

---

# Improved Spectroscopy for Microwave and Infrared Satellite Data Assimilation

**Vivienne Payne, Jean-Luc Moncet and Tony Clough\***

**JCSDA 6th Workshop on Satellite Data Assimilation**

**June 10-11 2008 ■ ■**

\*Currently at Clough Associates

# Acknowledgements

- **AER:** Mark Shephard, Jennifer Delamere, Karen Cady-Pereira and Eli Mlawer
- **UMBC:** **Larrabee Strow**, **Scott Hannon**
- **U. Wisconsin:** Dave Tobin, Dave Turner
- **NASA Langley:** Bill Smith's group
- **NASA JPL:** TES Algorithm Development Team
- **Paris XII, Creteil:** Jean Michel Hartmann's Group
- **UMass:** Bob Gamache
- **ANL:** Maria Cadeddu
- **Radiometrics:** Mike Exner
- **University of L'Aquila:** Nico Cimini
- **NOAA:** Ed Westwater

# Overview

- **Microwave**
  - **MonoRTM**
  - Comparisons with Rosenkranz model
  - Water vapor continuum validation
- **Infrared**
  - **Updates to LBLRTM**
    - » General update to latest HITRAN 2004 line parameters
      - Water vapor line widths
    - » CO2 line mixing
  - **Validation against satellite measurements**
    - » AIRS/SARTA/LBLRTM comparisons
    - » IASI comparisons
  - **Validation against ground-based measurements**
  - **Future plans**
- **Summary**

# What is 'Truth'?

- **'Truth'** at the Level Required is not readily available
  - sonde accuracies; spatial and temporal sampling
  - laboratory measurements
- **Spectral Residuals are Key!** (Clough perspective)
  - Consistency **within a band system**
  - Consistency **between bands**
    - » AIRS, 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**
  - Consistency **between infrared and microwave**
  - Validation using both **upwelling** and **downwelling** measurements

# Microwave

## Microwave topics

- MonoRTM
- Differences from the Rosenkranz model
- Update on line parameters
- Ongoing continuum validation

# MonoRTM

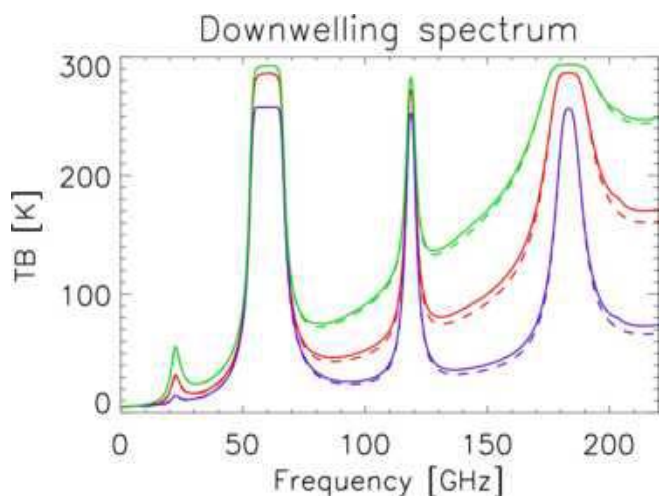
- **Microwave monochromatic radiative transfer model**
  - "laser" - i.e. single frequency - version of LBLRTM
- **Developed at AER (Clough et al., 2005)**
- **Useful range: 0-1648 GHz**
- **Spectroscopic parameters from external line file**
  - **HITRAN 2004 with specific updates/modifications**
    - » 22 GHz and 183 GHz line intensities from Clough et al (1973)
    - » Other 22 GHz and 183 GHz line parameters from Payne et al. (2008)
    - » Oxygen widths, line coupling parameters from Tretyakov et al (2005)
      - Ground-based validation of oxygen parameters in MonoRTM: Cadeddu et al. (2007)
- **Latest version: Monortm\_v3.3**
- **Lineshape: Van-Vleck Weisskopf**
- **Continuum: CKD\_2.4**

# MonoRTM: Recap from previous JCSDA Workshop

- **Work presented at 2007 Workshop:**
  - Tretyakov **O<sub>2</sub> parameters** (line widths, line mixing coefficients) validated using ground-based data
    - » Results now very similar to Rosenkranz
  - Had started validation of **water vapor line widths**
  - Had started validation of **water vapor continuum**
- **Important remaining differences between MonoRTM and Rosenkranz models:**
  - **Spectroscopic parameters**
    - » **Width of the 22 GHz water vapor line**
      - Ground-based validation supports MonoRTM width (Payne et al., 2008, IEEE TGRS)
    - » **Temperature dependencies of widths**
      - MonoRTM contains up-to-date values from state-of-the-art calculations
  - **Continuum**
    - » **Foreign & Self broadening**
      - Ground-based MWR data indicates parameters in Rosenkranz model are not consistent at 31.4 GHz
  - **Number of lines**
    - » **Rosenkranz does not include all lines or all species**
    - » **MonoRTM: line info from external file**
      - Can include/exclude lines according to speed/accuracy requirements
      - Weak water vapor lines can have non-negligible effect
      - Ozone can be important (e.g. AMSU Channel 18 (183 +/-1 GHz))
      - MonoRTM line file stores line parameters to greater precision
        - Leads to small differences (e.g. O2 line positions)

# Brightness temperature comparisons: MonoRTM vs RK

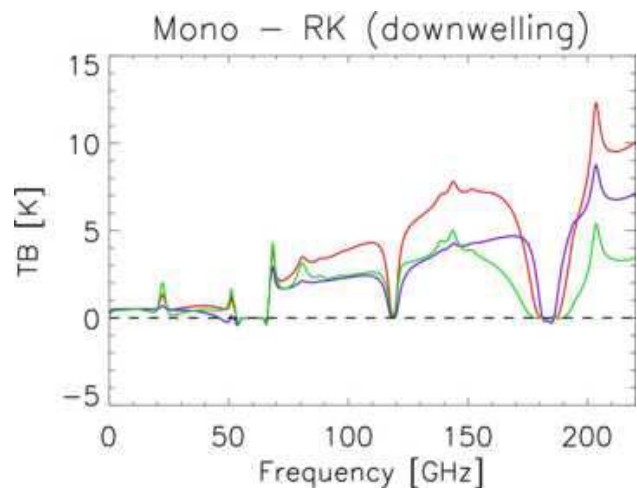
- Same RT code used (different models used for optical depth calculations).
- No ozone in either simulation.



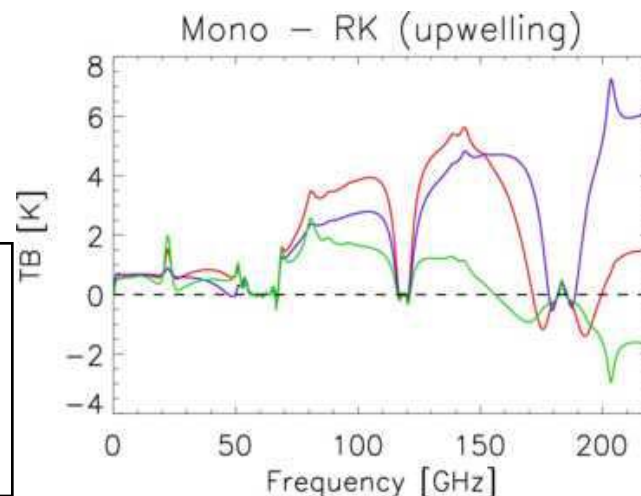
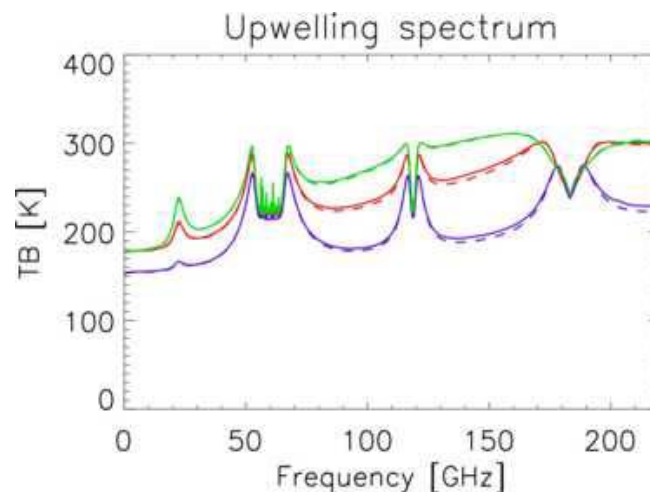
Mid-lat summer  
PWV = 2.9 cm

US standard  
PWV = 1.4 cm

Sub-arctic winter  
PWV = 0.41 cm



Upwelling:  
**Differences  
of up to 5K  
at 150 GHz!**

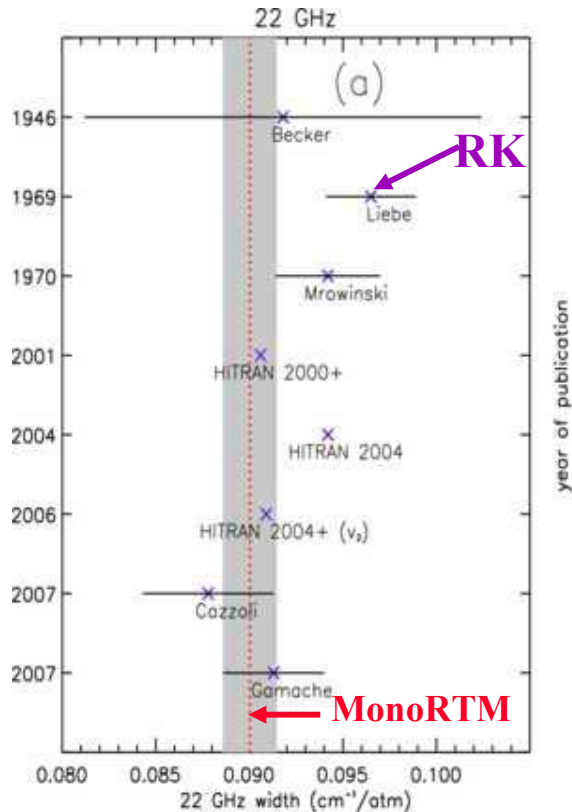




# Water vapor: Line widths

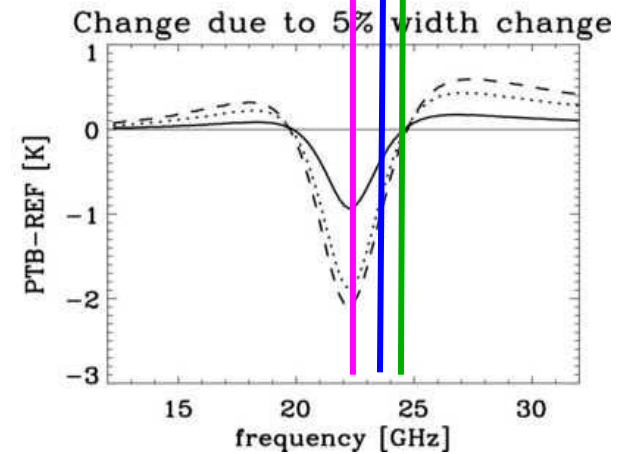
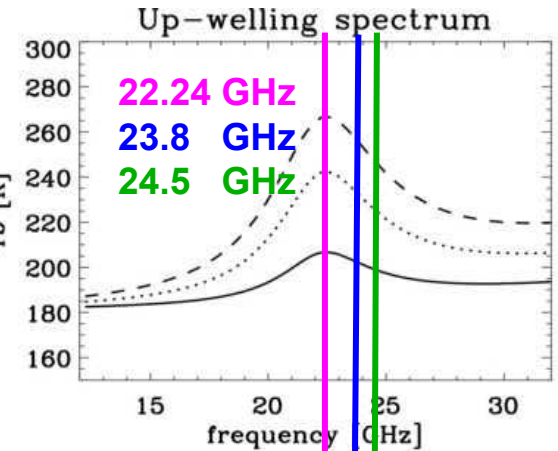
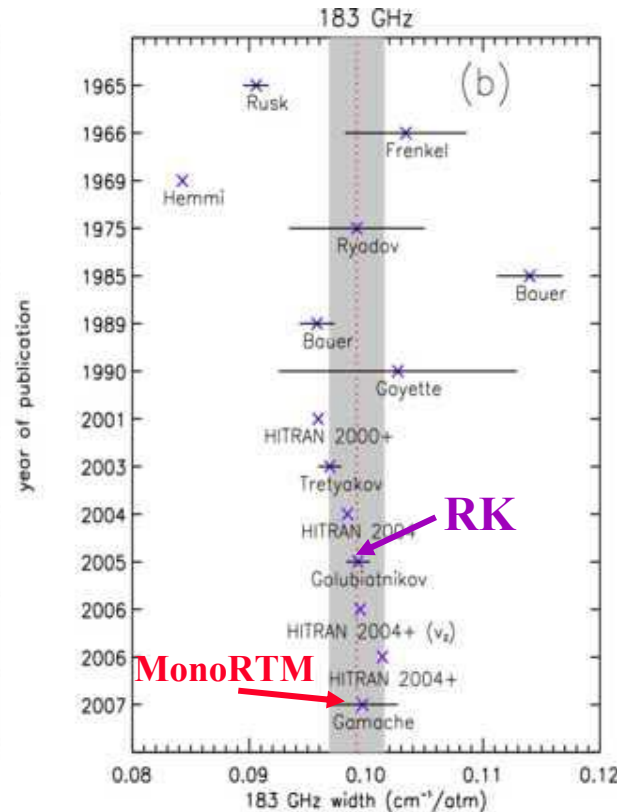
22 GHz:

MonoRTM 5% lower than RK



183 GHz:

MonoRTM ~ same as RK



**Payne et al., 2008, IEEE TGRS, in press**

**Incorrect specification of the 22 GHz width will lead to inconsistency between eg AMSU/AMSR-E and SSMIS!**

Additional evidence for lower 22GHz width value from upwelling radiation:

- »UK Met Office (W. Bell and P. J. Rayer - lower width improves SSMI biases)
- »Tom Wilheit (Texas A&M) - TMI and SSMI

# Water vapor continuum

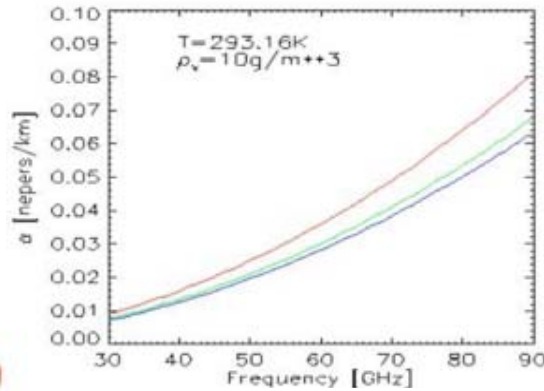
Clough and Cady-Pereira  
84 K

Ratios of absorption in models (Rosenkranz=1.0)

Thomas Meissner (RSS)

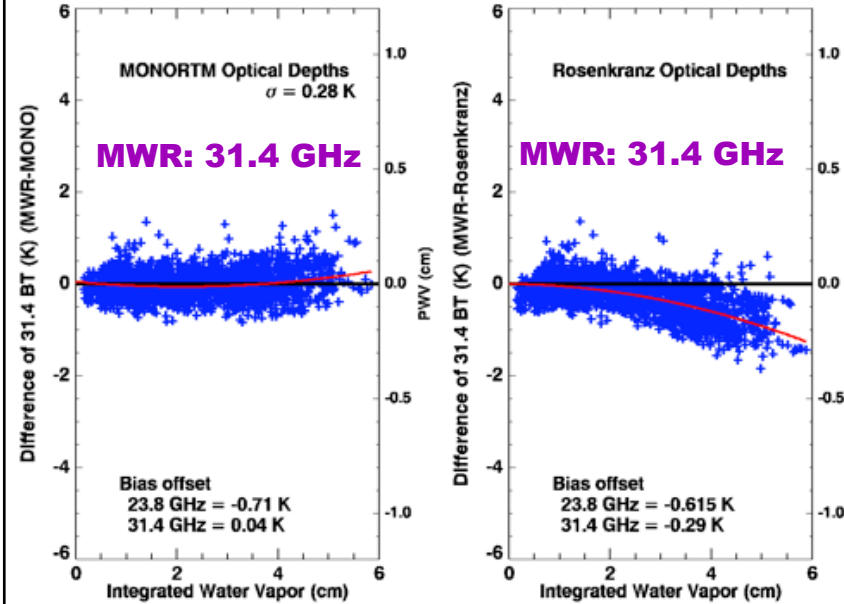
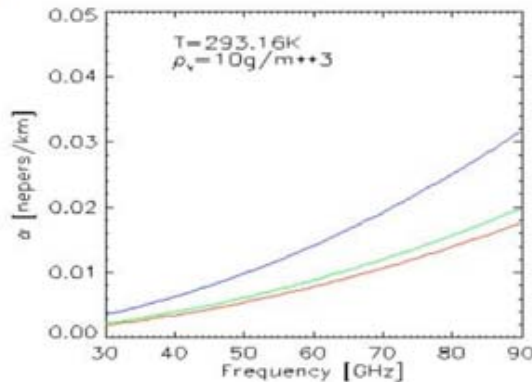
	FB T = 298 K	FB T = 278 K	SB T = 298 K	SB T = 278 K
Rosenkranz	1.00	1.00	1.00	1.00
MonoRTM	1.27	1.27	0.56	0.53
RSS	1.08	1.04	0.64	0.56

Foreign  
broadening  
(FB)

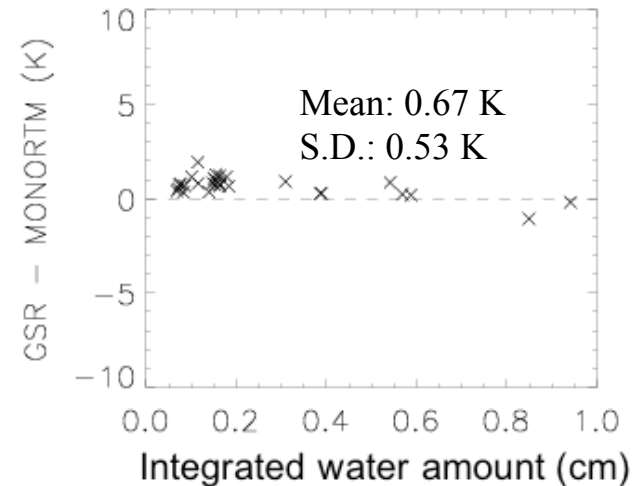


Rosenkranz  
AER MonoRTM  
RSS (AT80)

Self  
broadening  
(SB)



GSR 89 GHz

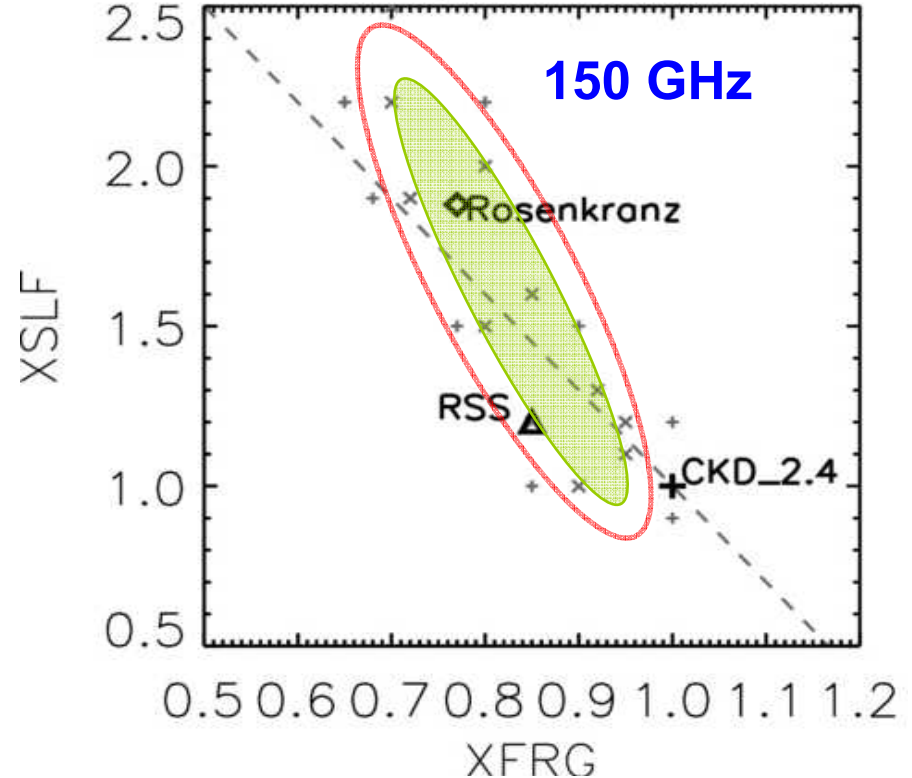
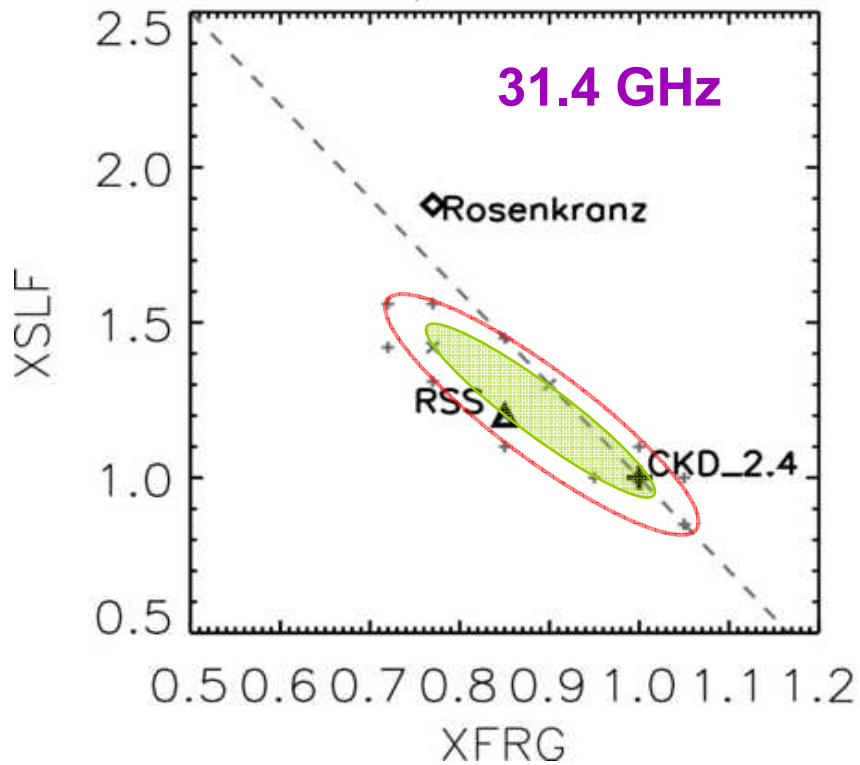
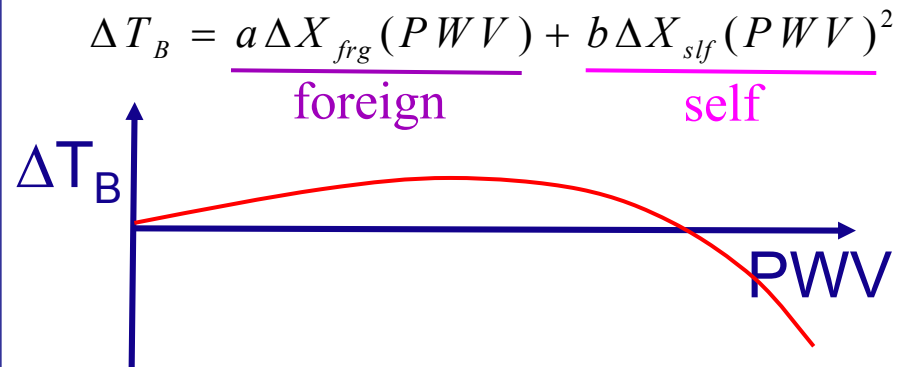


# Continuum uncertainty

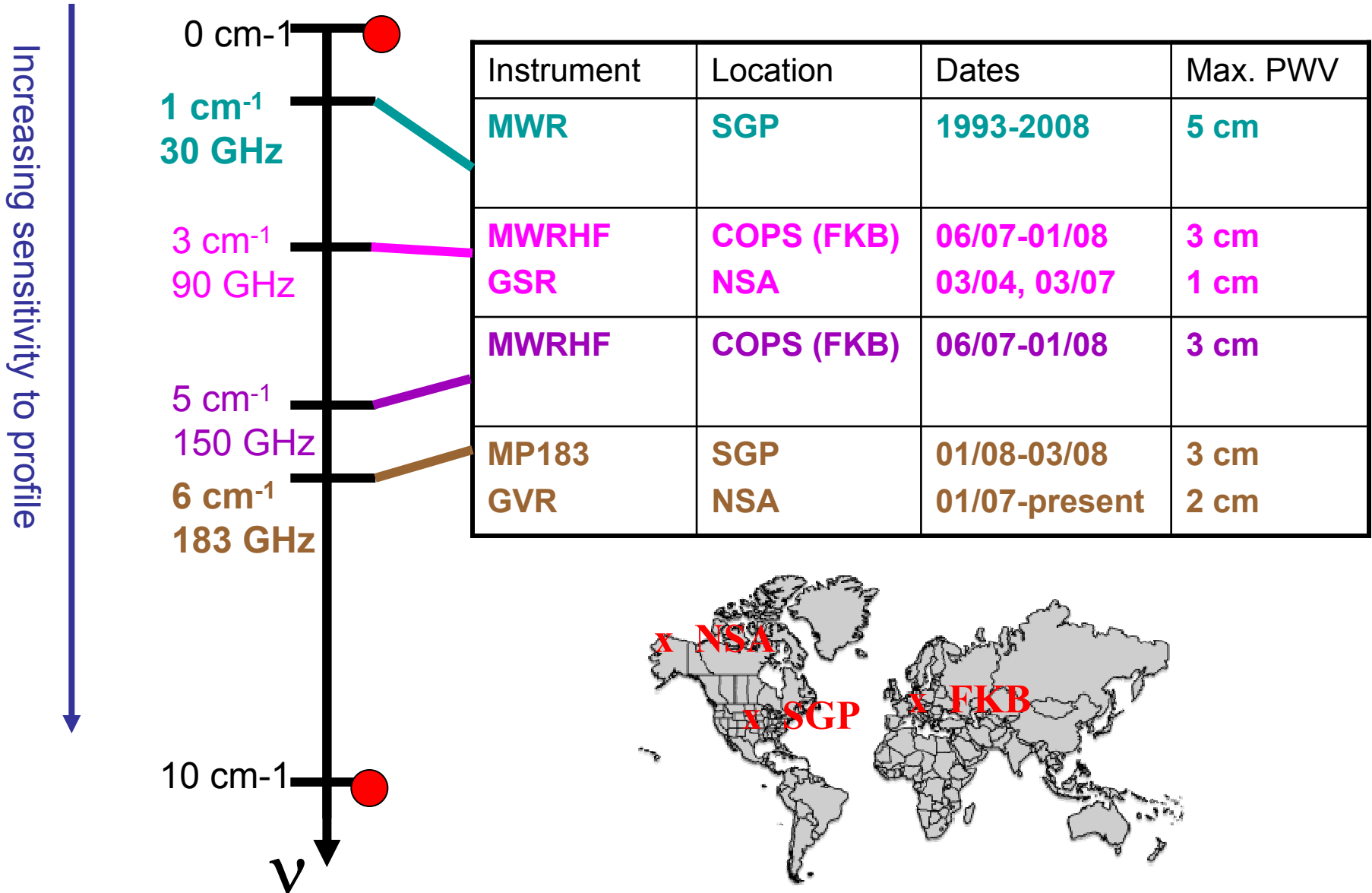
Extending the SGP MWR analysis

Within **green** area:  
Consistency with  
measurements **possible**

Outside **red** oval:  
consistency with  
measurements **impossible**



# Measurements



# Microwave Summary

- **Main differences between MonoRTM v3.3 and Rosenkranz (2007):**
  - Width of 22 GHz water vapor line
  - Water vapor continuum
  - Number of lines and input format
- **Ground-based validation supports MonoRTM 22 GHz line width**
  - Additional evidence from upwelling radiation:
    - » UK Met Office (W. Bell and P. J. Rayer - lower width value improves SSMI biases)
    - » Tom Wilheit (Texas A&M) - TMI & SSMI
- **Ongoing/future work:**
  - Continued validation at ARM sites
  - **“Best fit” water vapor continuum using a range of frequencies**
  - Consistency between microwave and infrared (AERI instrument at NSA)
  - **Zeeman line splitting**

# Infrared

## LBLRTM

### Line-by-line radiative transfer model

- Recent updates to LBLRTM
- Validation against satellite data
  - AIRS/LBLRTM/SARTA comparisons
  - IASI/LBLRTM comparisons
- Validation against ground-based data
  - AERI
- Working closely with Tony Clough

# LBLRTM: Line parameters

- **HITRAN: reference source for 'AER' Line Parameters**
  - Substitutions made only for very specific reasons and only with extensive validation
- **aer\_v\_2.0 (0 -22,656 cm-1)**

	2007	2008	Under investigation
<b>H<sub>2</sub>O</b>	HITRAN 2000	<b>HITRAN 2004 + updates</b> Updated widths AER co-authors on <b>Gordon et al., 2007</b>	Temperature dependence of widths ( <b>R. Gamache</b> ) Strengths ( <b>L. Coudert</b> )
<b>CO<sub>2</sub></b>	HITRAN 2000 P&R branch line coupling implemented for strongest bands ( <b>Niro et al., 2005, J-M Hartmann</b> )	HITRAN 2000 (Identical to HITRAN 2004 for v2 and v3 regions) <b>Niro et al. line coupling implemented for all CO<sub>2</sub> bands</b>	MIPAS CO2 v3 strengths and widths <b>(S. Tashkun, J-L. Teffo et al., J-M. Flaud et al.)</b> Corresponding update to line coupling, chi-factor, CO <sub>2</sub>
<b>O<sub>3</sub></b>	MIPAS (Wagner et al., Flaud et al.)	<b>HITRAN 2004</b>	continuum MIPAS vs ▪ ▪ HITRAN 2004

# LBLRTM: MT\_CKD\_2.1 Continuum

- **Water Vapor**
  - Self / Foreign
  - Single Line Shape for each
- **Carbon Dioxide**
  - Continuing Research Focus
  - in conjunction with CO<sub>2</sub> line parameters, line coupling and lineshape (chi-factor)
- **Nitrogen: Collision Induced**
  - 2330 cm<sup>-1</sup> Region
- **Oxygen: Collision Induced**
  - 1600 cm<sup>-1</sup> Region



# AIRS/model comparisons

# Models

- **LBLRTM v11.3**

- HITRAN 2004 line parameters, except for CO<sub>2</sub>
  - Includes water vapor width updates from Gordon et al. (2007)
- CO<sub>2</sub>
  - line parameters are HITRAN 2000 (consistency with line mixing)
  - Q / P&R branch line mixing from Niro et al. (2005)
  - Chi-factor currently set to 1.0
- Continuum: MT\_CKD\_2.1

- **SARTA v1.05**

- version 4 of AIRS RTA, January 2004
- Line parameters based on HITRAN 2000 (Strow et al. 2006)
- Line mixing / chi factors
  - Tobin (1996), De Souza-Machado et al. (1999)
- H<sub>2</sub>O continuum loosely based on MT\_CKD
  - but with large modifications (scaling by up to 10x in selected regions)
- **Transmittances tuned to agree with the dataset in these comparisons**

# Measurements

- AIRS validation, phase 1
  - ARM Tropical Western Pacific at Nauru
  - **Over ocean**
    - Avoid issues of modeling of land emissivity
  - **Night-time**
    - Avoid non-LTE effects and reflected solar radiation
  - **“Clear-sky” AIRS overpasses**
    - Sonde launches within 1 hour, 30km of AIRS measurement
    - 39 AIRS spectra (multiple AIRS match-ups for each sonde)
    - 8 distinct radiosonde profiles
      - PWV range: 4.0 to 5.6 cm

# Specification of atmospheric state

- **Layer profiles supplied by L. Strow**
  - Temperature, H<sub>2</sub>O
    - ARM “best estimate” files below 60 mbar (Tobin et al., 2006)
      - Constructed from sondes launched at times around AIRS overpasses
    - AIRS retrieval (uses SARTA) above 60 mbar
  - CO<sub>2</sub> VMR set to 370 ppmv
  - Other trace gases
    - O<sub>3</sub> from ECMWF (Strow et al 2006)
    - CH<sub>4</sub> and CO columns have been fitted
    - All other molecules from US standard atmosphere

# Layering

- 100 layers
- Layering is fine enough that switching on/off the “linear-in-tau” approximation in LBLRTM has negligible impact

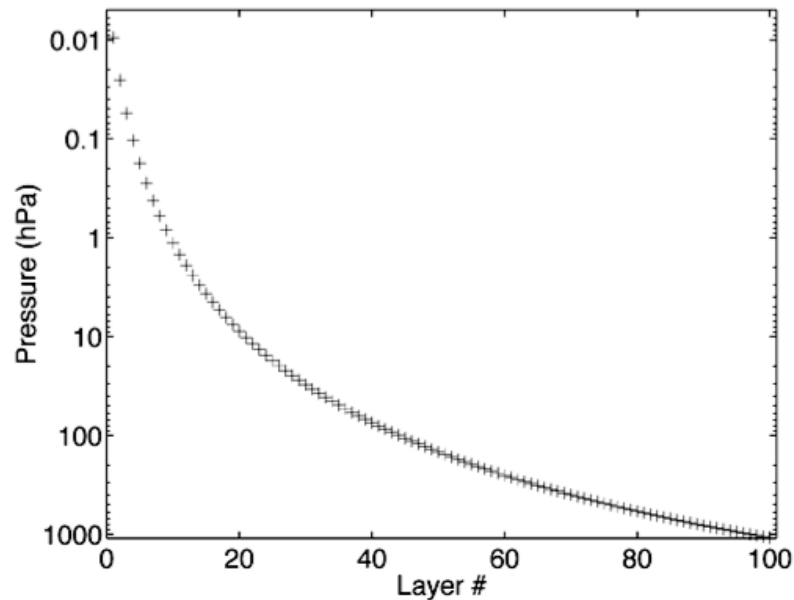
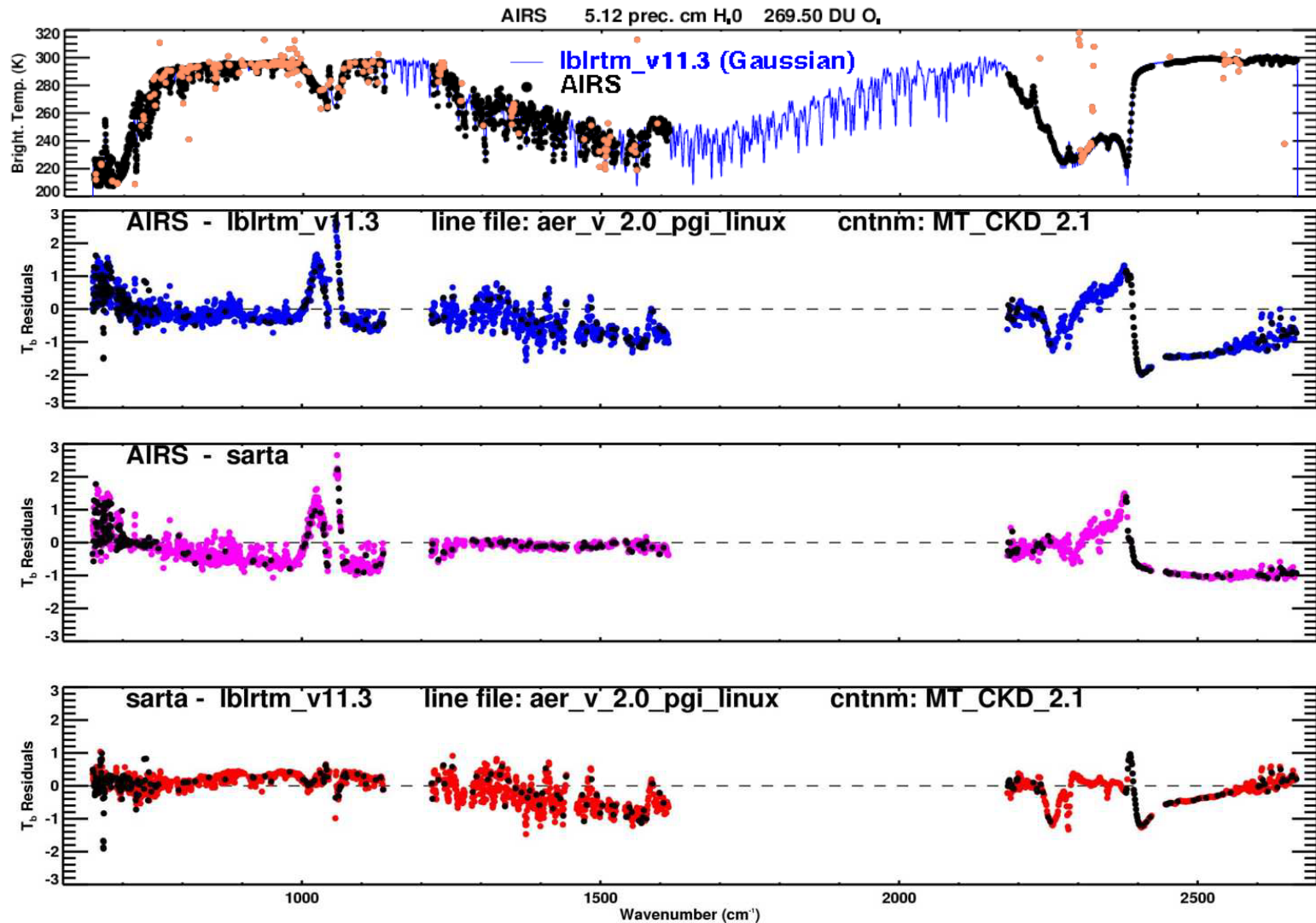


Fig. 1 from Strow et al. (2003): Mean layer pressures used in the AIRS radiative transfer model

# AIRS/model comparisons:

Mean differences for 39 AIRS match-ups at ARM TWP



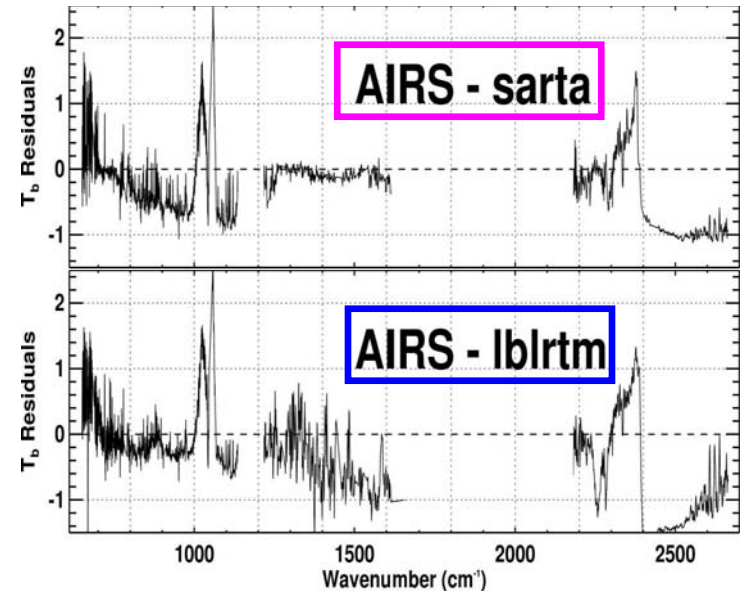
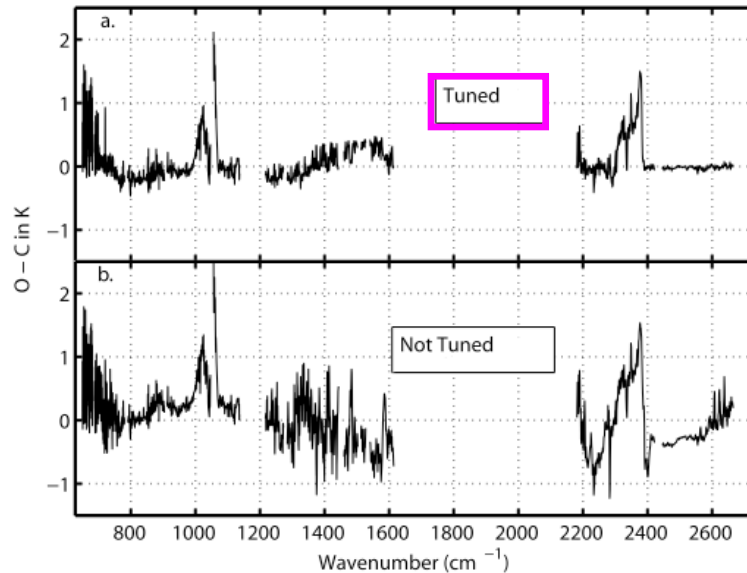
Lower 3 plots: Black dots show subset of 281 channels used by NCEP

# Comparison to results shown in Strow et al. (2006)

Strow et al (2006): ARM TWP  
ABOVE (Chesapeake Bay)  
Minnet (Carribean)

This work: Phase 1 TWP only

STROW ET AL.: VALIDATION OF THE AIRS RTA



**Figure 9.** (a) Biases relative to all clear-sky RS-90 sondes, using version 4 RTA, which has been tuned using ARM-TWP Phase 1 observations. (b) Biases relative to all RS-90 sondes but with no empirical adjustments/tuning made. Note that little adjustment is made to channels below  $690 \text{ cm}^{-1}$  (see text).

- Similar features in “untuned” SARTA and LBLRTM residuals
- To do:
  - Direct comparison of LBLRTM with “untuned SARTA” results for same dataset

# CO<sub>2</sub> 667 cm<sup>-1</sup> Q branch

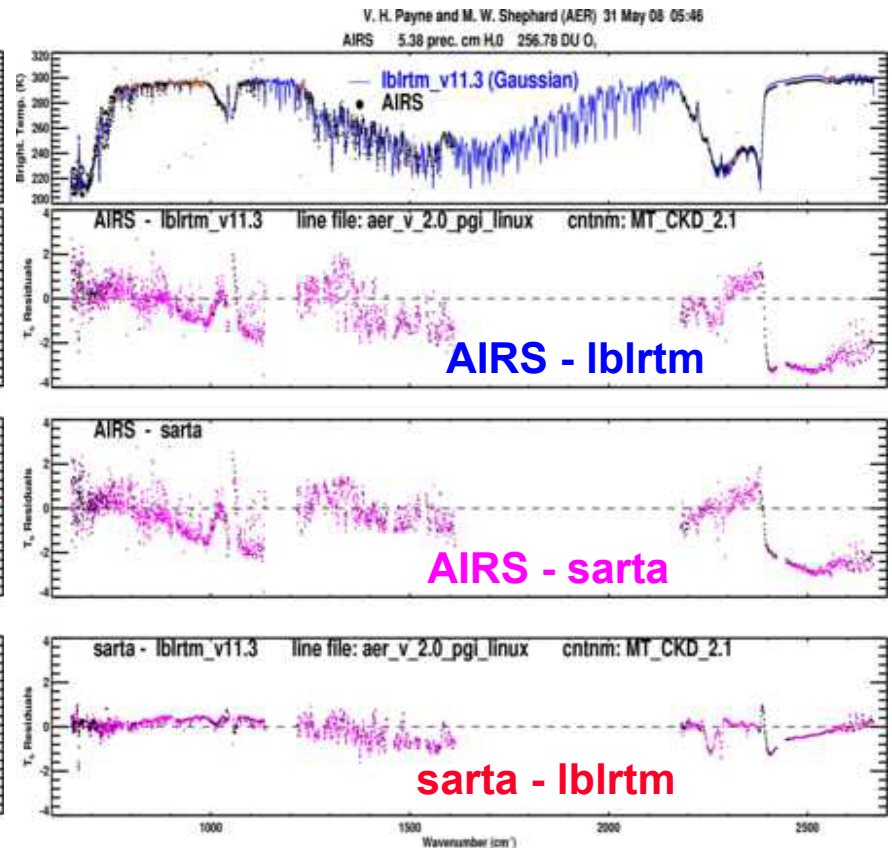
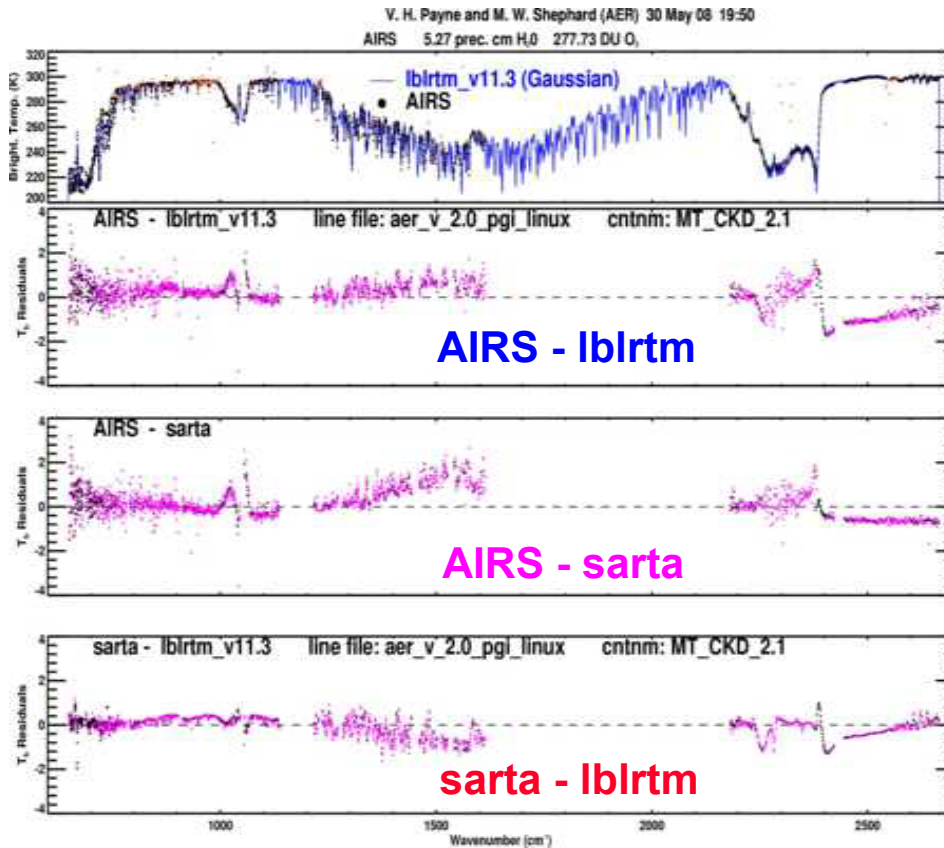
- **LBLRTM currently using 1st order perturbation theory**
  - not sufficient for sharp 667 cm<sup>-1</sup> Q-branch
- Exact calculation is very time consuming
  - Niro et al., 2005
- Approaches to be investigated:
  - 2nd order perturbation
  - parameterization of Niro et al.



# Residuals at 2500 cm<sup>-1</sup>: “Good” and “bad” ARM TWP Phase 1 cases

“Good”: Case 003

“Bad”: Case 034



- “Bad” case:

- Sonde T, H<sub>2</sub>O profile does not accurately represent atmospheric state observed by AIRS?
- Influence of cloud?
- Demonstrates importance of careful selection of cases in addition to ensembles for RT model validation

# AIRS/model comparisons

## – CO<sub>2</sub> residuals:

### •Tropospheric

- Sonde provides good estimate of “true” temperature
- **v2 region agrees well with sonde in troposphere**
- v3 region - issues with modeling outer edges of the band
  - » Both in LBLRTM and “untuned” SARTA

### •Stratospheric

- “True” temperature is more difficult to determine
- **Models essentially not yet validated in the stratosphere**
- LBLRTM/SARTA agree well (apart from 667cm<sup>-1</sup> Q branch)
  - » LBLRTM uses first order perturbation for line coupling
  - » First order perturbation not enough for 667 cm<sup>-1</sup> Q branch

## – H<sub>2</sub>O residuals

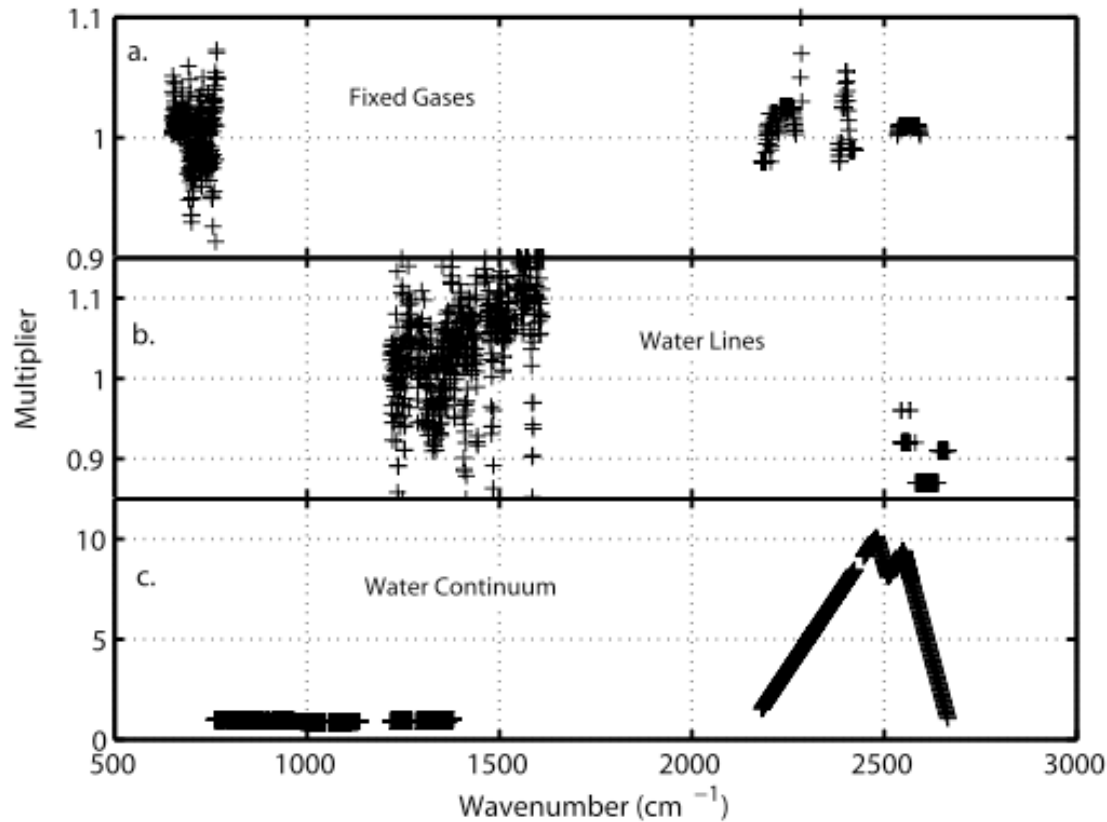
### • **Sonde should not be regarded as “truth”**

- Sonde biases
- Variation of H<sub>2</sub>O on small temporal and spatial scales

### – H<sub>2</sub>O continuum:

- » Known to within a few percent at 900 cm<sup>-1</sup>
- » Larger uncertainty at 2500 cm<sup>-1</sup>

## Figure from Strow et al (2006)



**Figure 8.** Multipliers to the channel-averaged absorption coefficients in the version 4 RTA. Different multipliers were derived for the RTA fixed gases, water lines, and water continuum using the ARM-TWP Phase 1 observations.

**AERI comparisons also indicate possible evidence of H<sub>2</sub>O dependence for  $\nu > 2385 \text{ cm}^{-1}$  (past CO<sub>2</sub>  $\nu_3$  bandhead)**

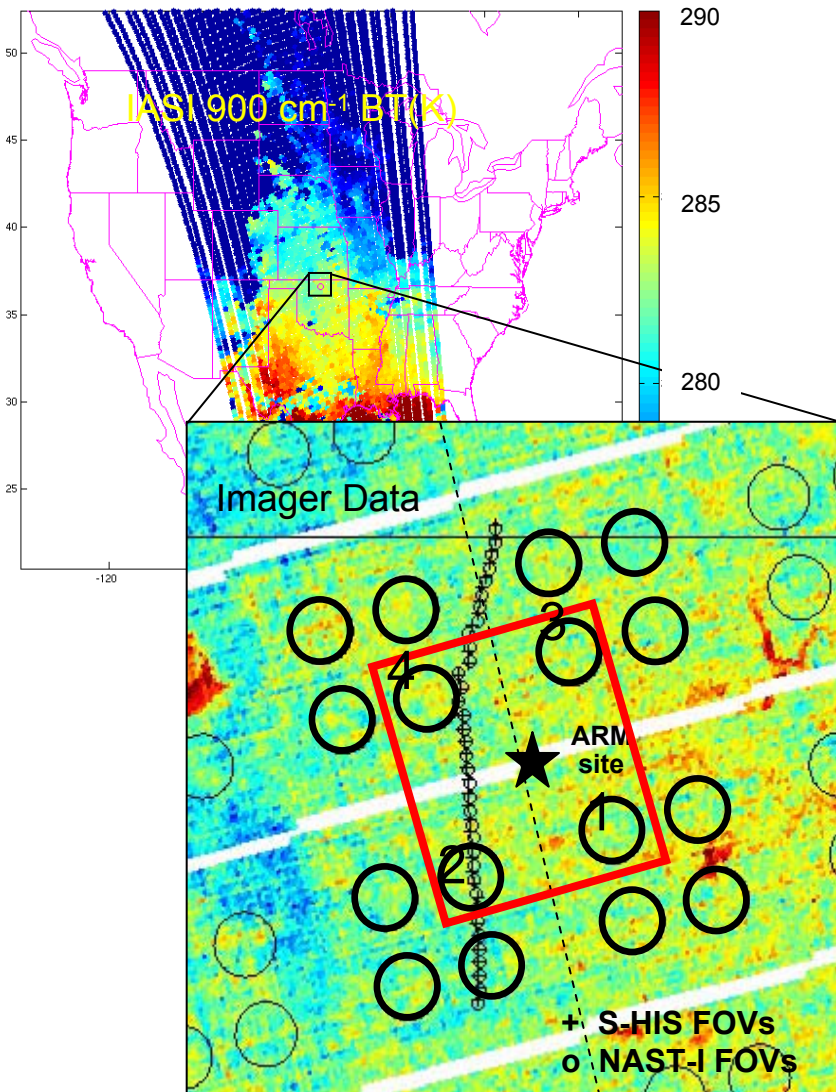
# IASI/LBLRTM comparisons

# IASI/LBLRTM comparisons

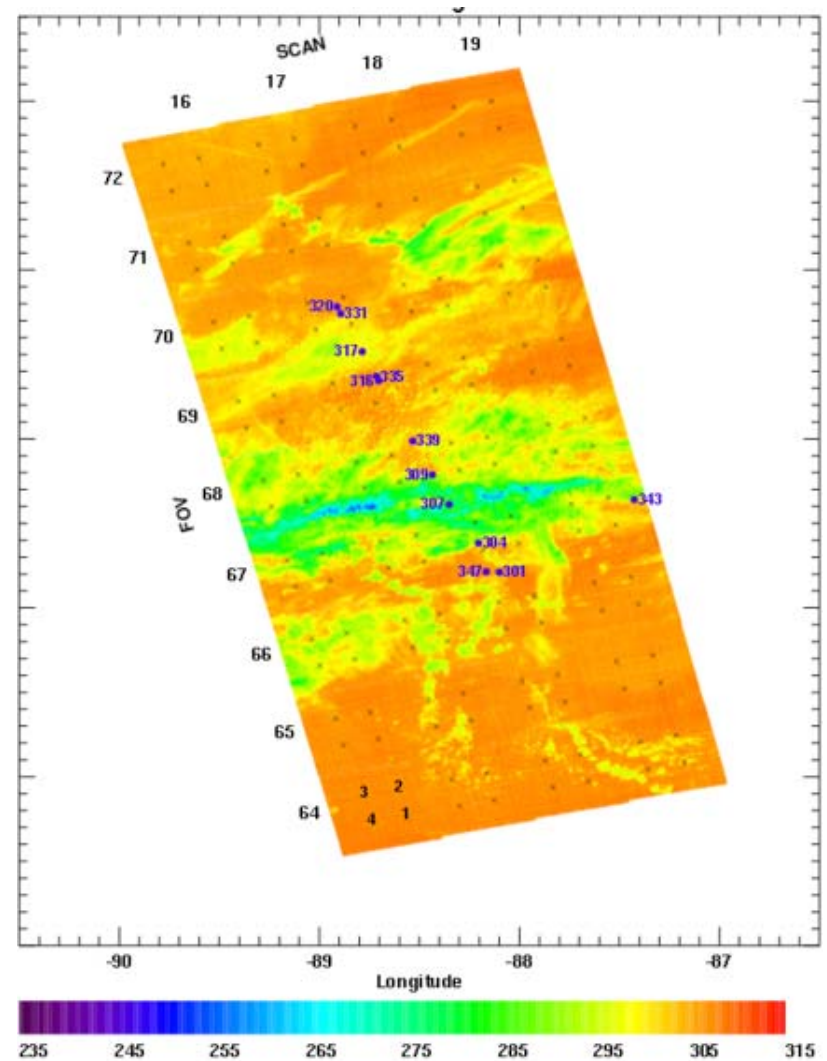
Mark Shephard, Tony Clough

- **Night-time data from JAIVEx campaign (April/May 2007)**
- **Land case**
  - Over ARM SGP site
  - Radiosonde profiles as initial guess for temperature, H<sub>2</sub>O
  - Initial guess surface emissivity supplied by Bill Smith (NASA Langley)
  - Retrievals of surface emissivity, temperature, H<sub>2</sub>O and other trace gases
- **Ocean cases**
  - **Gulf of Mexico**
  - Drop-sondes as initial guess for temperature, H<sub>2</sub>O
    - » Maximum altitude ~9 km
  - Surface should be well characterized
  - Retrievals of temperature, H<sub>2</sub>O, other trace gases

*JAIVEx 19 Apr 2007*  
*SGP (03:35 UTC)*

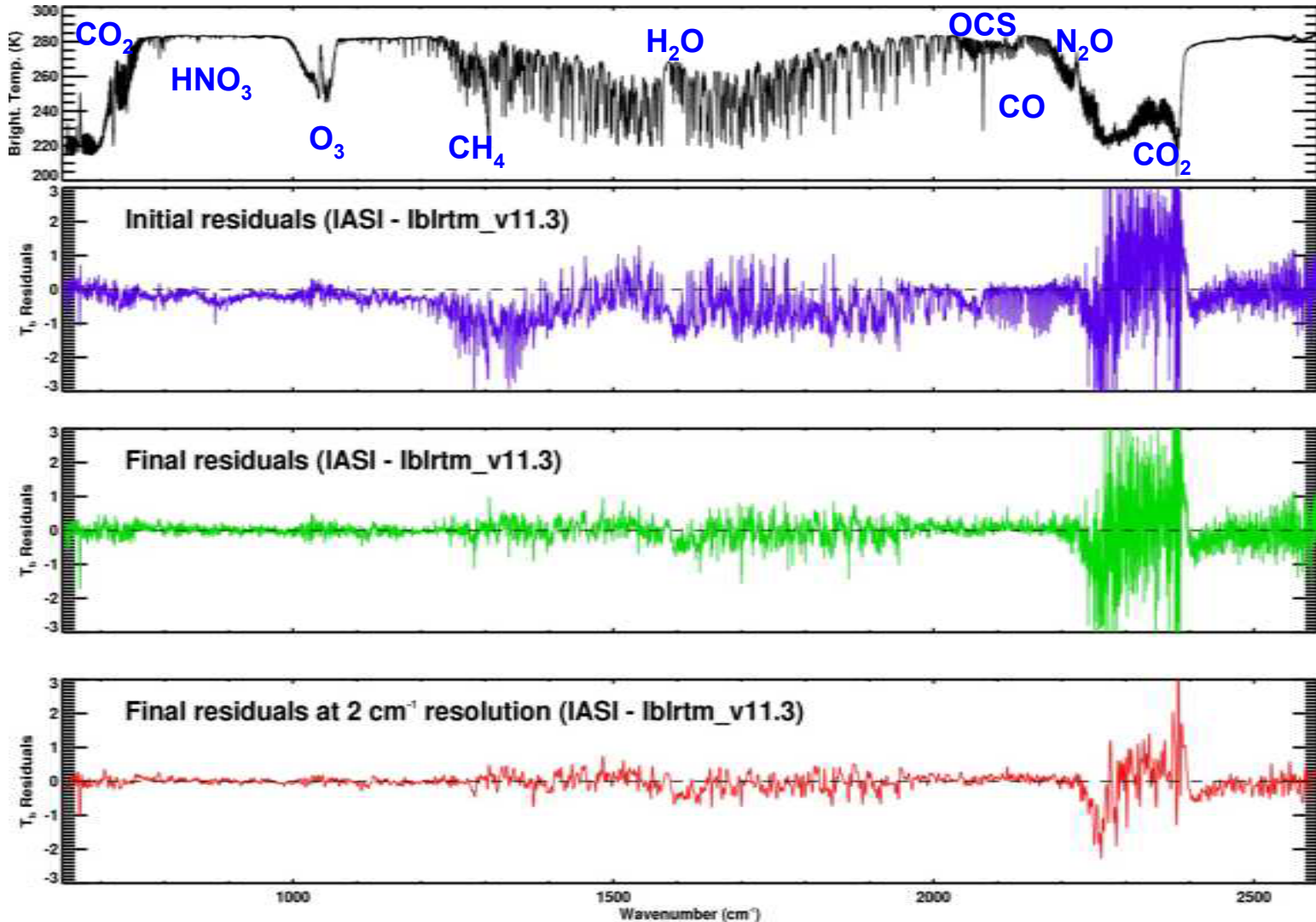


*JAIVEx 20 Apr 2007*  
*Gulf of Mexico (~03:35 UTC)*

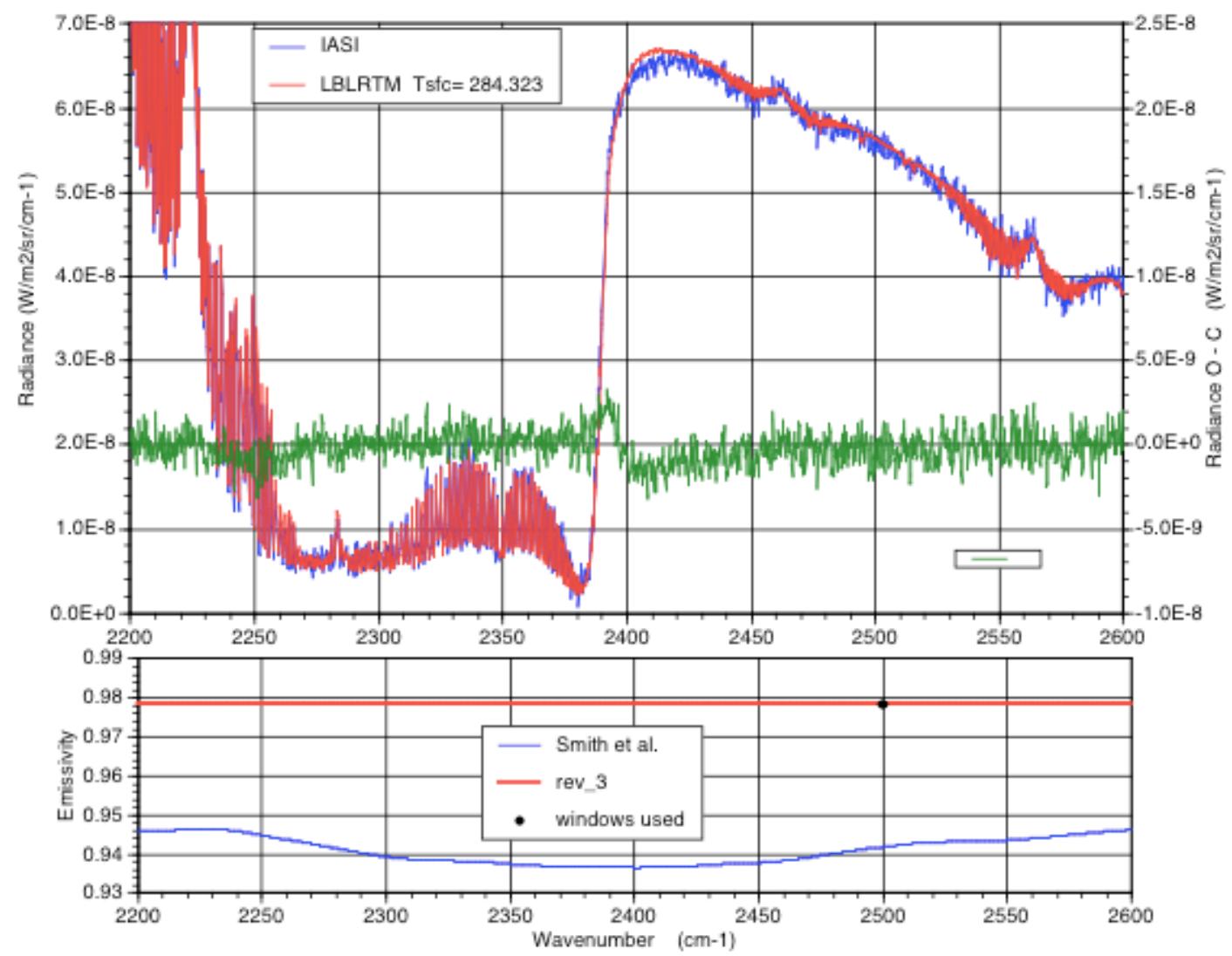


Figures from Bill Smith

# IASI: ARM SGP

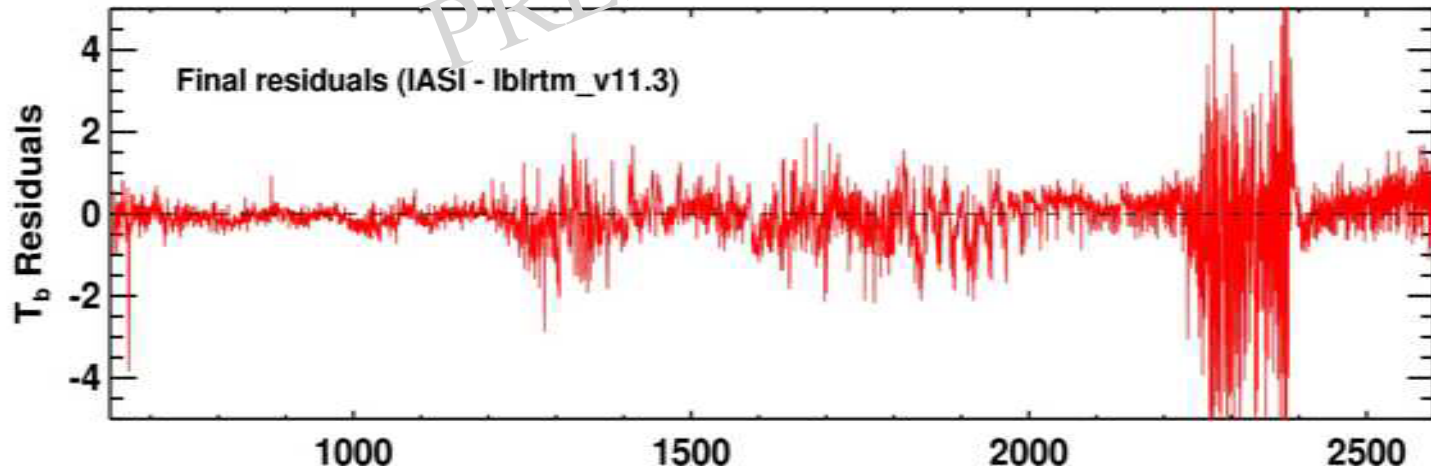
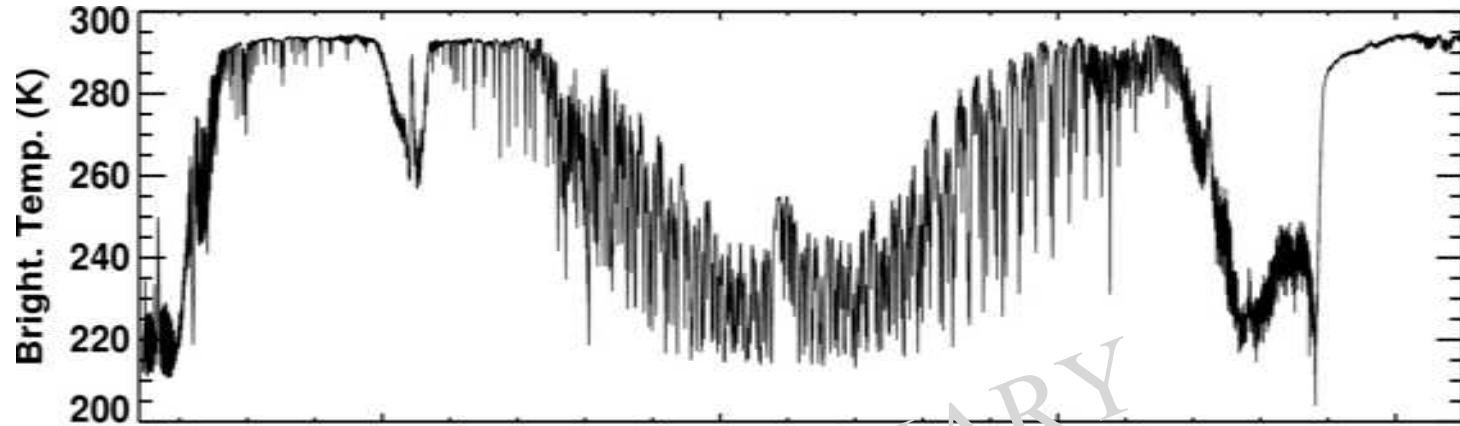


▪ Tony Clough, Mark Shephard





# IASI: Gulf of Mexico



# IASI/LBLRTM comparisons

- **IASI measurements are excellent!**
- **Experience with ocean cases:**
  - “Good” high H<sub>2</sub>O cases show negative residual at 2500 cm<sup>-1</sup>
  - “Good” low H<sub>2</sub>O cases show positive residual at 2500 cm<sup>-1</sup>
  - Can’t attribute both to the H<sub>2</sub>O continuum
    - » Residual contribution due to H<sub>2</sub>O continuum would go to zero for low PWV profiles
  - H<sub>2</sub>O continuum is not the only piece of the answer at 2500 cm<sup>-1</sup>.....
- **Residuals in H<sub>2</sub>O region remain large after retrieval**
  - **Issues with HITRAN H<sub>2</sub>O line parameters?**
  - Laurent Coudert:
    - » New measurements indicate HITRAN strengths may be 5% to low for strong lines
  - Bob Gamache
    - » Temperature dependences of widths in HITRAN are out of date
    - » Large impact in upper troposphere

# Future Plans

- **LBLRTM:**
  - **Update CO<sub>2</sub> v<sub>3</sub> line parameters**
    - HITRAN\_MIPAS database: line parameters from Tashkun, Teffo, Flaud et al
      - Validated by Flaud et al. using MIPAS spectra
    - **Update line coupling, continuum and chi-factor accordingly**
    - Initial validation using laboratory spectra (J. Johns)
  - Re-assessment of H<sub>2</sub>O self continuum in region of 2500 cm<sup>-1</sup>
  - **Validation using AIRS, IASI and AERI**
  - **Validation of LBLRTM in the stratosphere**
  - Comparisons with “untuned” SARTA
  - Investigation of alternative sets of v<sub>2</sub> water vapor line parameters
    - Line strengths from L. Coudert
    - Temperature dependences of widths from R. R. Gamache

# Improved Spectroscopy for Microwave and Infrared Satellite Data Assimilation

P.I.: J.-L. Moncet, AER, Inc.

## Summary of Accomplishments

- **Microwave**
  - Publication on water vapor line widths
  - Validation of water vapor self & foreign H<sub>2</sub>O continuum using ground-based measurements
- **Infrared**
  - Implementation of P&R branch line coupling for all CO<sub>2</sub> bands
  - Updated water vapor line widths
  - AIRS/LBLRTM/SARTA comparisons
  - IASI/LBLRTM comparisons

## Future Work

- **Microwave**
  - Find optimal fit for self and foreign H<sub>2</sub>O continuum
  - Zeeman splitting
- **Infrared**
  - Update CO<sub>2</sub> v3 line parameters
    - Update CO<sub>2</sub> line coupling, lineshape and continuum
    - Validation using up- & down-welling measurements
  - Assessment of H<sub>2</sub>O continuum in 2500 cm<sup>-1</sup> region using upwelling, & downwelling measurements
  - Validation of LBLRTM in the stratosphere
  - Comparisons with “untuned SARTA”
  - Investigate alternative H<sub>2</sub>O line parameters

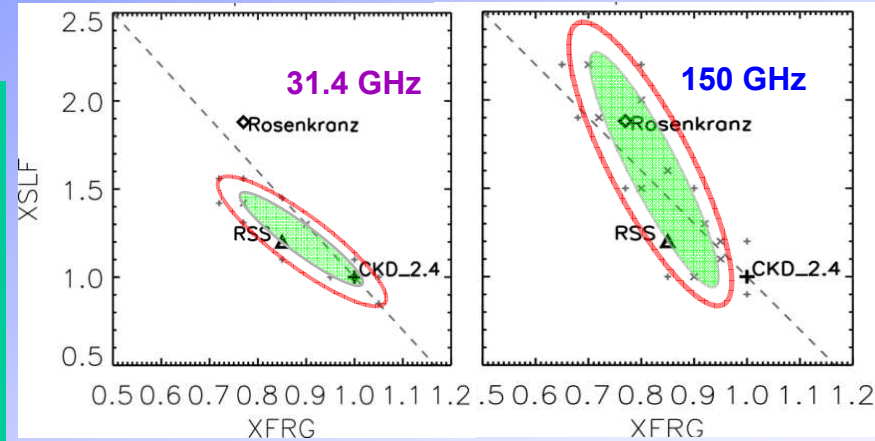


Figure 1: Current uncertainty on MW water vapor continuum

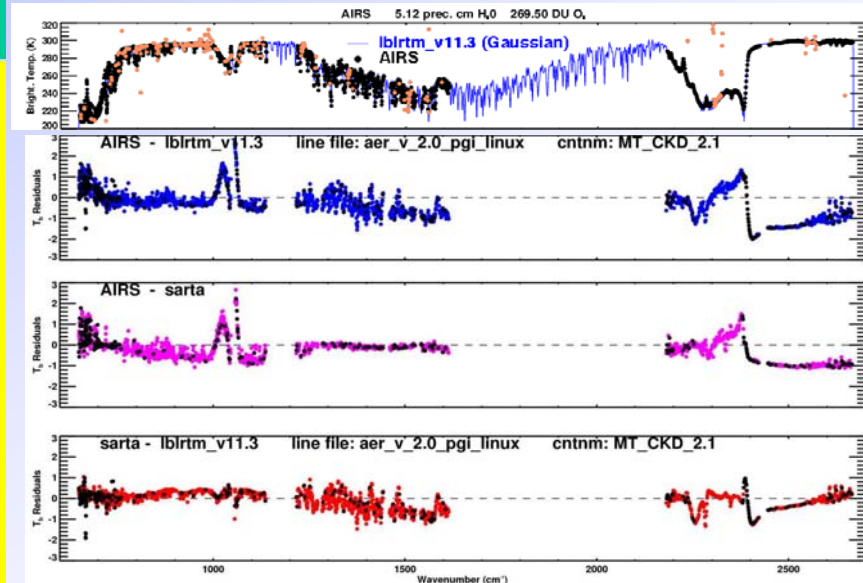


Figure 2: AIRS/LBLRTM/SARTA comparisons for ARM TWP