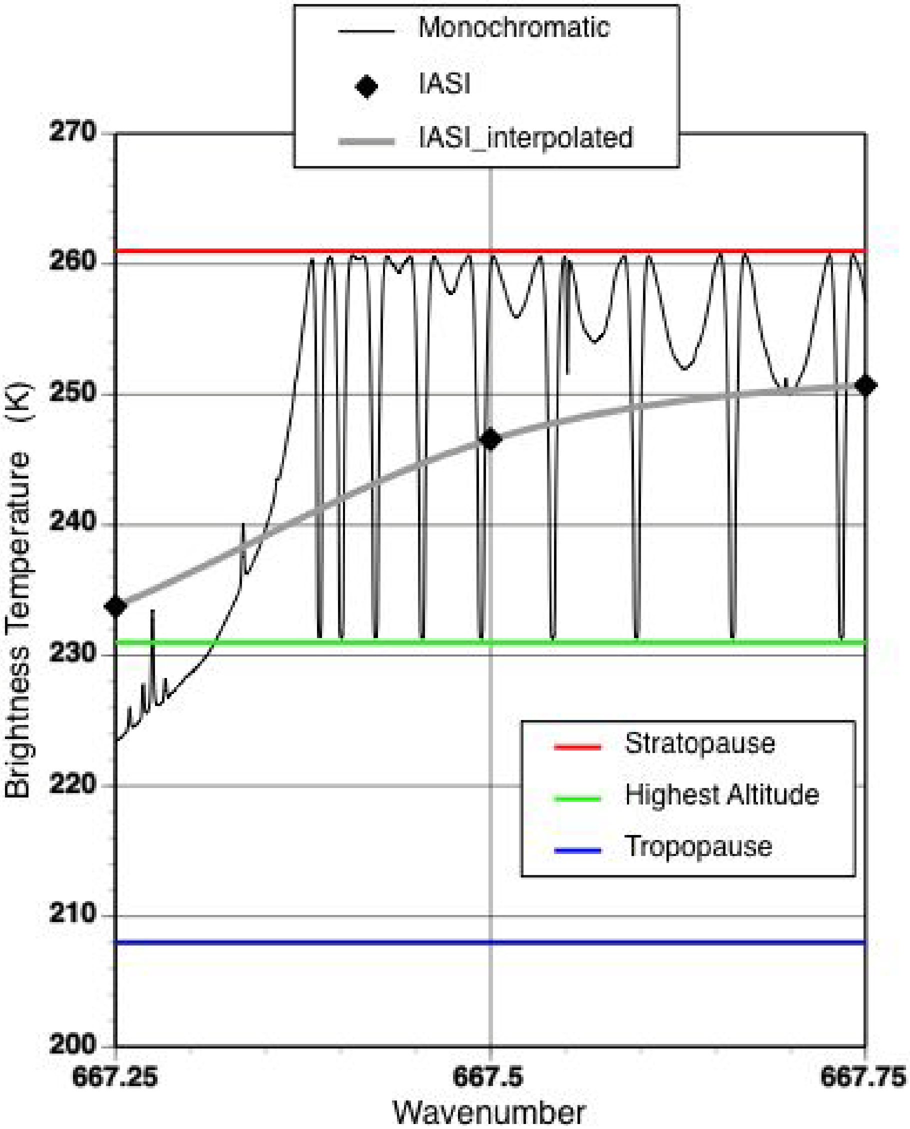




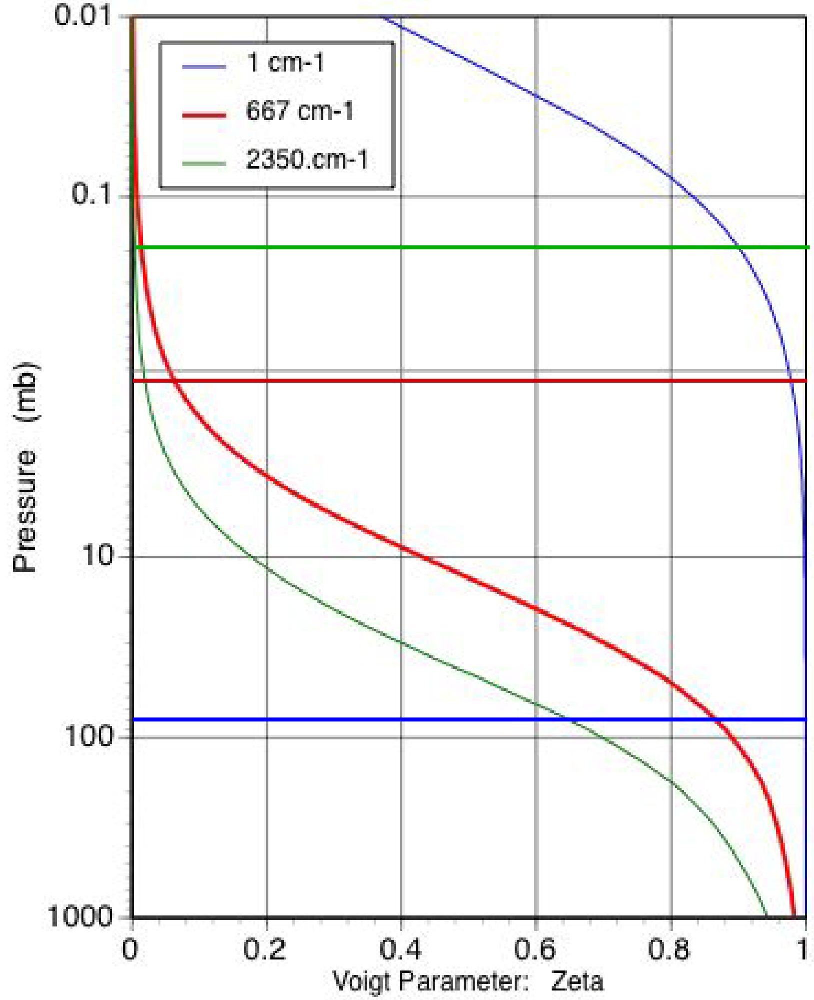
IASI 19 Apr 2007 CO_2 Q-Branch
Sensitivity to Upper Stratosphere



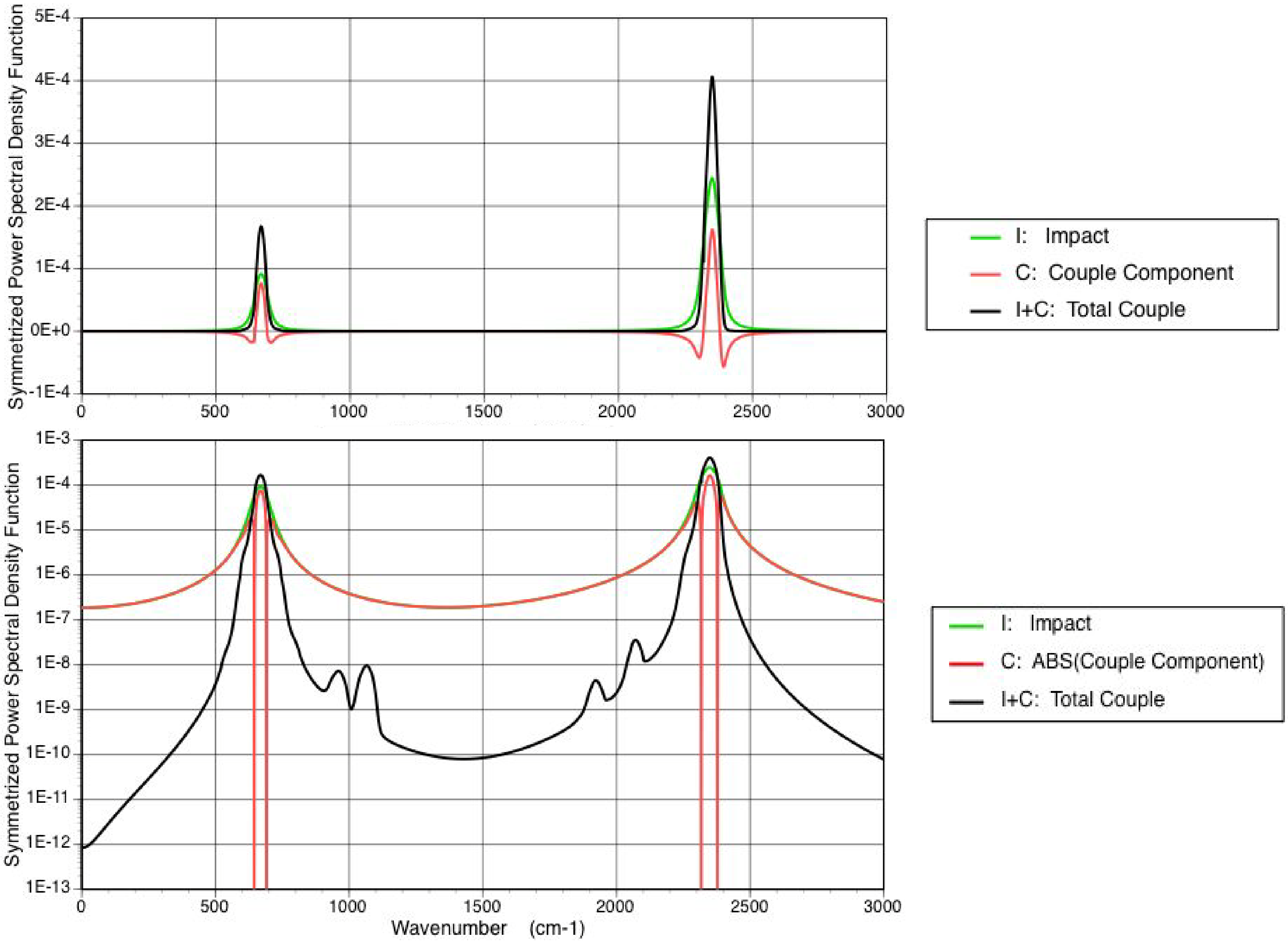
Voigt Parameter and Q Branch Monochromatic Spectrum



$$\zeta = \frac{\alpha_C}{\alpha_C + \alpha_D}$$

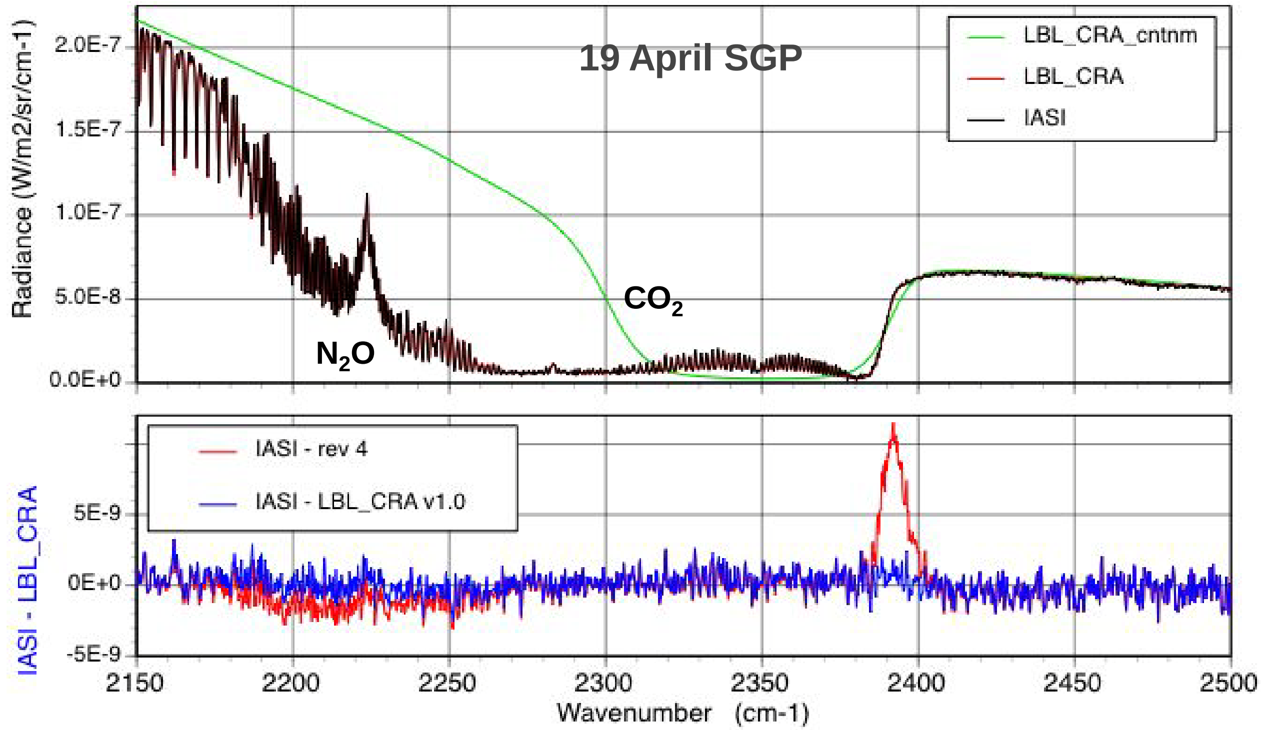


Effect of Line Coupling on CO_2 Continuum

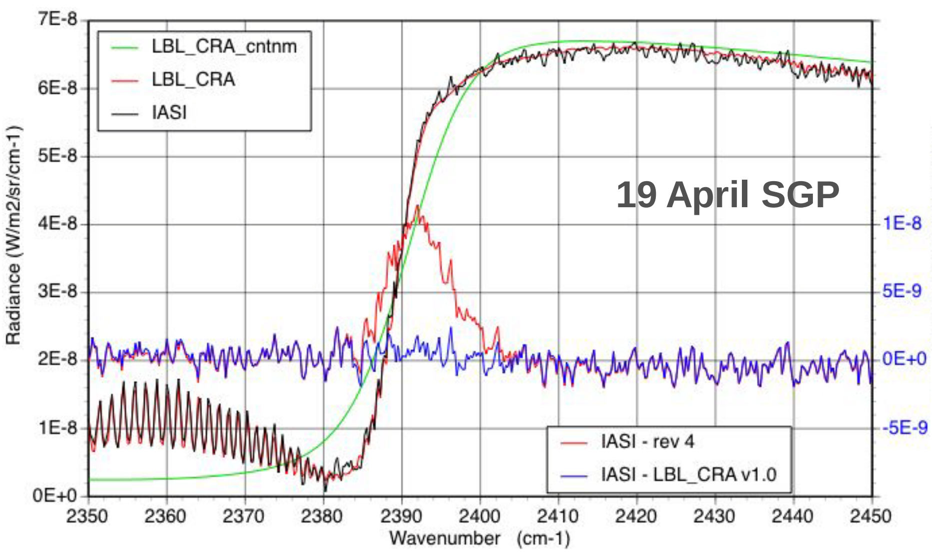


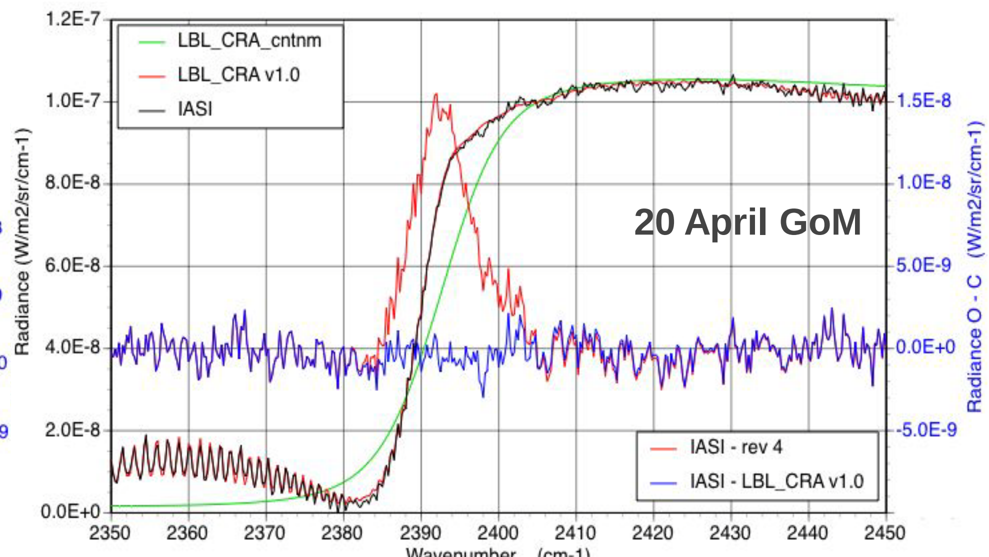
ν_3 Bands of N_2O and CO_2

2150 - 2500 cm-1



LBL_CRA: N_2O increased by 1.04





CO_2 Line Coupling

- **Line Parameters:**
  - P, Q, & R line coupling for bands of importance
  - 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.
  - 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

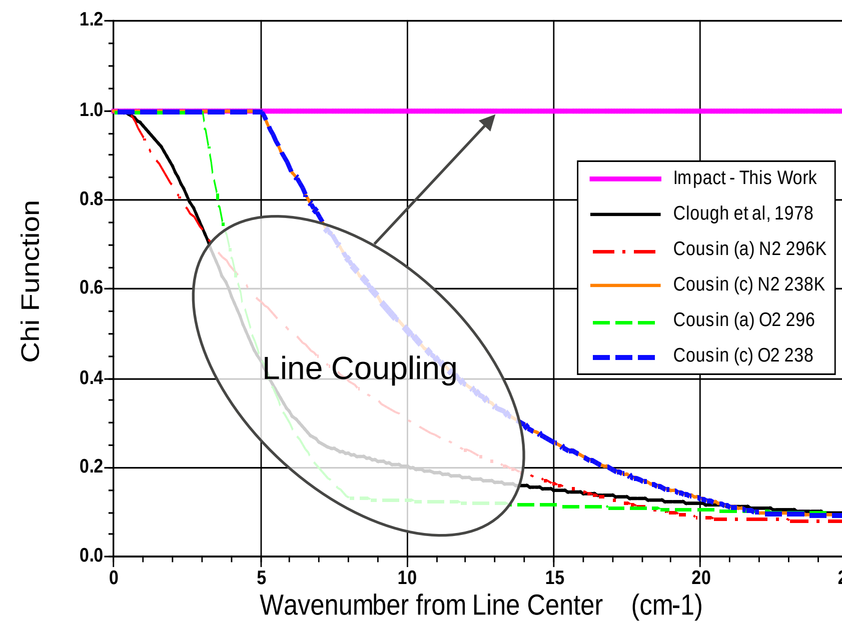
- **Line Shape:**
  - Impact Approximation
  - Duration of collision effects under study

- **Continuum:**
  - Band head: 2385 cm-1

Chi Factor

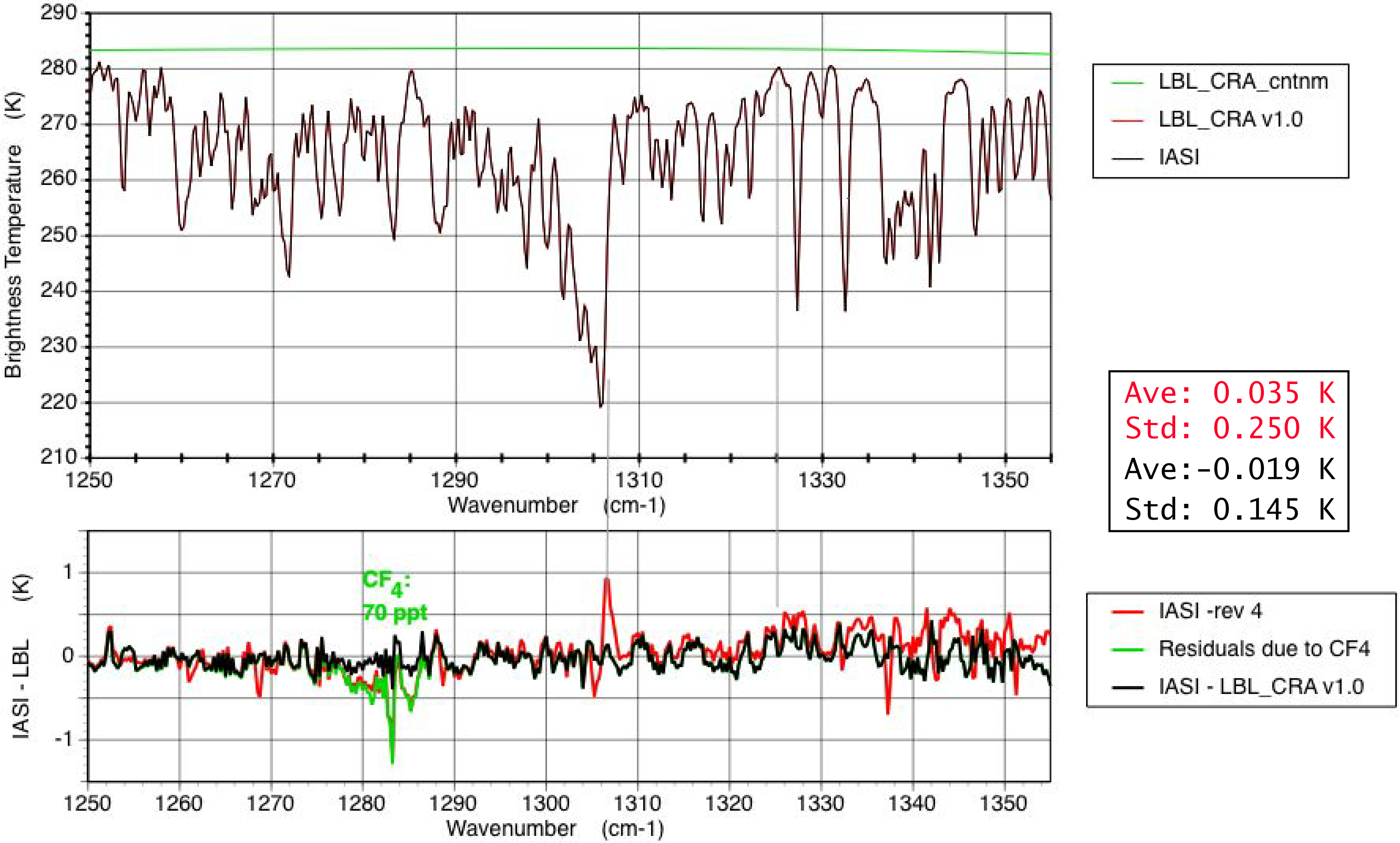
Line Coupling - Duration of Collision

Clough/ Burch/Benedict based on ν3 band



Line Coupling in Methane

Tran et al., JQSRT, 2006



Water Vapor: 'The Most Important Greenhouse Gas'

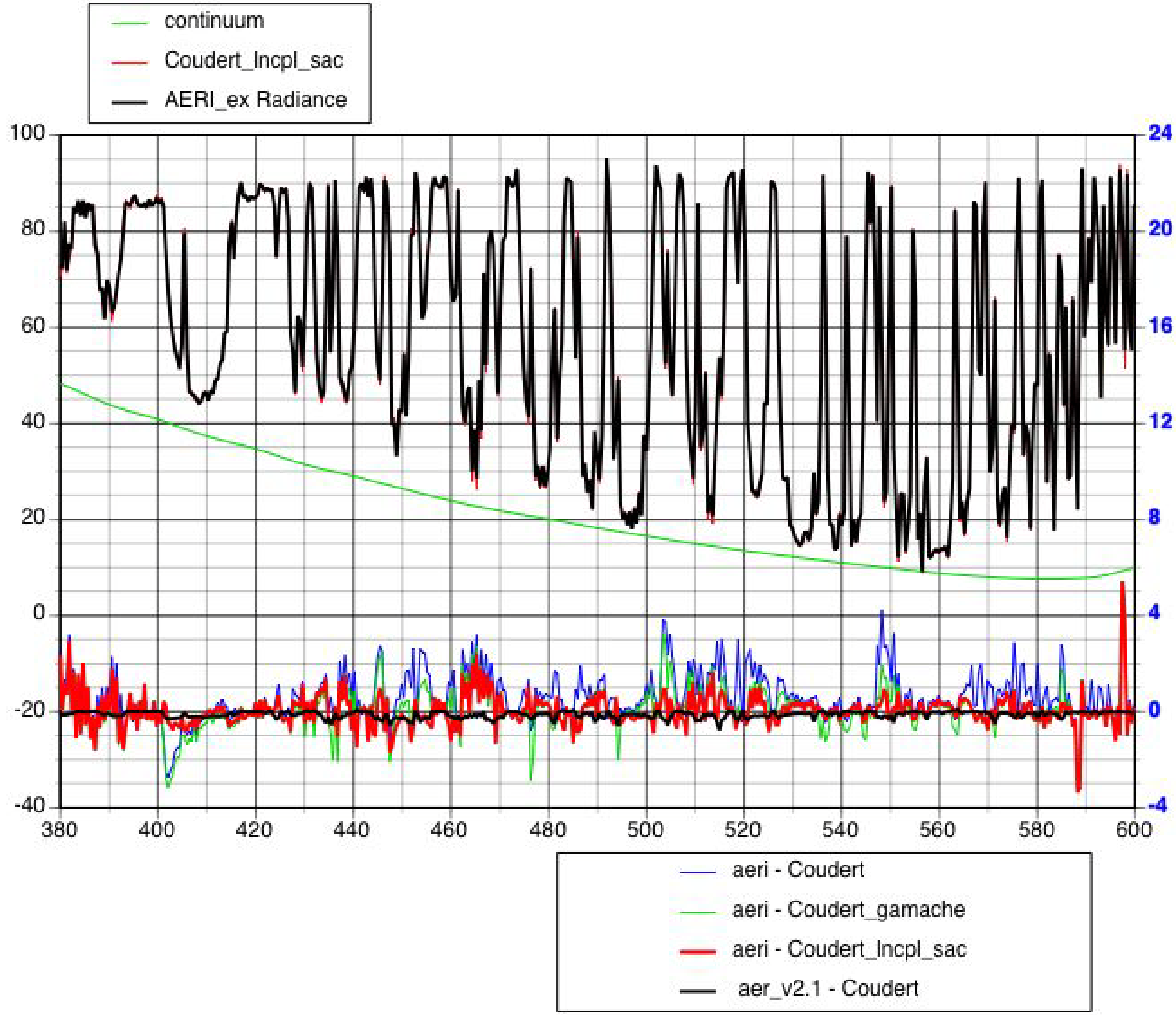
Critical for NWP and Climate

- **Line Strengths**
  - 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 >> 2.5 (water only)
  - Scaled in selected regions of the water band by ~5%

AERI Downwelling Radiances I

ARM NSA Site

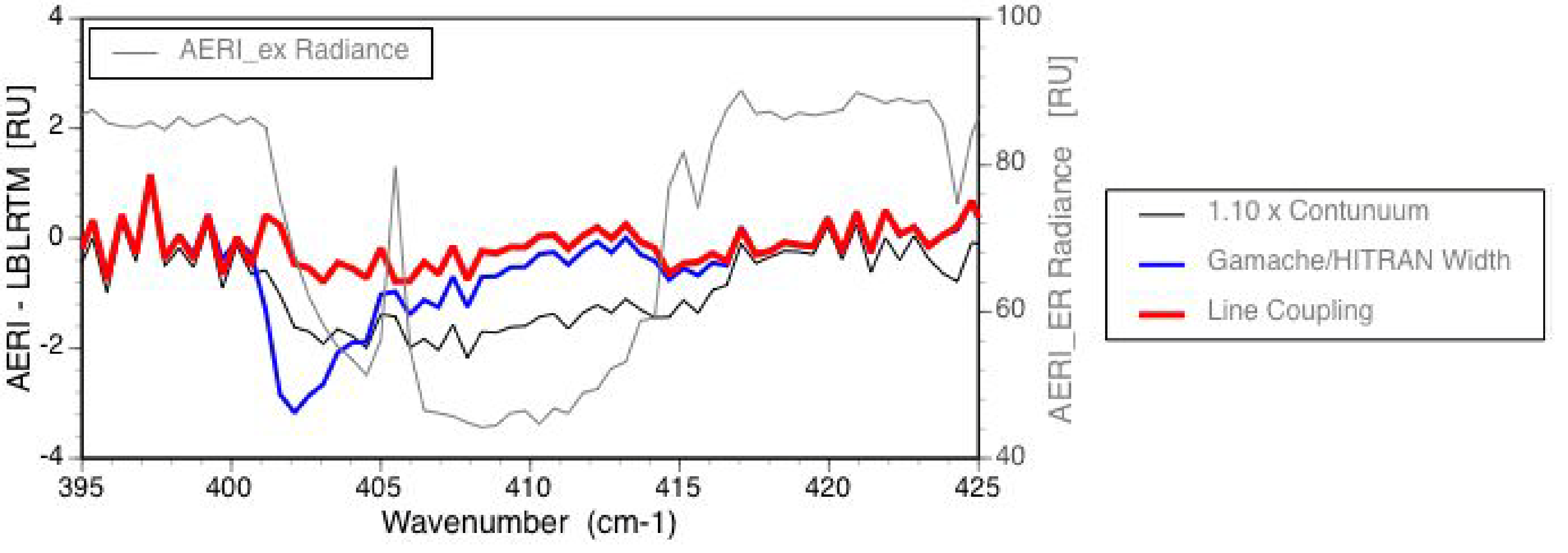
PWV: 1.866 mm



AERI Downwelling Radiances II

ARM NSA Site

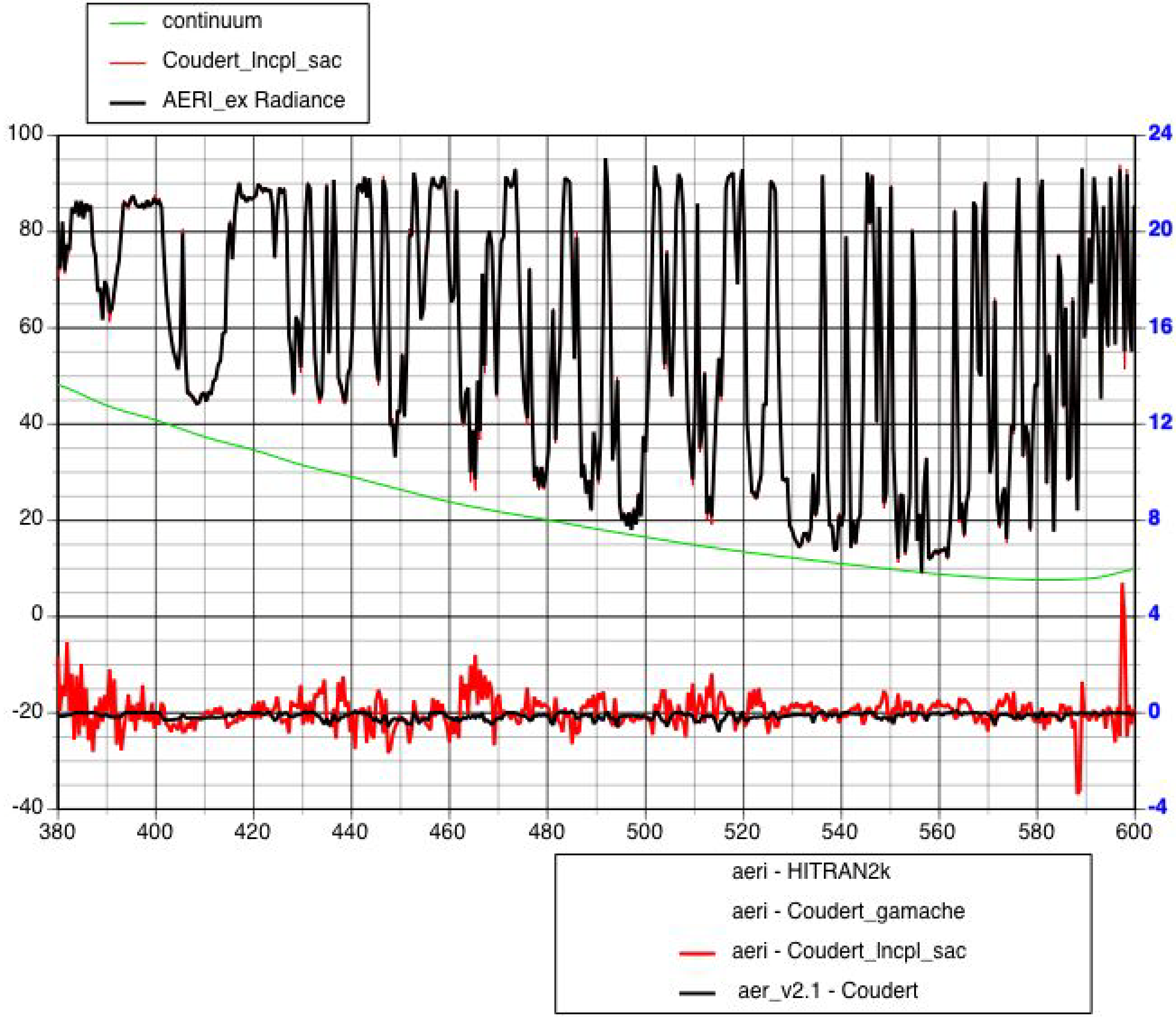
Line Coupling



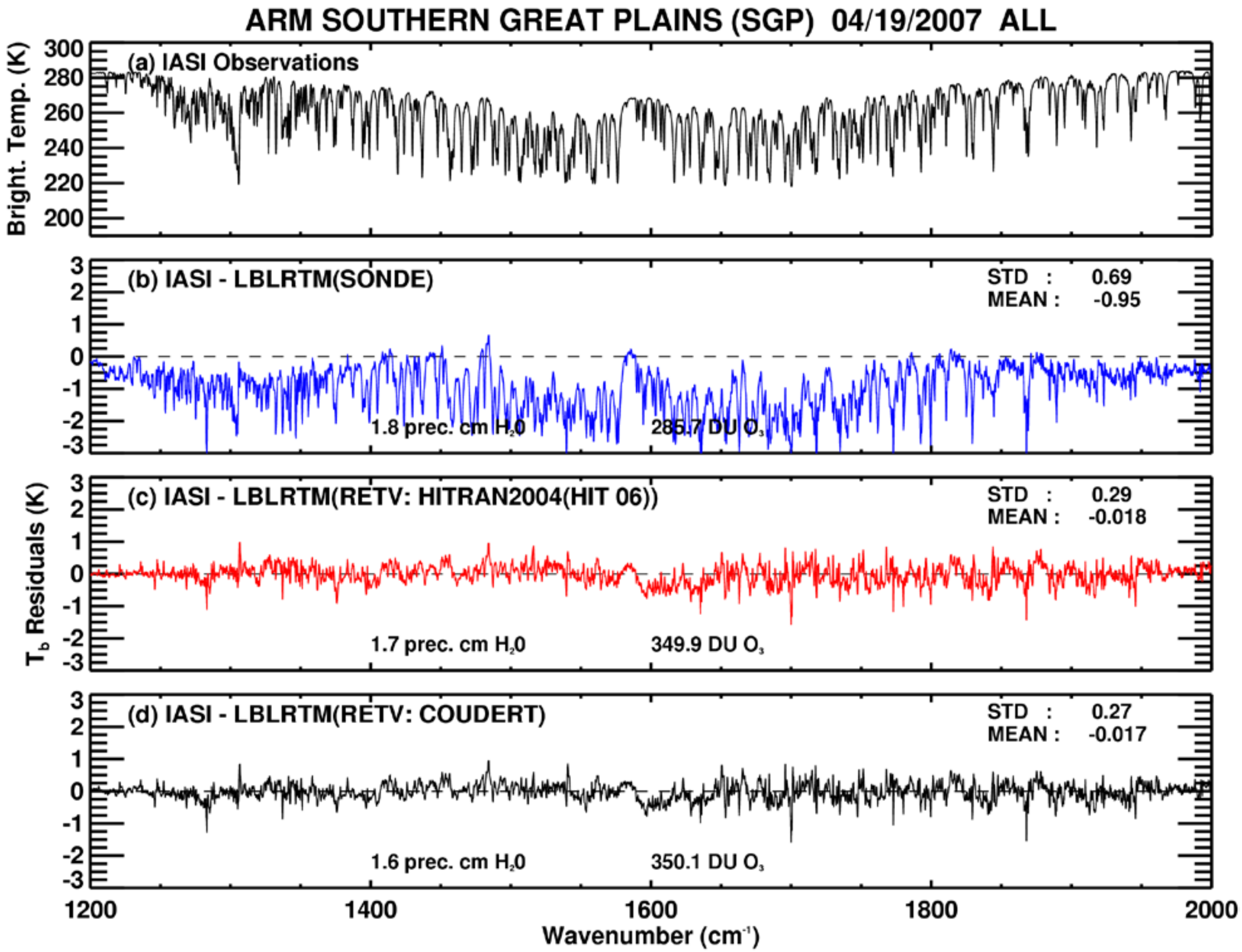
AERI Downwelling Radiances III

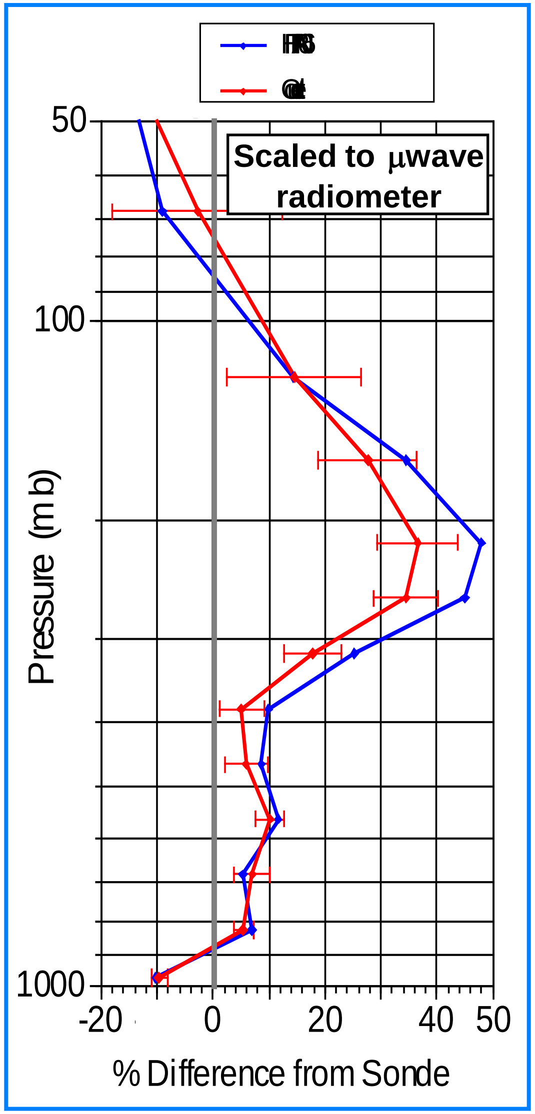
ARM NSA Site

PWV: 1.866 mm

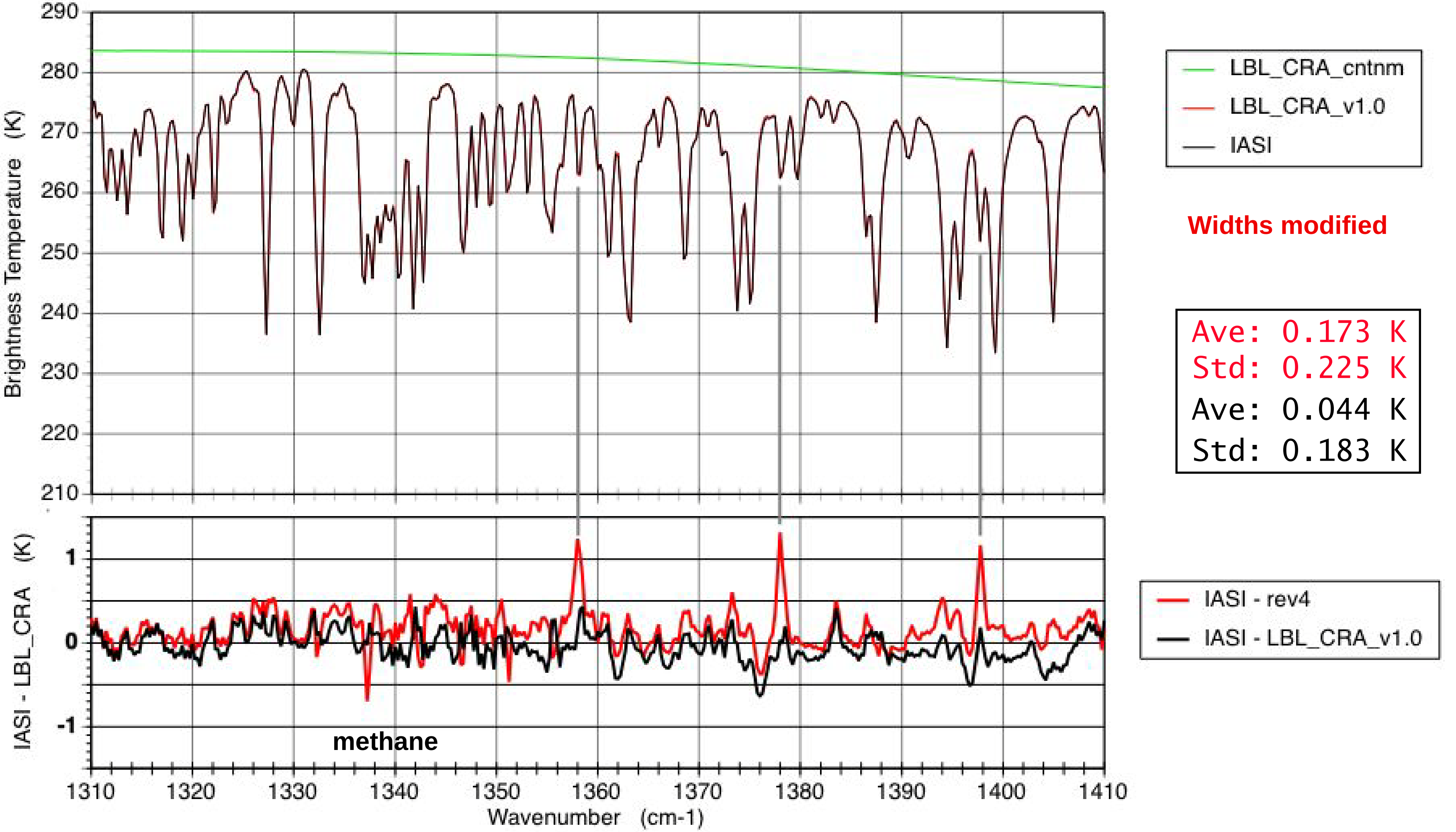


Water Vapor ν_2 Region : Impact of Coudert Intensities

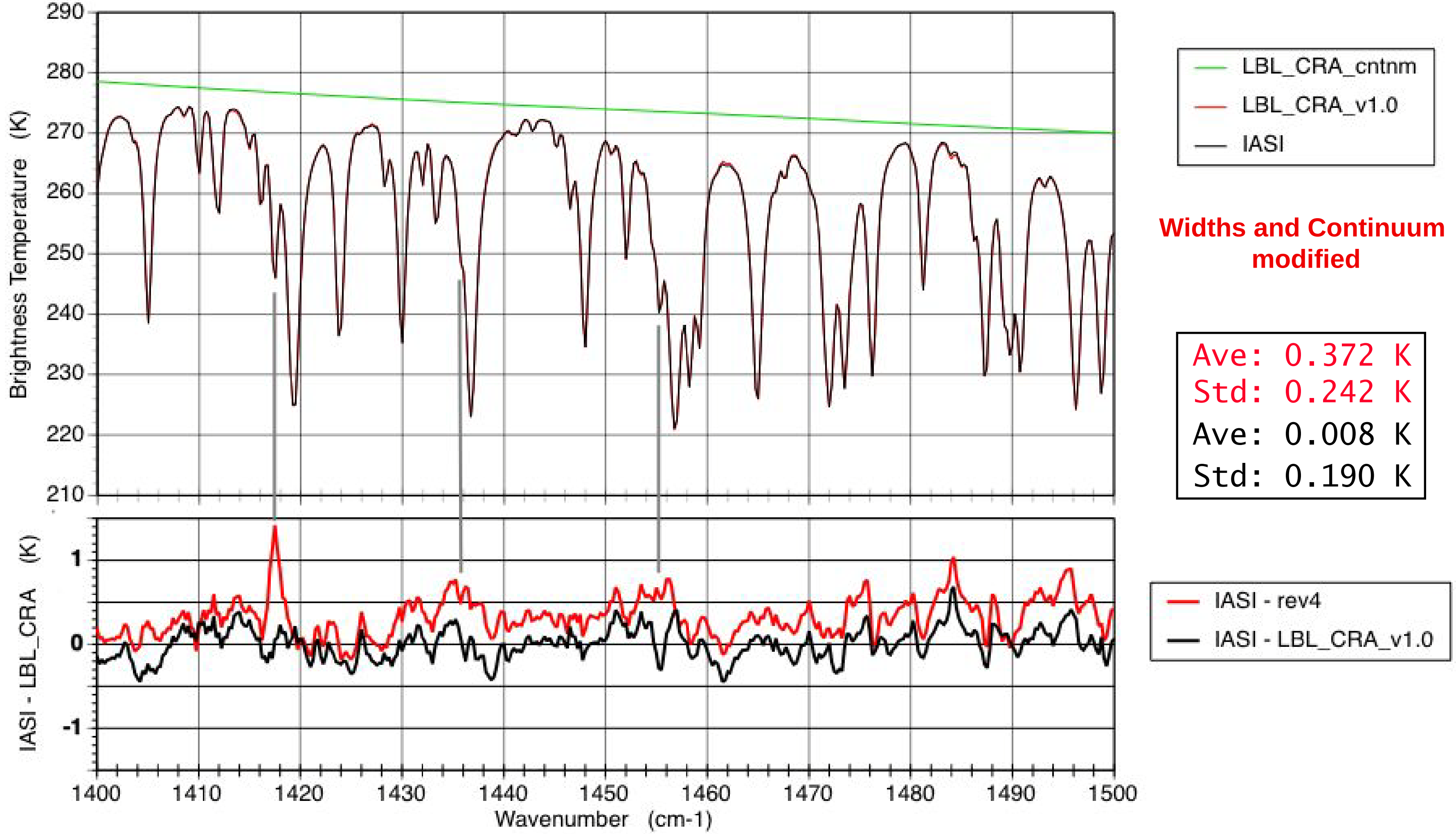




Water Vapor P-Branch: 1310 -1410 cm-1



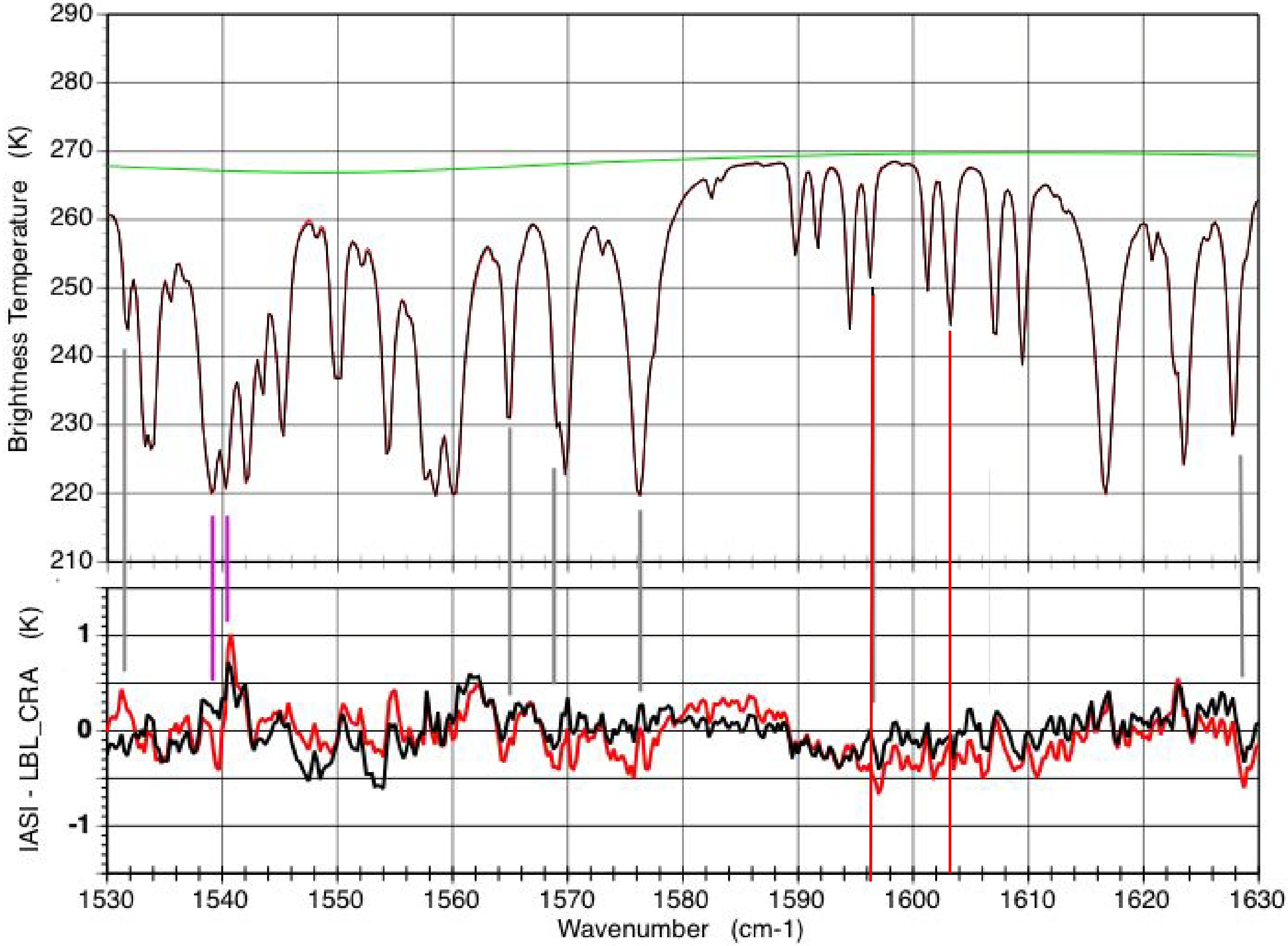
Water Vapor P-Branch: 1400 -1500 cm-1



Widths and Continuum modified

Ave: 0.372 K
Std: 0.242 K
Ave: 0.008 K
Std: 0.190 K

Water Vapor Band Center: 1530 -1630 cm-1

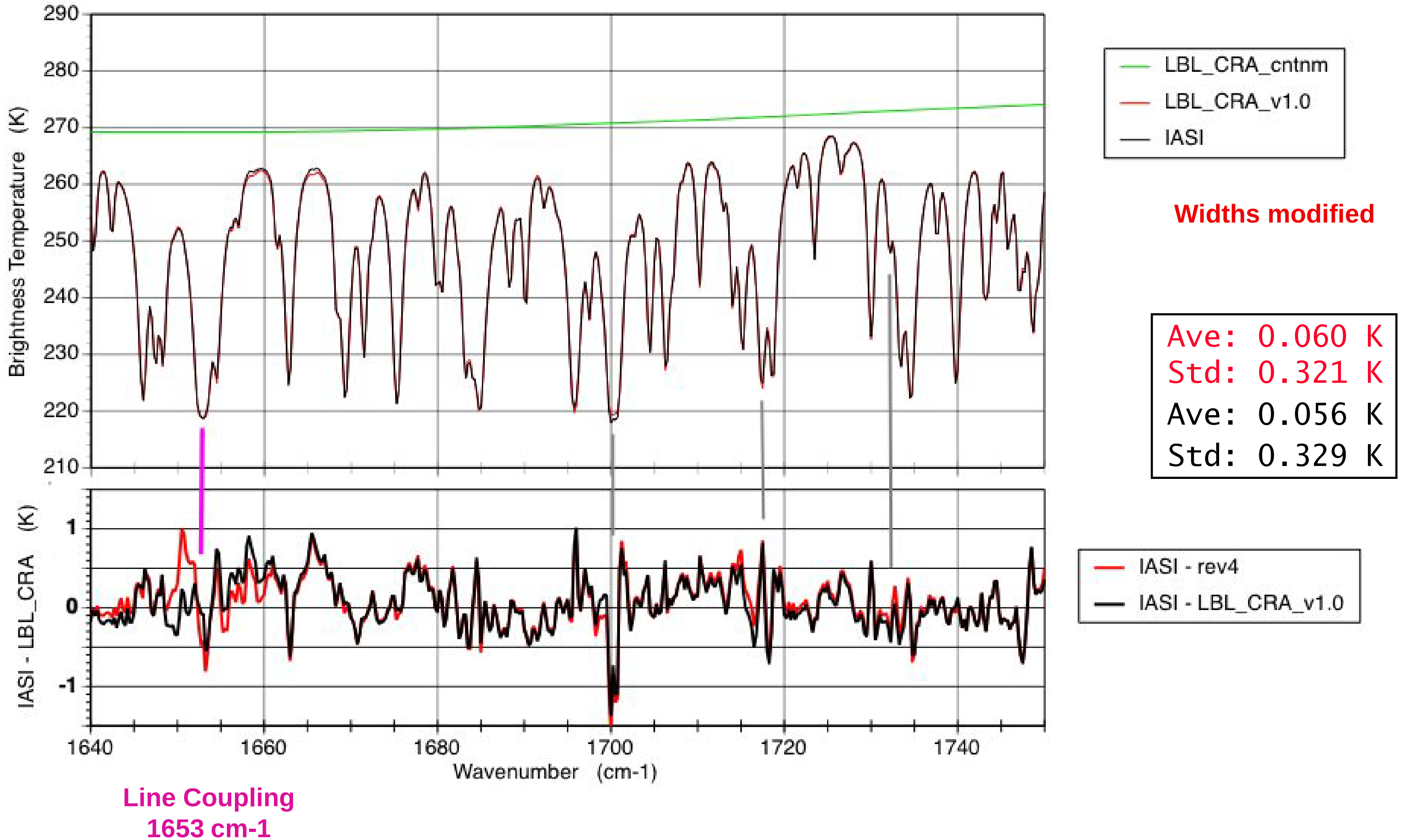


Widths and Continuum modified

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

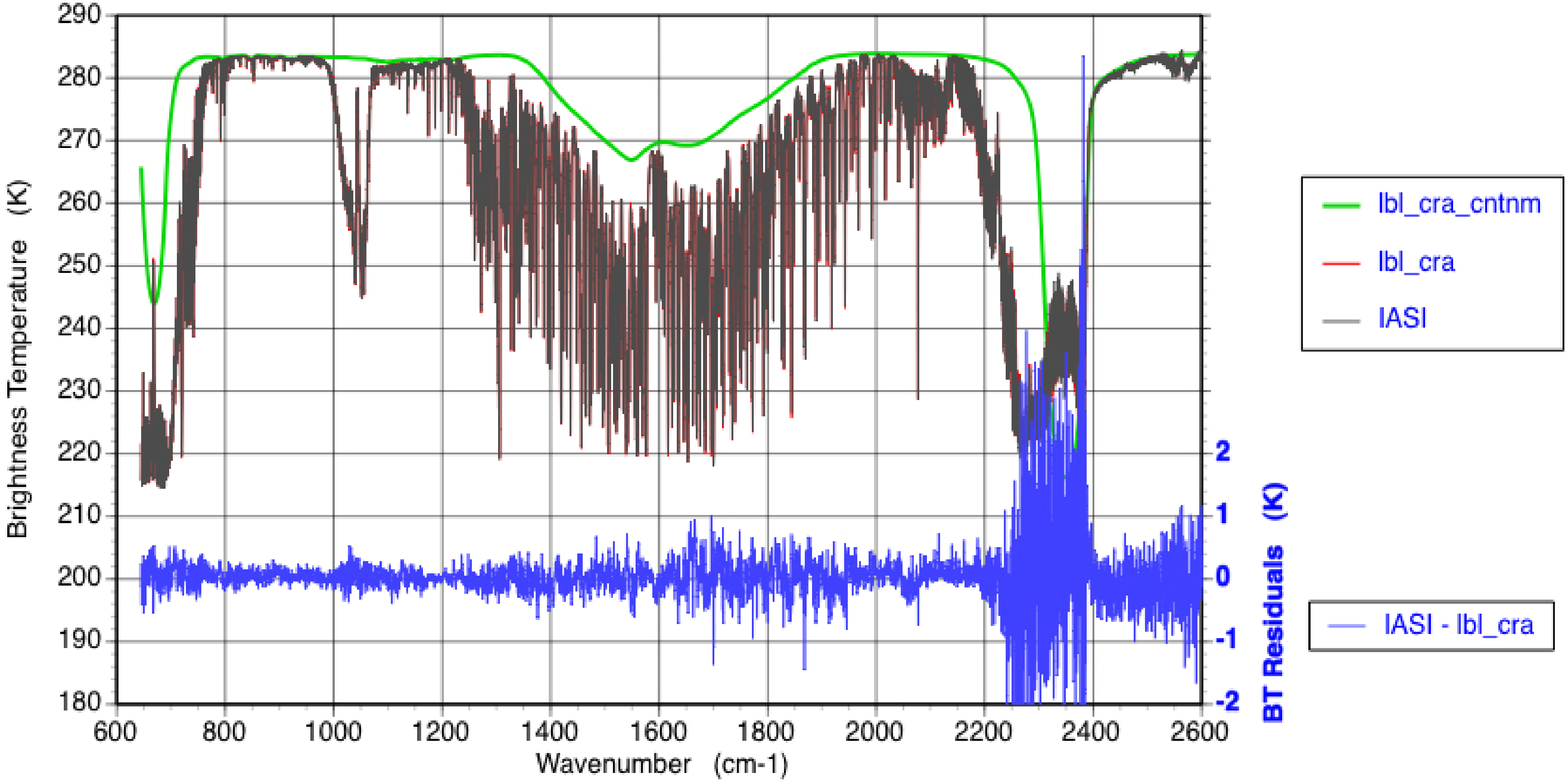
Line Coupling 1540 cm-1

Water Vapor R-Branch: 1640 -1750 cm-1



Overall Comparison of LBL_CRA with IASI

19 Apr 2007 SGP case



Summary - 1

- **Temperature**
  - **Carbon Dioxide**
    - » **Line Parameters: Tashkun et al. JQSRT, 2009**
    - » **Line Coupling:**
      - **Niro et al., JQSRT, 2005 J.M.Hartmann**
      - **Q-Branch 667 cm-1: Niro * 1.2**
    - » **Band Head 2385 cm-1 Robust for 19 April and 20 April (low water cases)**
      - **Line Coupling > Continuum**
    - » **Good agreement between CO_2 ν_2 and CO_2 ν_3**
  - **Nitrous Oxide**
    - » **Agreement between CO_2 ν_2 and N_2O ν_3 / CO_2 ν_3**
    - » **N_2O profile scaling required: 19 April case: 1.04**
      20 April case: 1.02
    - » **N_2O shows more variability than expected**
- **Methane**
    - » **Residuals significantly reduced with line coupling: Tran * 1.5**
      - **Tran et al., JQSRT, 2006 J.M.Hartmann**

Summary - 2

- Water Vapor
  - » Sondes provide an excellent first guess / structure (nothing more)
  - » Coudert strengths
    - Residuals unchanged; retrieved water in upper trop reduced 10%
  - » Widths are the current major issue
    - Gamache widths: 350 - 1600 cm-1
    - Widths of a series of weak high J low Ka P-Branch lines reduced by ~50%
  - » Widths and continuum are inextricably linked
  - » Three coupled lines observed so far (accidental line resonances)
  - » P-Branch has much lower residuals than R-Branch. Why ???
    - Gamache Widths ???
  - » 19 April 2007 case is superb for FM improvement
  - » Due to the resolution of IASI there is a limit to the spectroscopic improvements that can be achieved

Summary - 3

- Next Steps
  - Resolve R-Branch Issues for water vapor
  - More Cases
    - Night time with high water
    - Day time cases for impact of NLTE on 720 cm-1 Q-Branch
  - Line Shape issues are the dominant problem
  - Spectroscopy needs greater support to take full advantage of the data
  - Thinking of the real world as our laboratory
  - Implement line parameter retrieval scheme using spectral residuals

Performance of LBL_xxx is generally gratifying

(said in not quite all modesty?)

10 years ago I wouldn't have envisioned that we would be modeling at this level

Line Coupling: Accidental Line Resonances

400 cm-1 Tony Clough

```
11  398.976493 5.556D-20 2.283E+01.0360.3283 1411.61150.29-.000910 1  1 9 7 2    8 6 3   5552433 5
11  400.221796 1.070D-20 4.643E+00.0791.3009 1216.23130.710.004940 1  110 4 6    9 3 7   5552433-1
1 1.456529E-01           1.365260E-01          1.300000E-01          1.248789E-01             -1
11  400.481057 1.071D-20 1.636E+01.0510.3009 1474.98080.30-.000770 1  110 6 4    9 5 5   5552433-1
1-2.671053E-01          -1.725650E-01         -1.303796E-01         -1.064366E-01             -1
11 1337.897589 9.576D-23 5.903E+00.0261.1905 1806.67180.05-.000970 2  112 012   13 113   3556443 0
```

Y: 200K 250K 296K 340K

1540 cm-1 Linda Brown

```
11 1539.060760 2.255D-19 1.153E+01.1053.4643   79.49640.79-.004100  2  1 1 0 1    2 1 2   3555433-1
1 1.098843E-02           1.048538E-02           1.012000E-02          9.829722E-03             -1

11 1540.299806 1.767D-19 7.175E+00.0971.5173  136.76170.79-.000020  2  1 2 1 2    3 0 3   3577443-1
1-1.604015E-02          -1.409560E-02          -1.292537E-02         -1.211058E-02             -1
```

1630 cm-1 Linda Brown

```
11 1539.060760 2.255D-19 1.153E+01.1053.4643   79.49640.79-.004100  2  1 1 0 1    2 1 2   3555433-1
1 1.098843E-02           1.048538E-02           1.012000E-02          9.829722E-03             -1
11 1540.299806 1.767D-19 7.175E+00.0971.5173  136.76170.79-.000020  2  1 2 1 2    3 0 3   3577443-1
1-1.604015E-02          -1.409560E-02          -1.292537E-02         -1.211058E-02             -1
```