Line-by-line modeling at AER: Perspectives and recent spectroscopy studies

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CNR: Luca Palchetti

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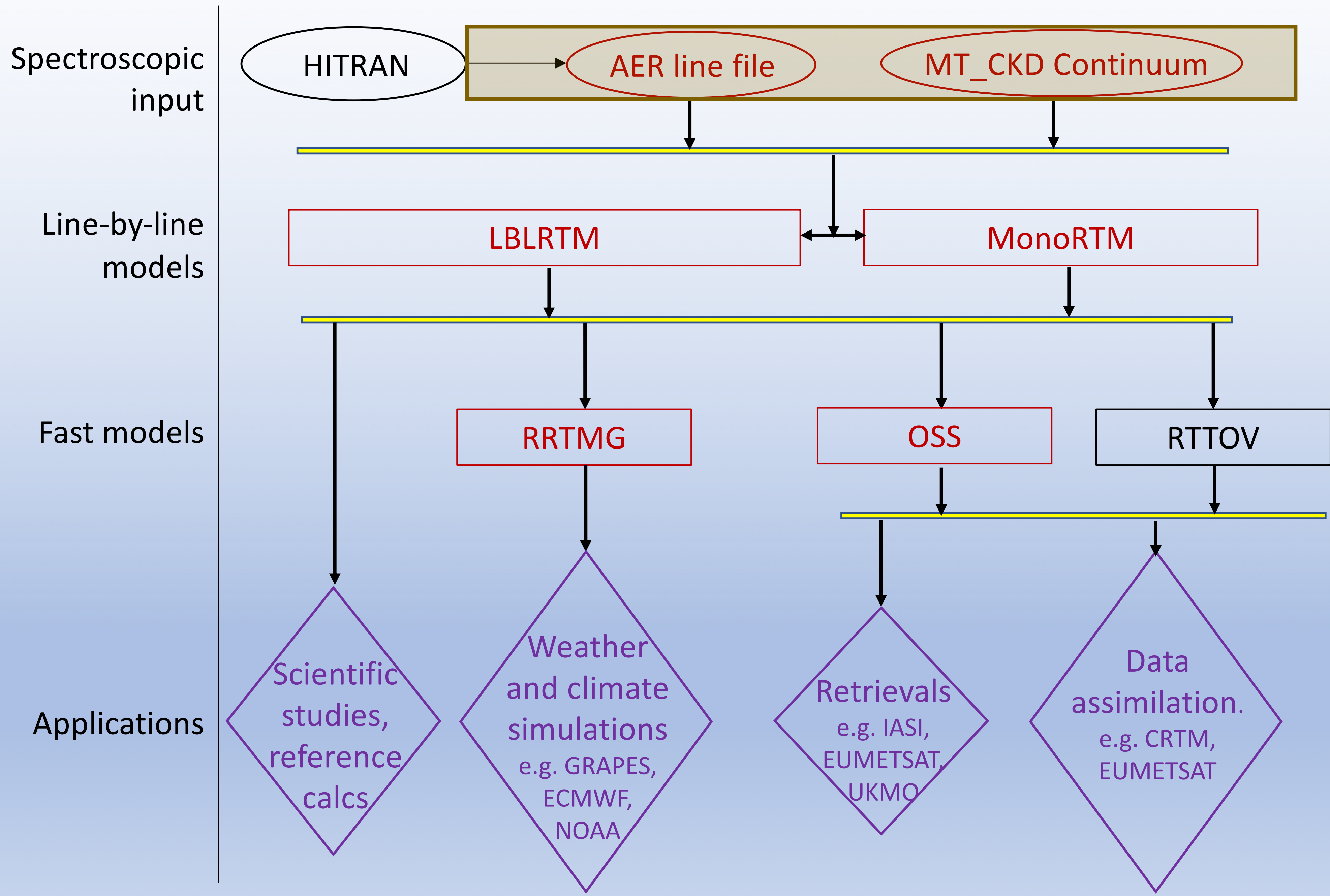
Texas A&M: Jeff Mast

DoE ANL: Maria Cadeddu

AER's radiative transfer models and databases

available from AER, see rtweb.aer.com



Perspectives on validation and model improvement

- ❖ Validation of absorption/RT models not straightforward
  - Radiometric measurements and atmospheric profiles may not be accurate

- ❖ What is "truth"?
  - **'Truth' at the level required is not readily available**
  - Laboratory measurements
  - Theoretical calculations
  - Radiosonde accuracies, spatial and temporal sampling

- ❖ **Consistency is key** (Tony Clough perspective)
  - Consistency between instruments
  - Validation using both upwelling and downwelling measurements
  - Consistency between spectral bands, regions (e.g. IR & MW)

Our main approach is to use detailed radiative closure studies with field measurements to evaluate and improve spectroscopic parameters.

Topics

Radiative closure study examples

1) Water vapor line widths and continuum in microwave

2) Water vapor line widths and continuum in far-infrared

3) Other examples of issues with water vapor line widths

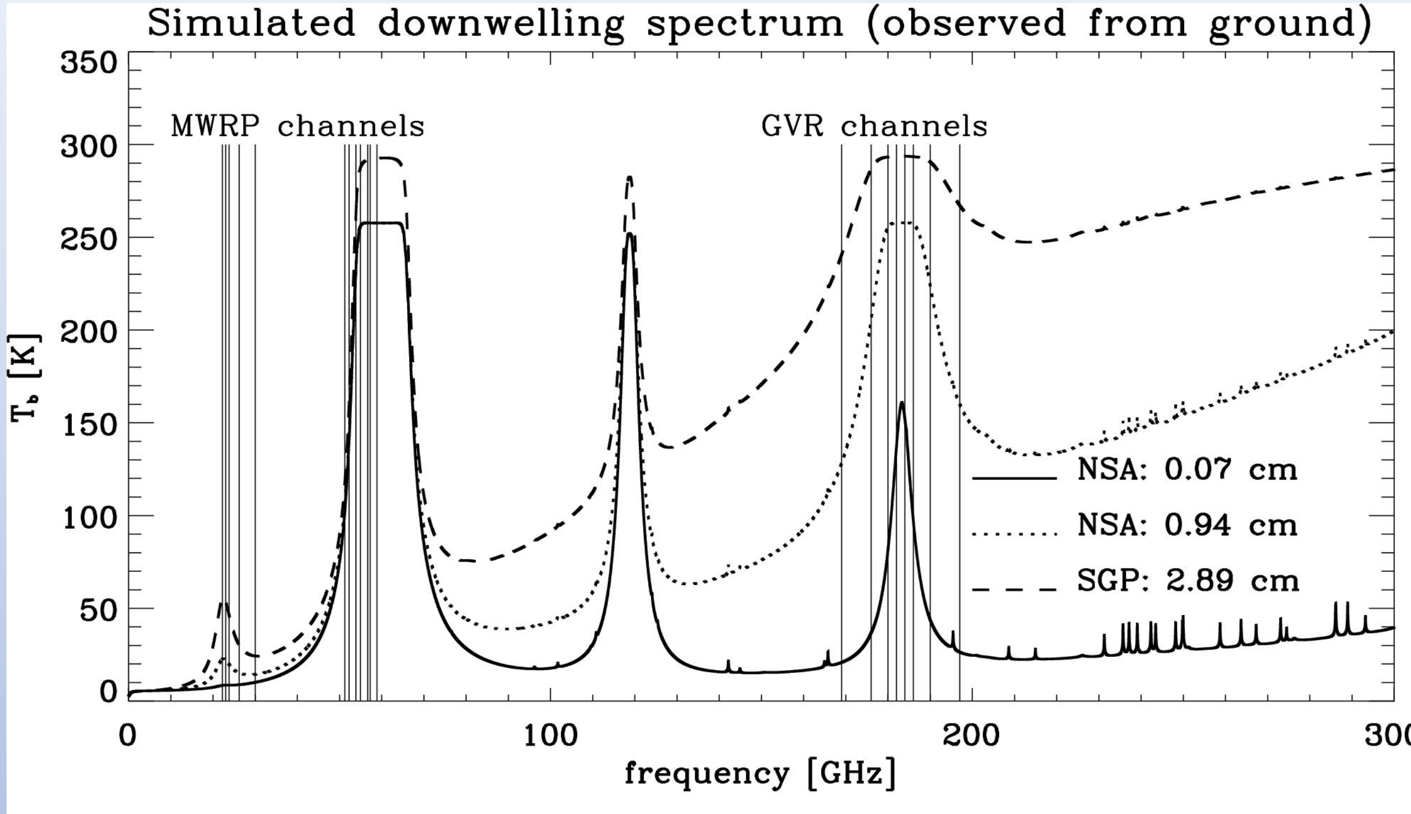
Improving water vapor spectroscopy in the microwave

- Ground-based microwave radiometers (MWRs) have been and **continue to be** used to derive key spectroscopic parameters of water vapor in the microwave

- Previous studies
  - Widths of 22 GHz and 183 GHz lines – **Payne et al. 2008**
    - 22 GHz width has an impact on continuum analysis
  - Microwave water vapor continuum – **Payne et al. 2011**

- **Ongoing studies**
  - Widths of 22 GHz and 183 GHz lines
    - Re-evaluate in light of new line parameters in HITRAN
  - Microwave water vapor continuum
    - Comprehensive new analysis using more recent measurements from MWRs, including more moist cases

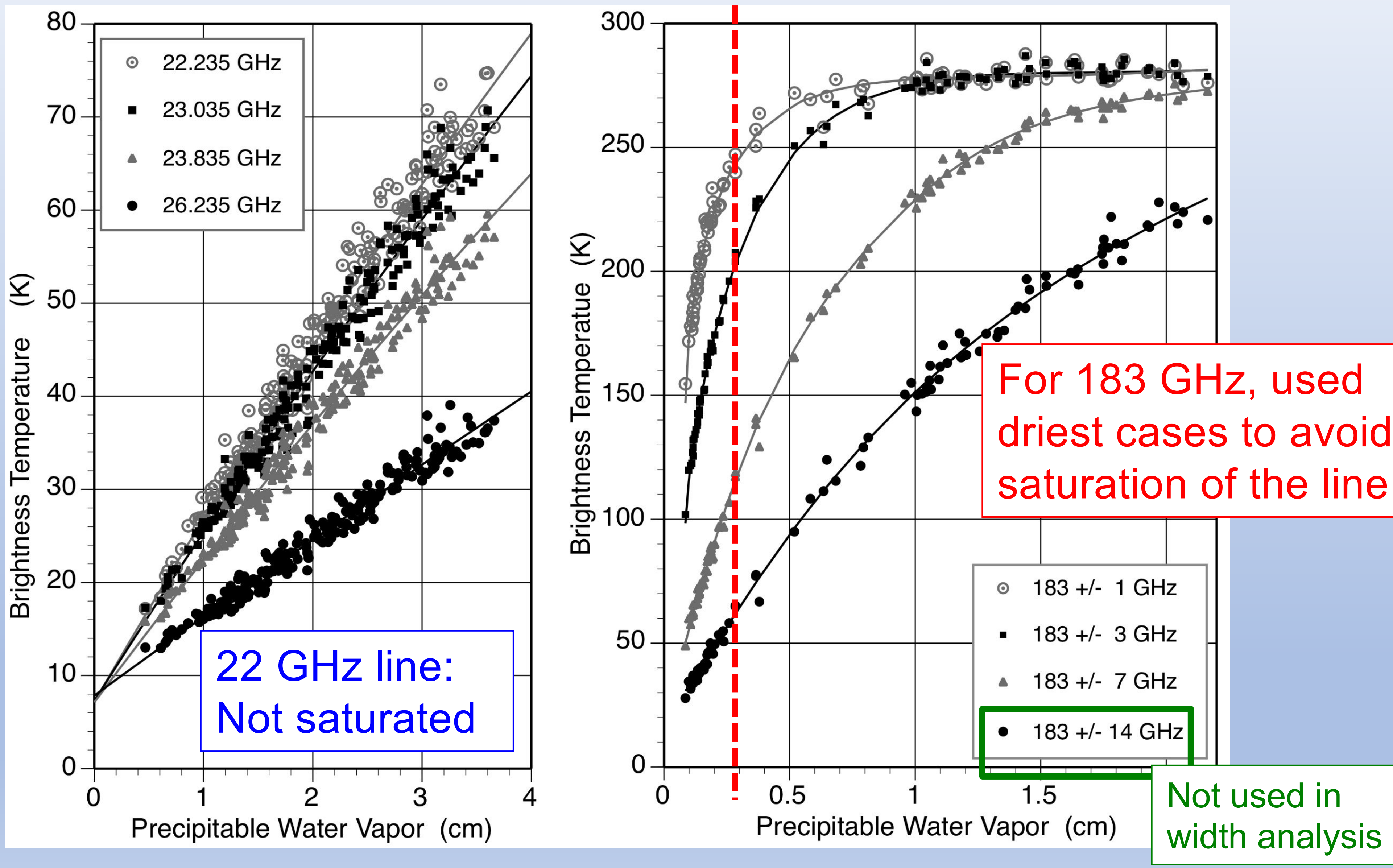
Instruments used for line width determination



- **Compare MonoRTM with radiometer measurements**
  - Model the instrument bandpass characteristics
  - Use radiosonde temperature and humidity profiles as input
  - Radiosonde humidity measurements show variability and biases
    - » **Use radiometer to scale the total precipitable water vapor**

Payne et al., 2008

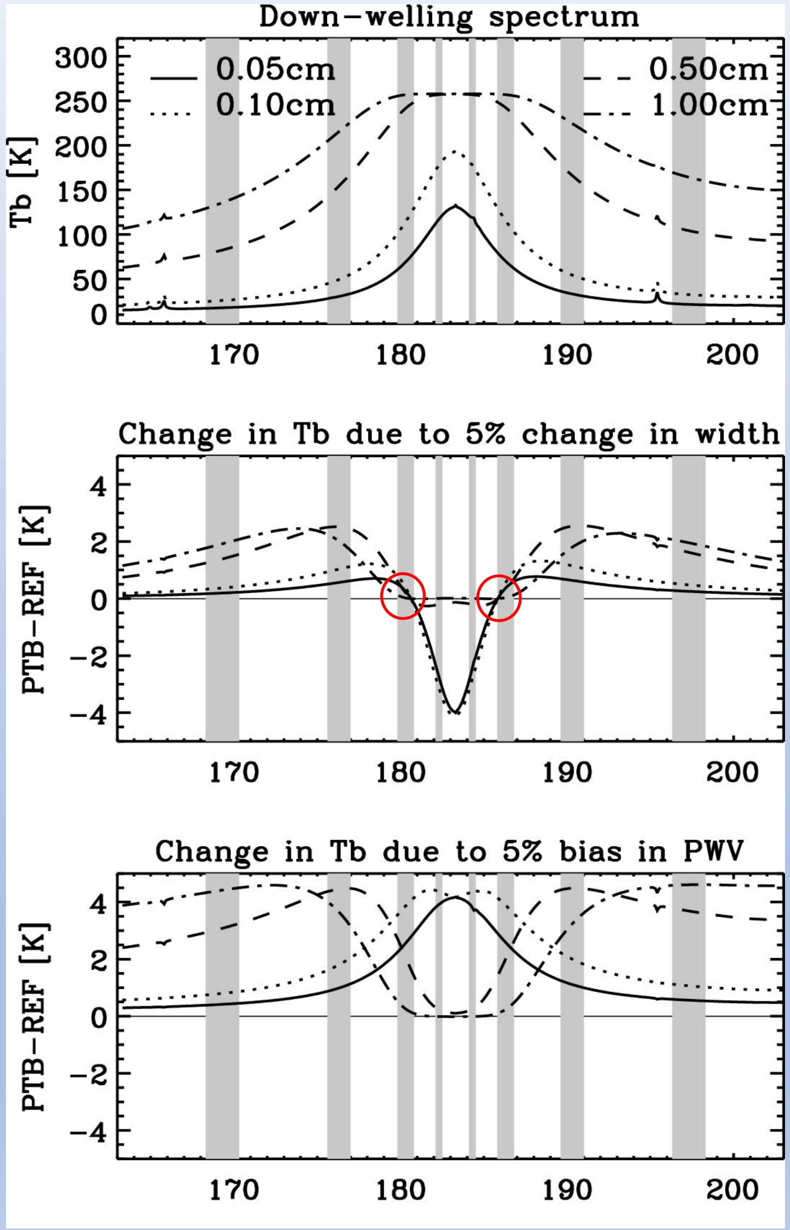
Ground-based radiometer measurements



Determination of line widths from ground-based data

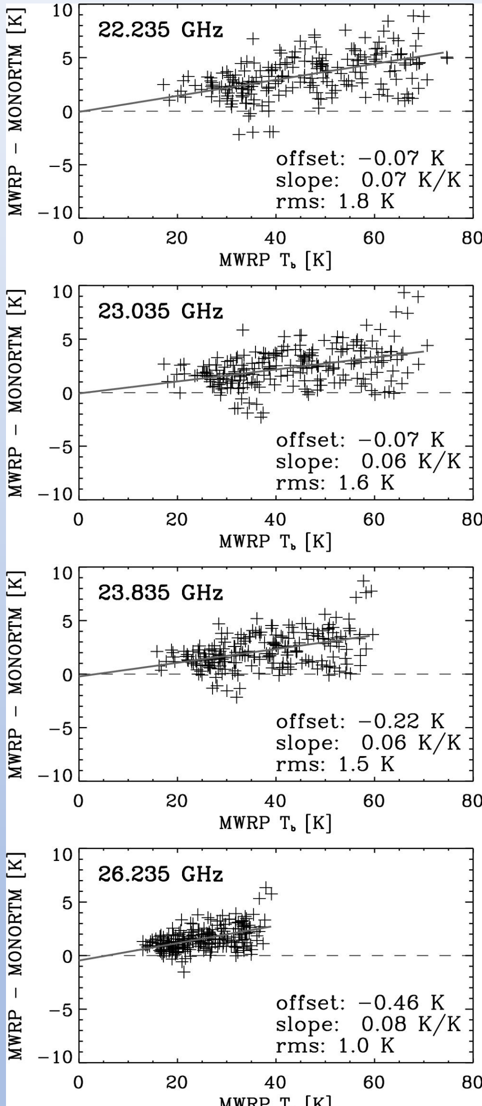
- **"Pivot point"**
  - Frequency where T_b insensitive to line width
  - GVR: 183+/-3 channel least sensitive
  - MWRP: 23.835 channel least sensitive
- **Channels on both side of "pivot point"**
  - Different response to width, PWV
  - **Crucial for information on width**

- **Width determination**
  - Run model using radiosondes as input
  - Retrieve PWV scaling from channel least sensitive to width uncertainty
  - Retrieve width value from remaining channels

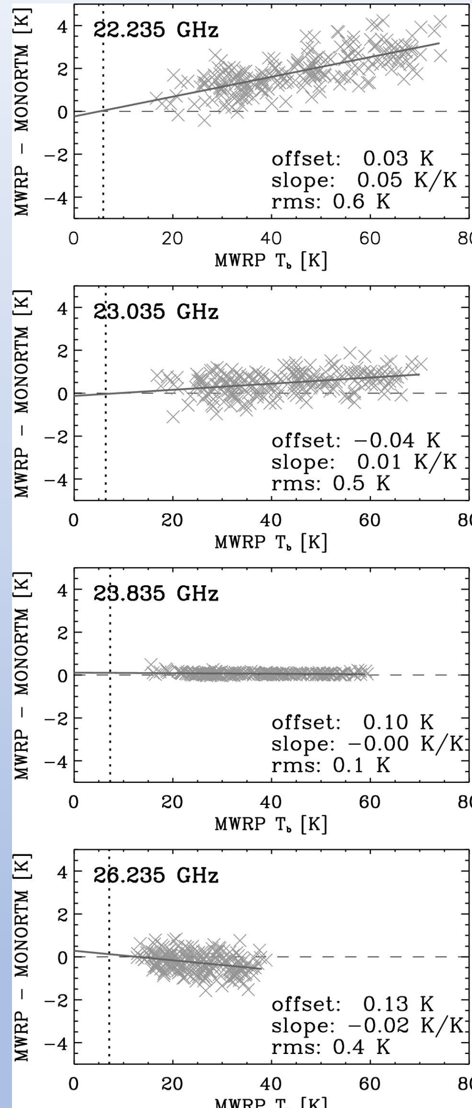


Payne et al., 2008

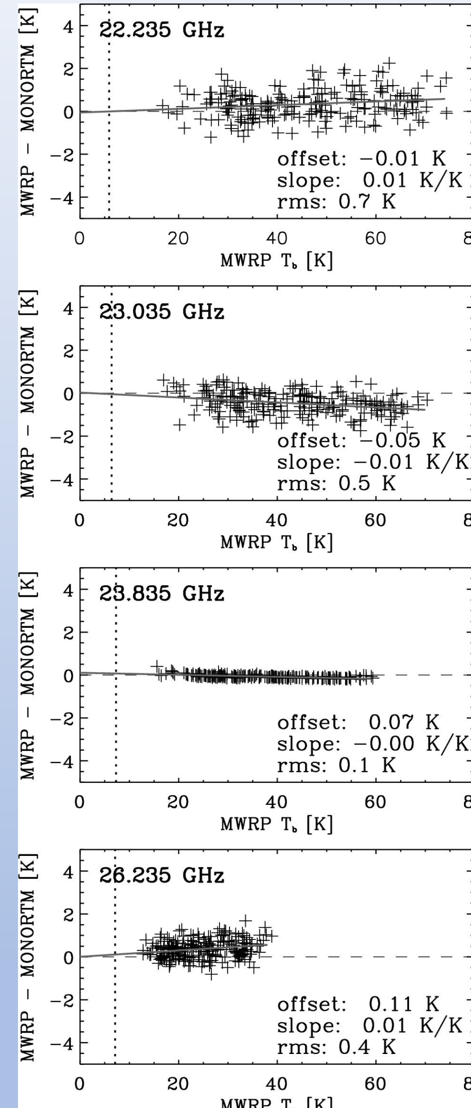
Determination of line widths from ground-based data



Original radiosondes, original width



Scaled Radiosondes, original width



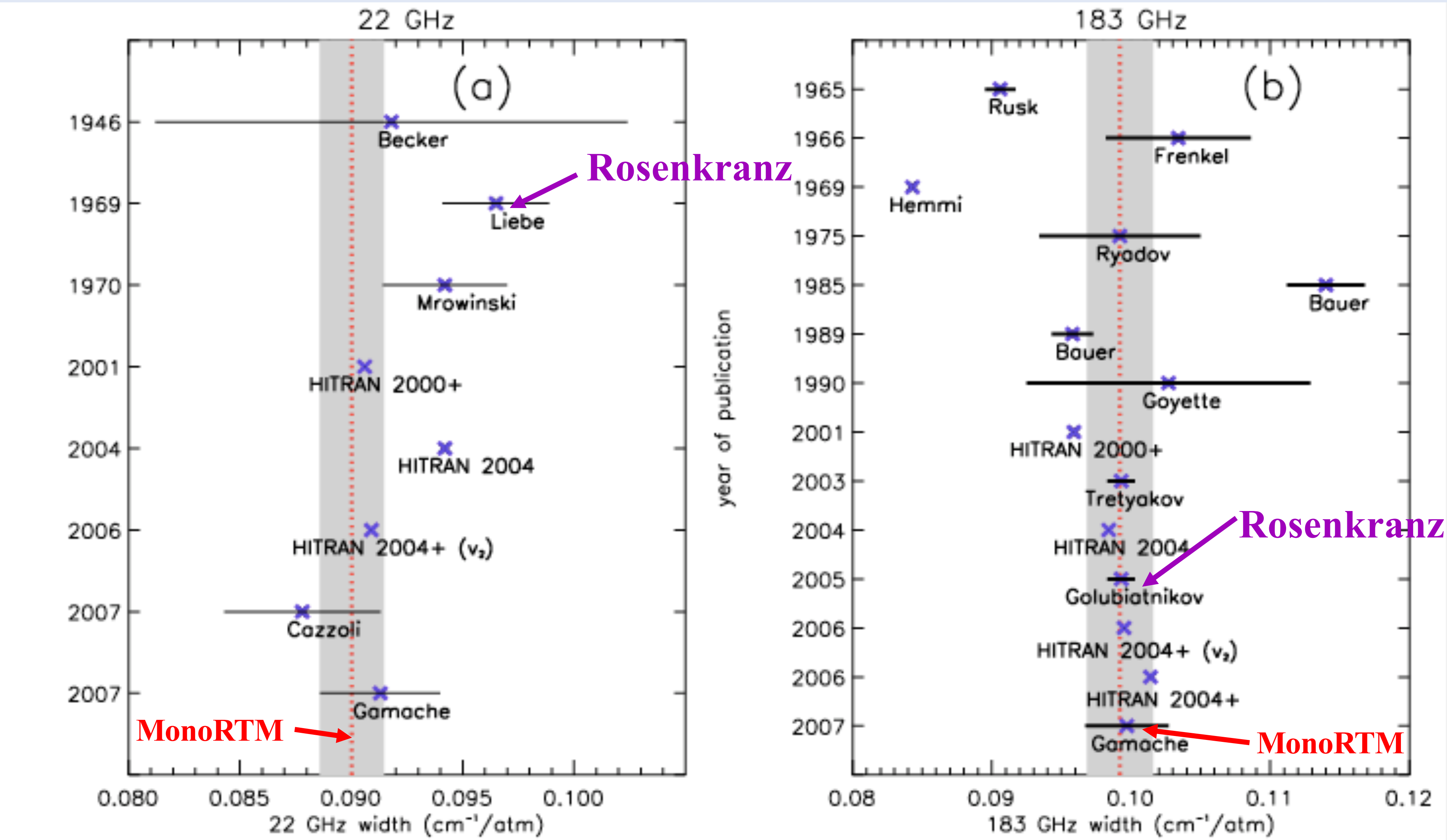
Scaled radiosondes, derived width

Payne et al., 2008

Water vapor line widths

22 GHz:
MonoRTM 5% lower than Rosenkranz (at that time)

183 GHz:
MonoRTM ~ same as Rosenkranz



Payne et al., 2008

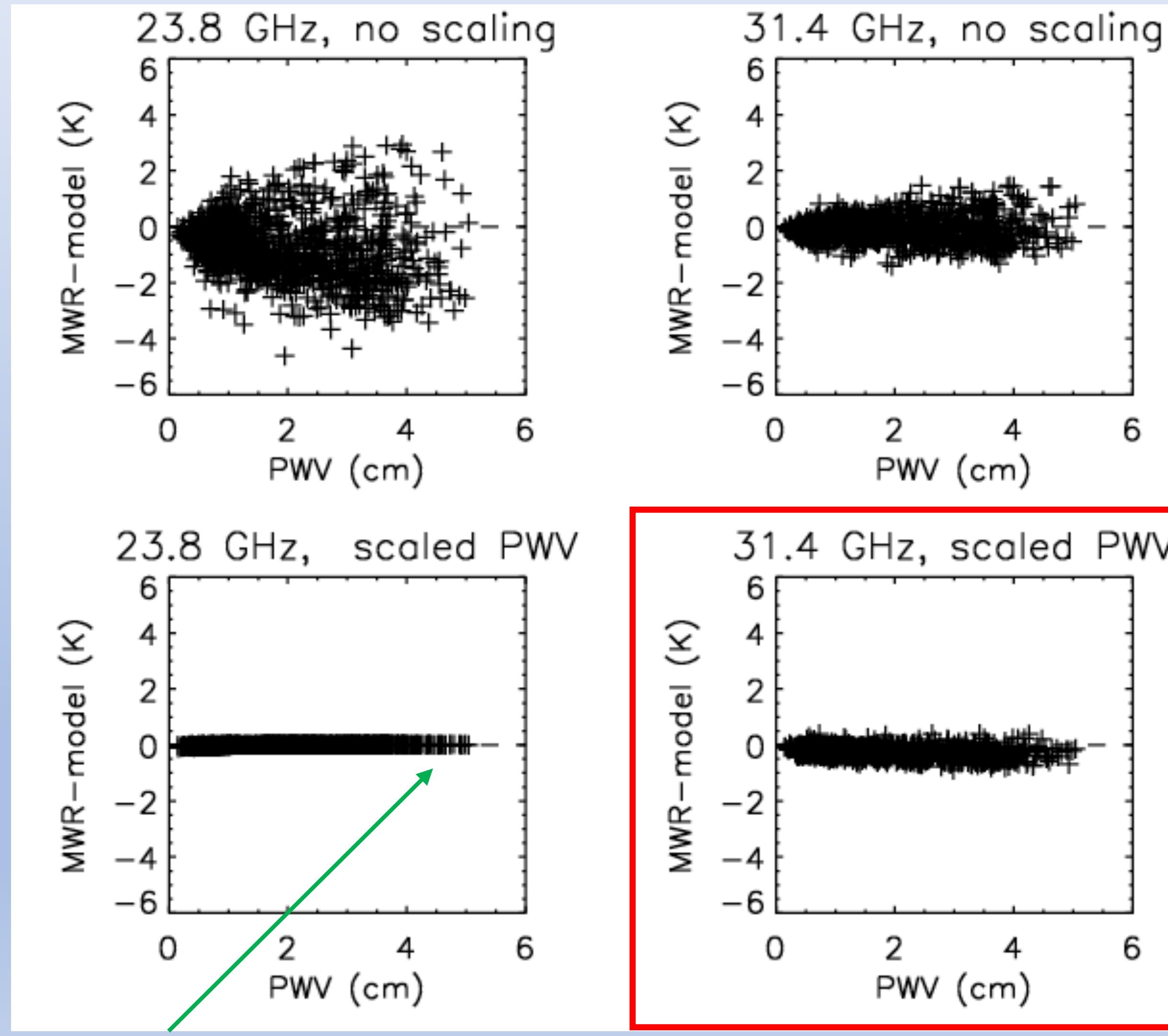
Determining the water vapor continuum in the microwave

MicroWave Radiometer

Built by Radiometrics
Two channels: 23.8 and 31.4 GHz
Measurement accuracy: 0.3 K
Long and successful use in ARM program

- Providing PWV and LWP retrievals at ARM sites for over 15 years
- An MWR is deployed at all ARM sites
- **Payne et al. (2011)**: 3 years of data from the **Southern Great Plains**
- Wide range of atmospheric conditions encountered

Scaling of PWV using MWR

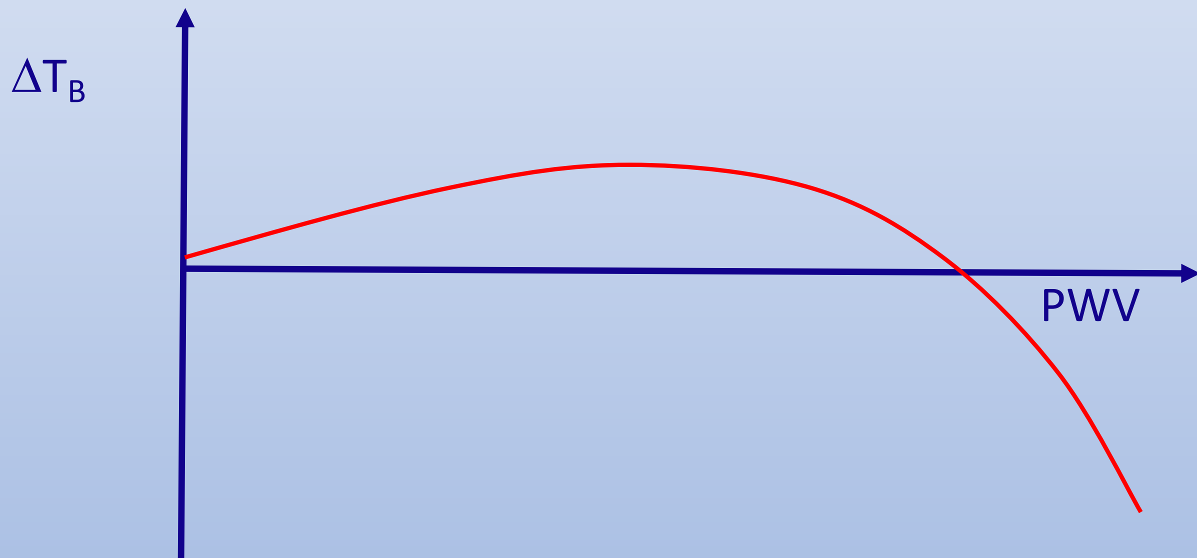


Not too many cases with PWV > 4 cm

Continuum uncertainty

Extending the SGP MWR analysis

$$\Delta T_B = \underbrace{a\Delta X_{frg}(PWV)}_{\text{foreign}} + \underbrace{b\Delta X_{slf}(PWV)^2}_{\text{self}}$$

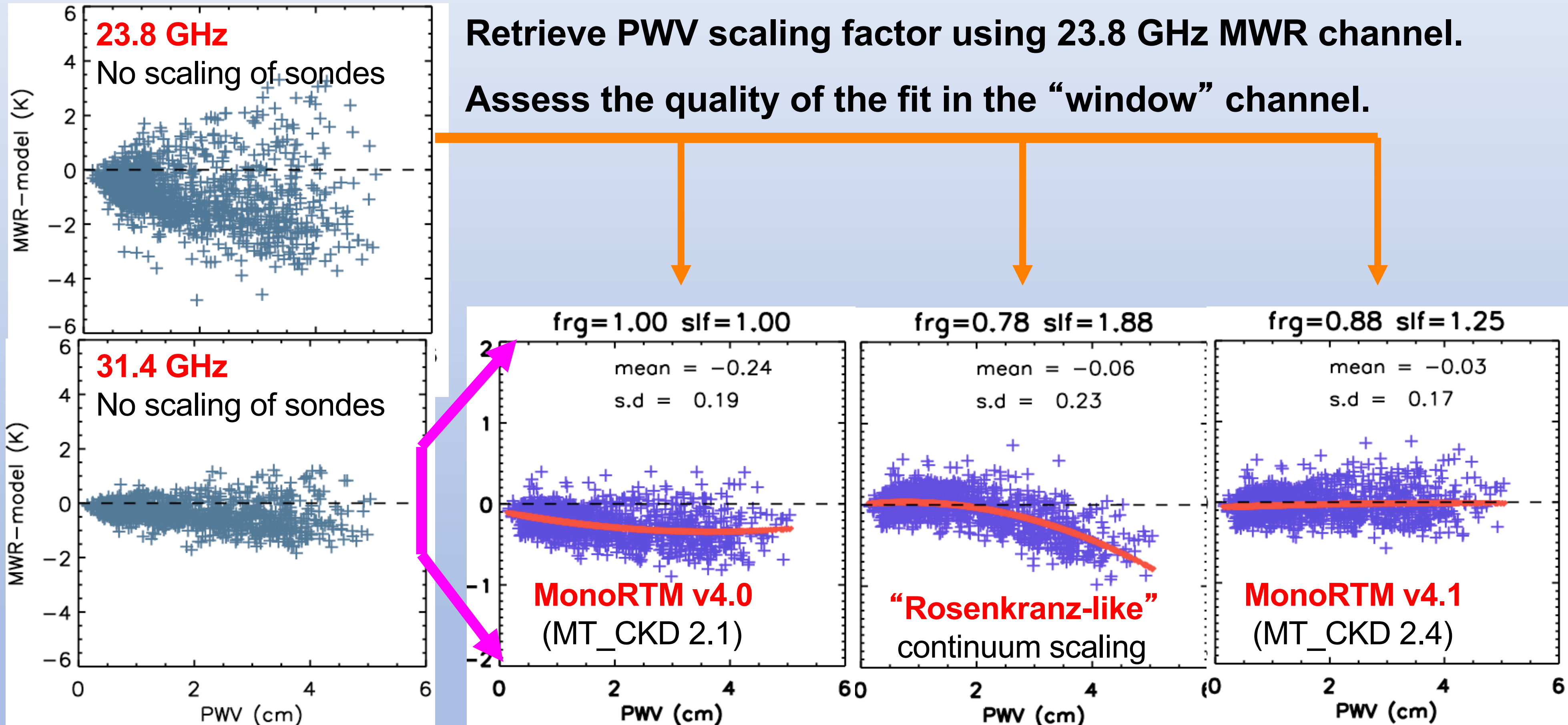


Measurements at higher PWV (>3.0 cm) needed to constrain the self continuum

Fitting the water vapor self and foreign continuum

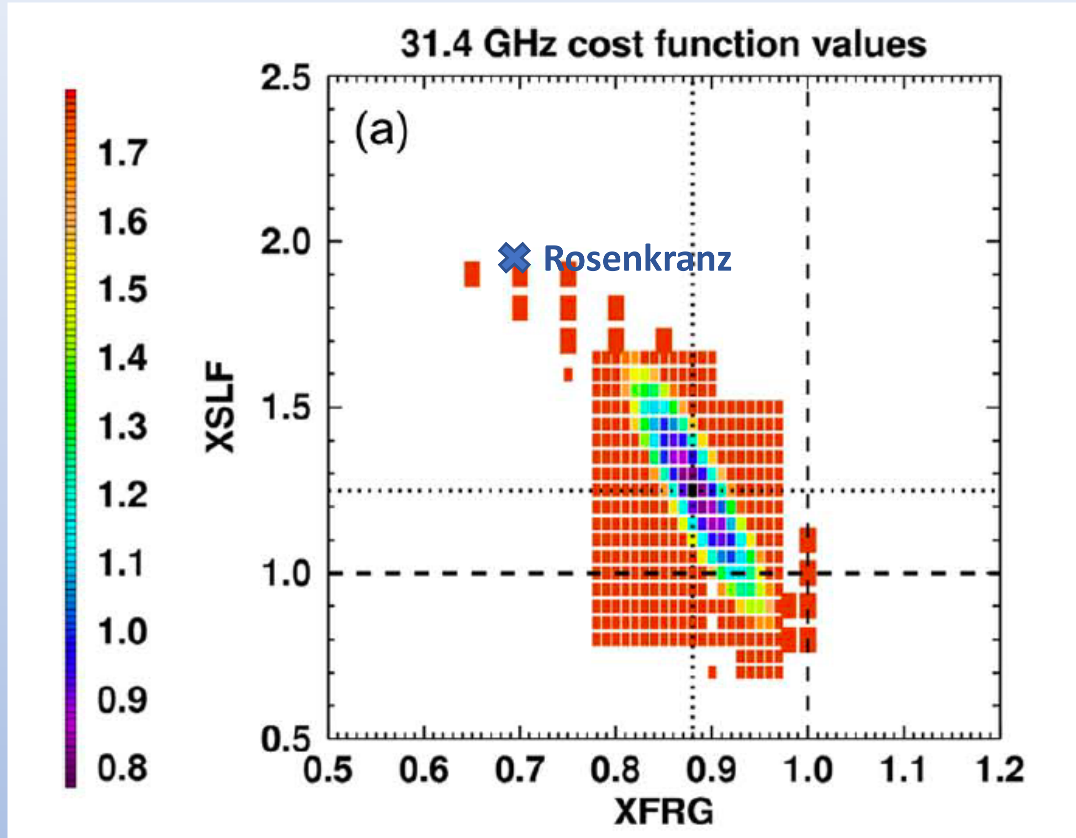
Retrieve PWV scaling factor using 23.8 GHz MWR channel.

Assess the quality of the fit in the "window" channel.



Payne et al., 2011

Cost function values of water vapor continuum fits



Cost function includes terms for residuals, plus the slope and curvature of fit to residuals.

Payne et al., 2011

New analysis includes cases with even higher PWV values

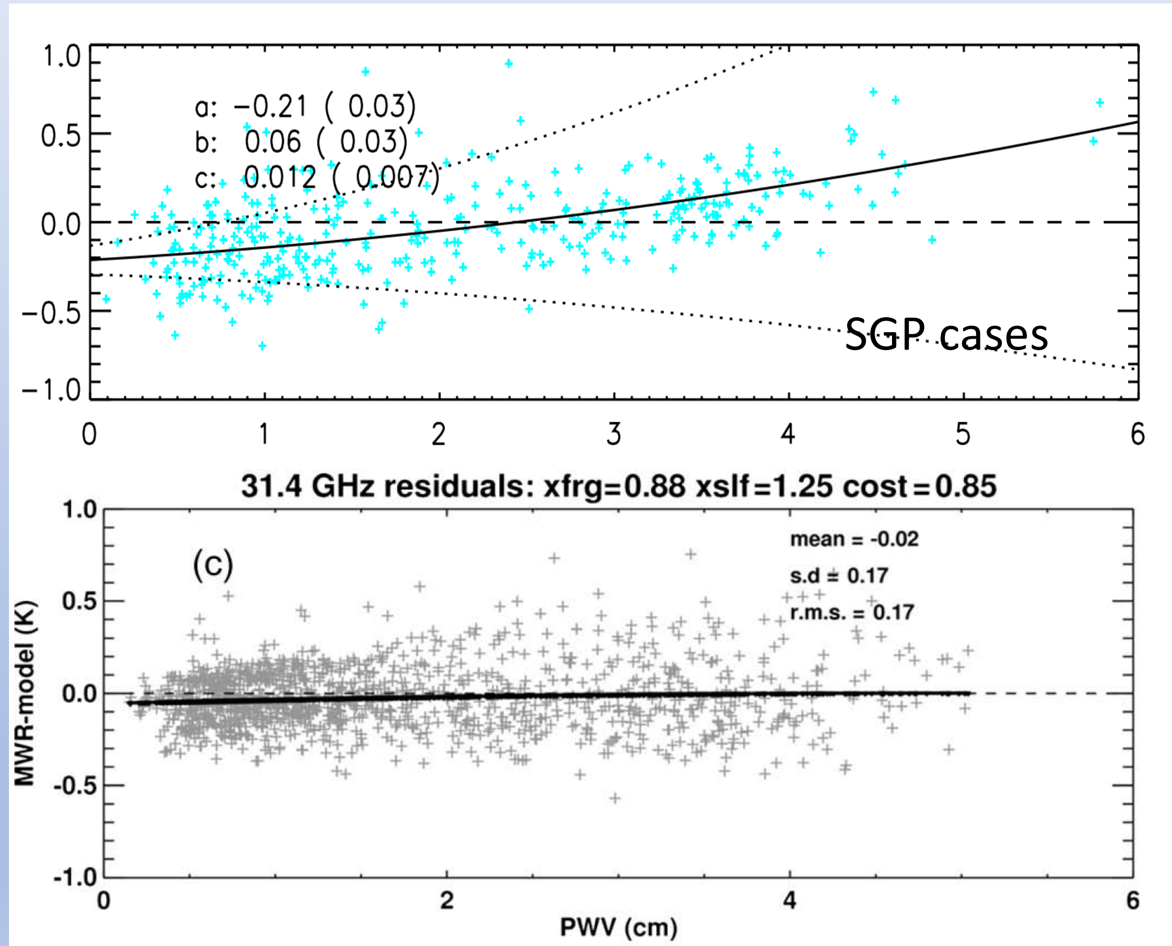
Site	Date ranges	Number of clear sondes	PWV range [cm]	Instruments
AMF_GoAmazon	06/2015-12/2015	637	2.85-6.25	MWR
SGP	01/2014-12/2014 10/2016 - 9/2017	1475	0.11-6.25	MWR

SGP MWR datasets: current study vs. Payne et al. (2011)

Measurement – calculation differences with MonoRTM v4.2, MT_CKD v2.4

Current analysis

Payne et al. (2011)



31.4 GHz

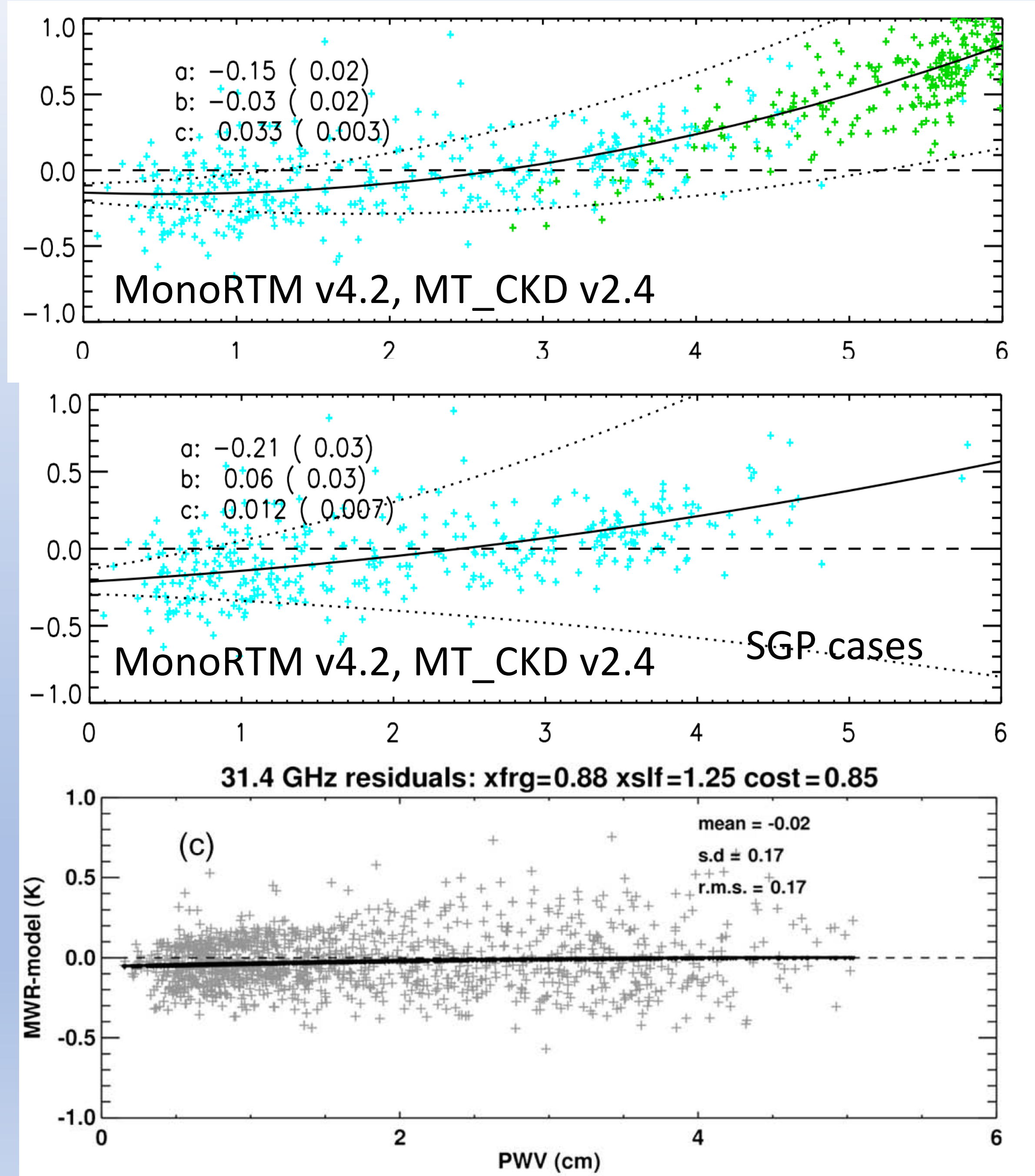
Including GoAmazon measurements in current analysis

31.4 GHz measurement – calculation (existing model)

GoAmazon + new SGP

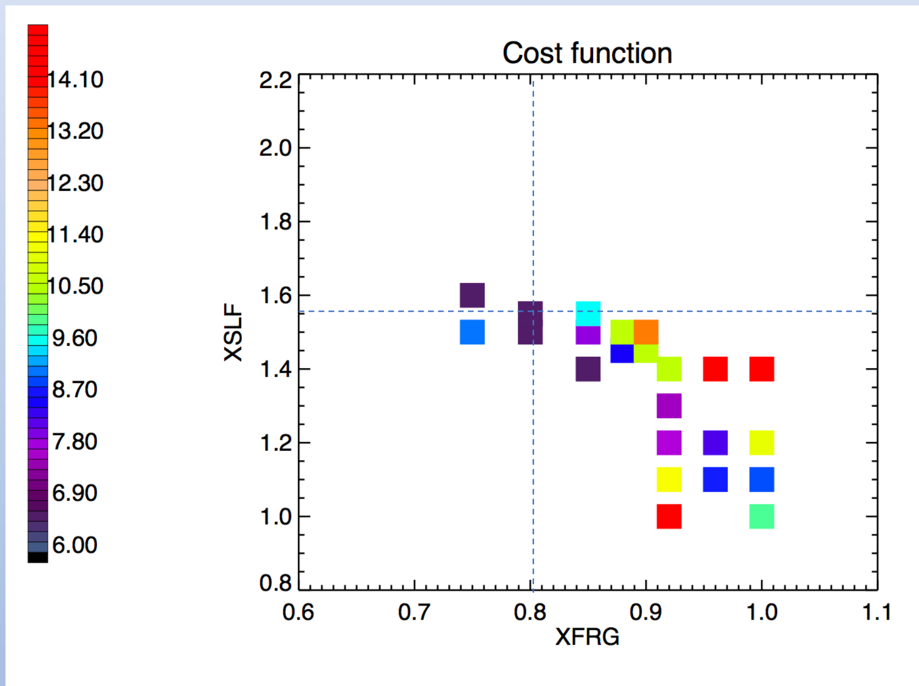
New SGP

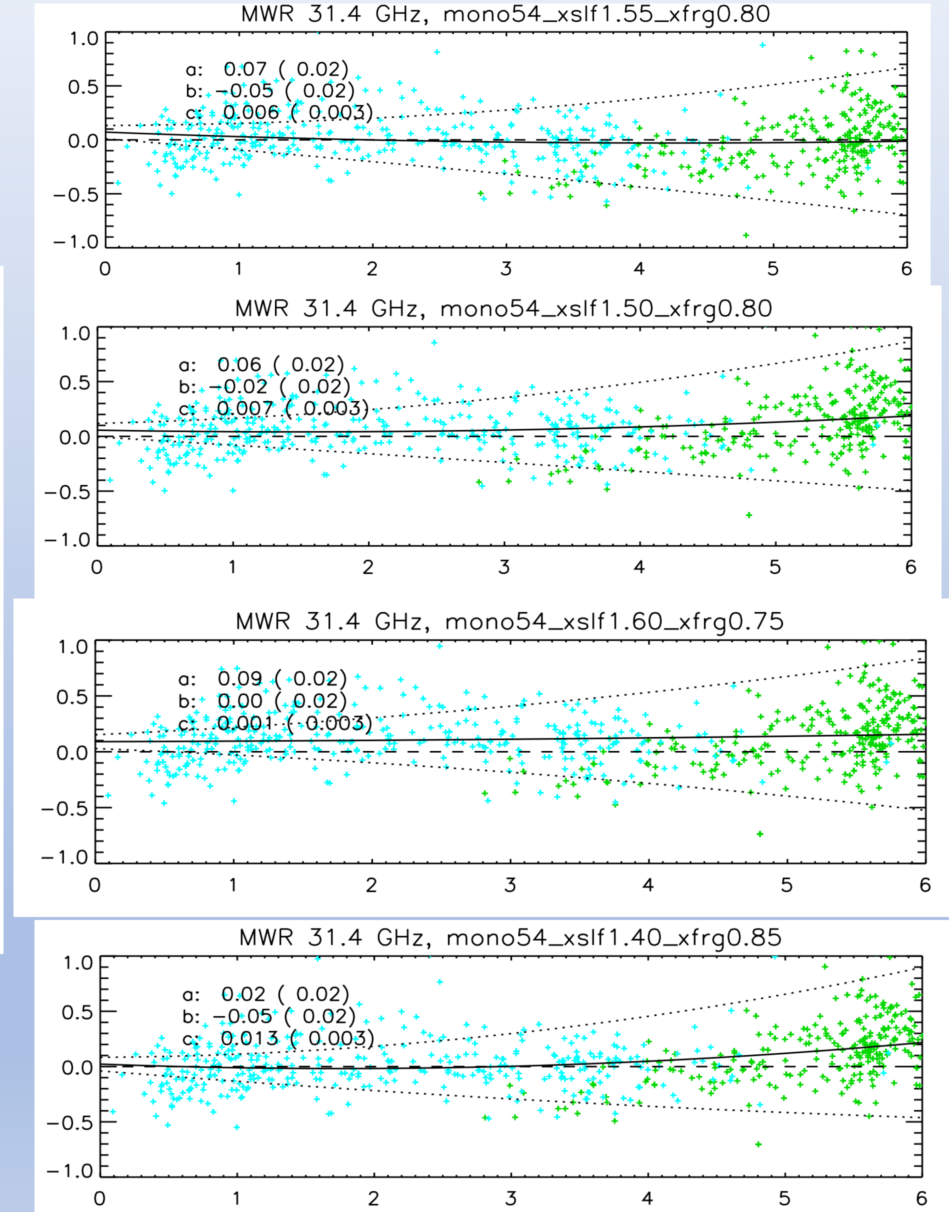
Older SGP



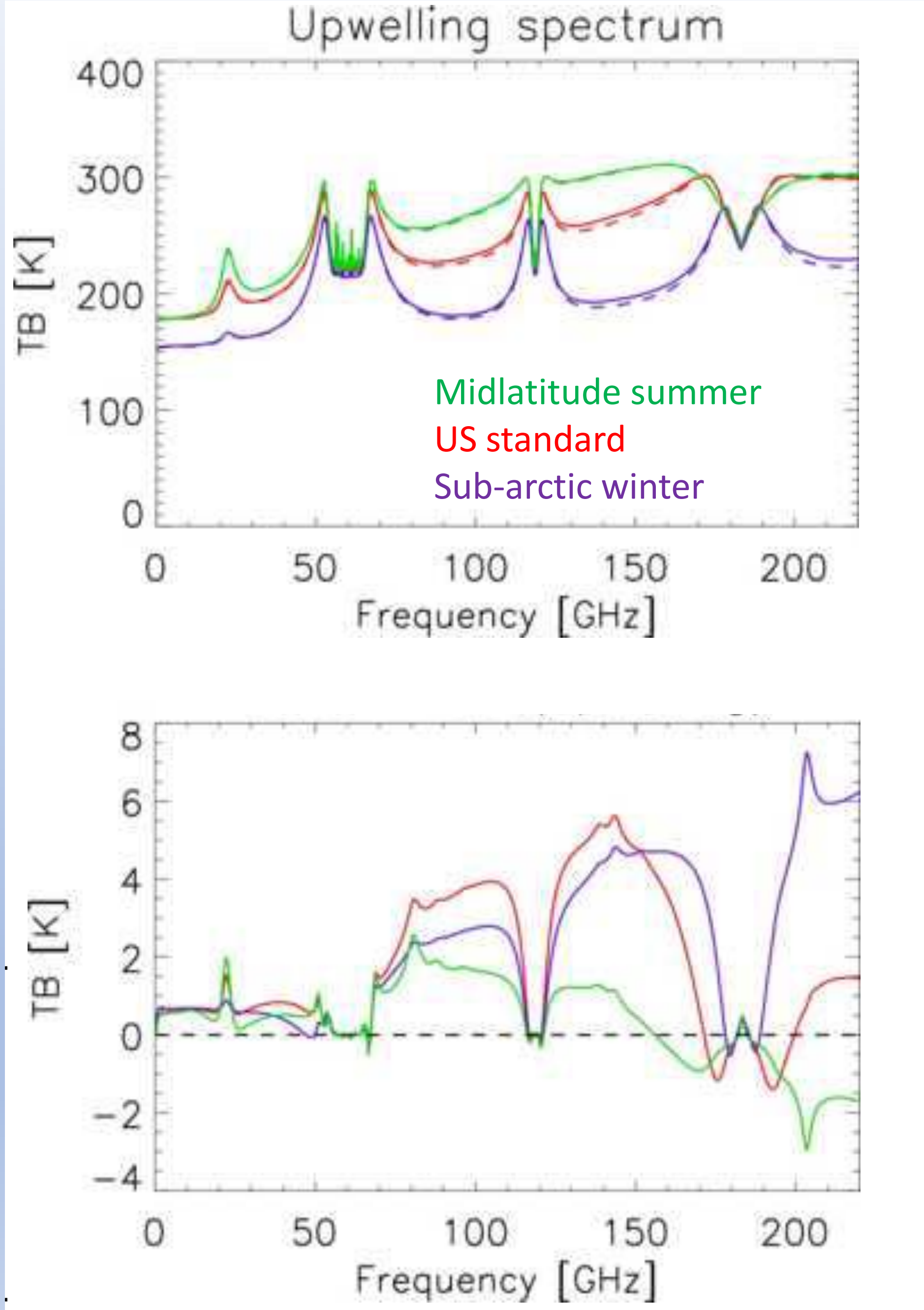
Preliminary results

Large changes to MW H_2O continuum appear to be needed





Brightness temperature comparison



Changes in upwelling brightness temperatures from anticipated continuum change will be large

Main points

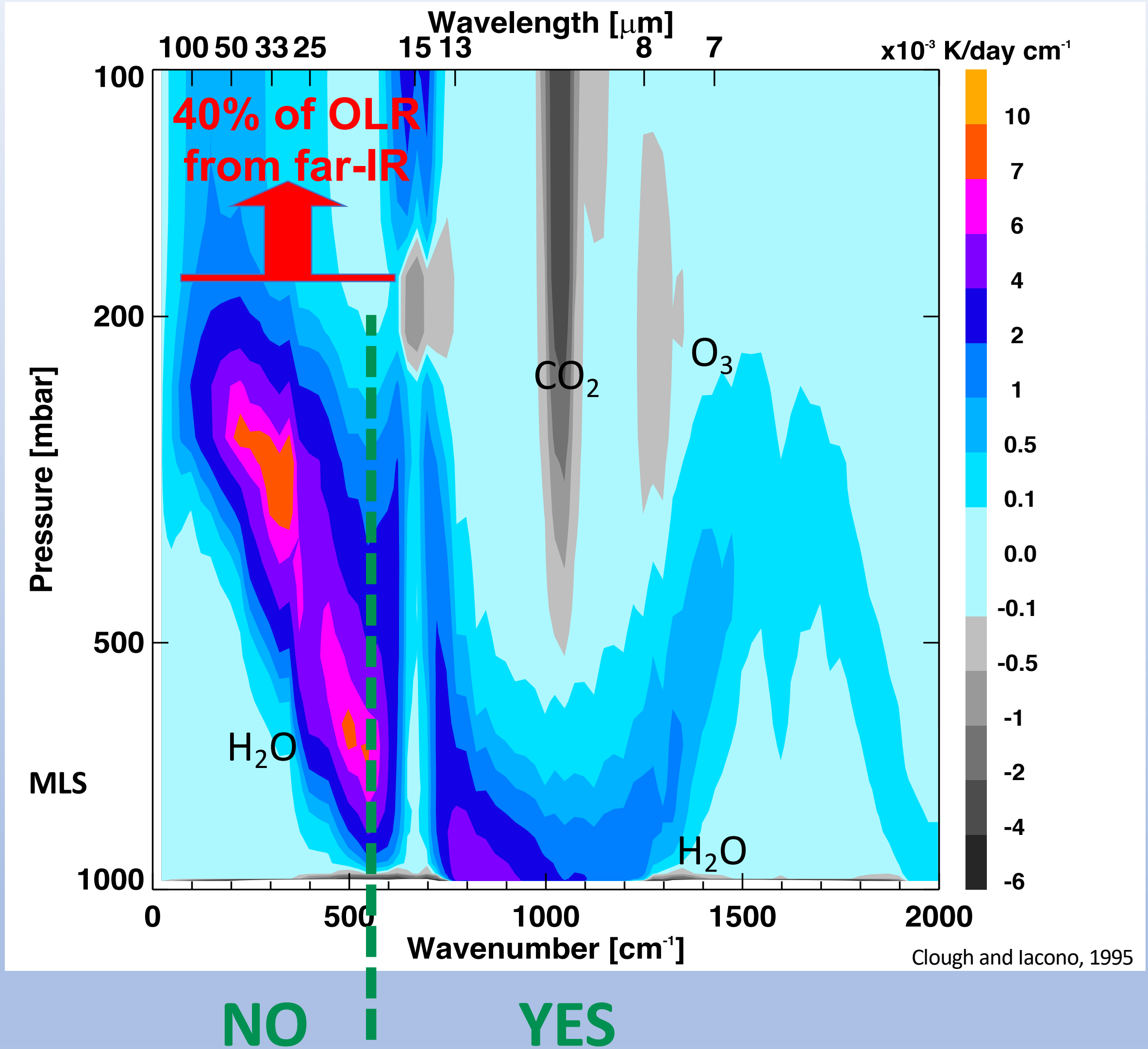
- Radiative closure experiments continue to play an important role in improving and validating spectroscopic input to radiative transfer calculations

- Accurate water vapor continuum values derived from these closure studies can lead to improved retrieval products and, most likely, improved results from data assimilation.

The importance of the far-IR

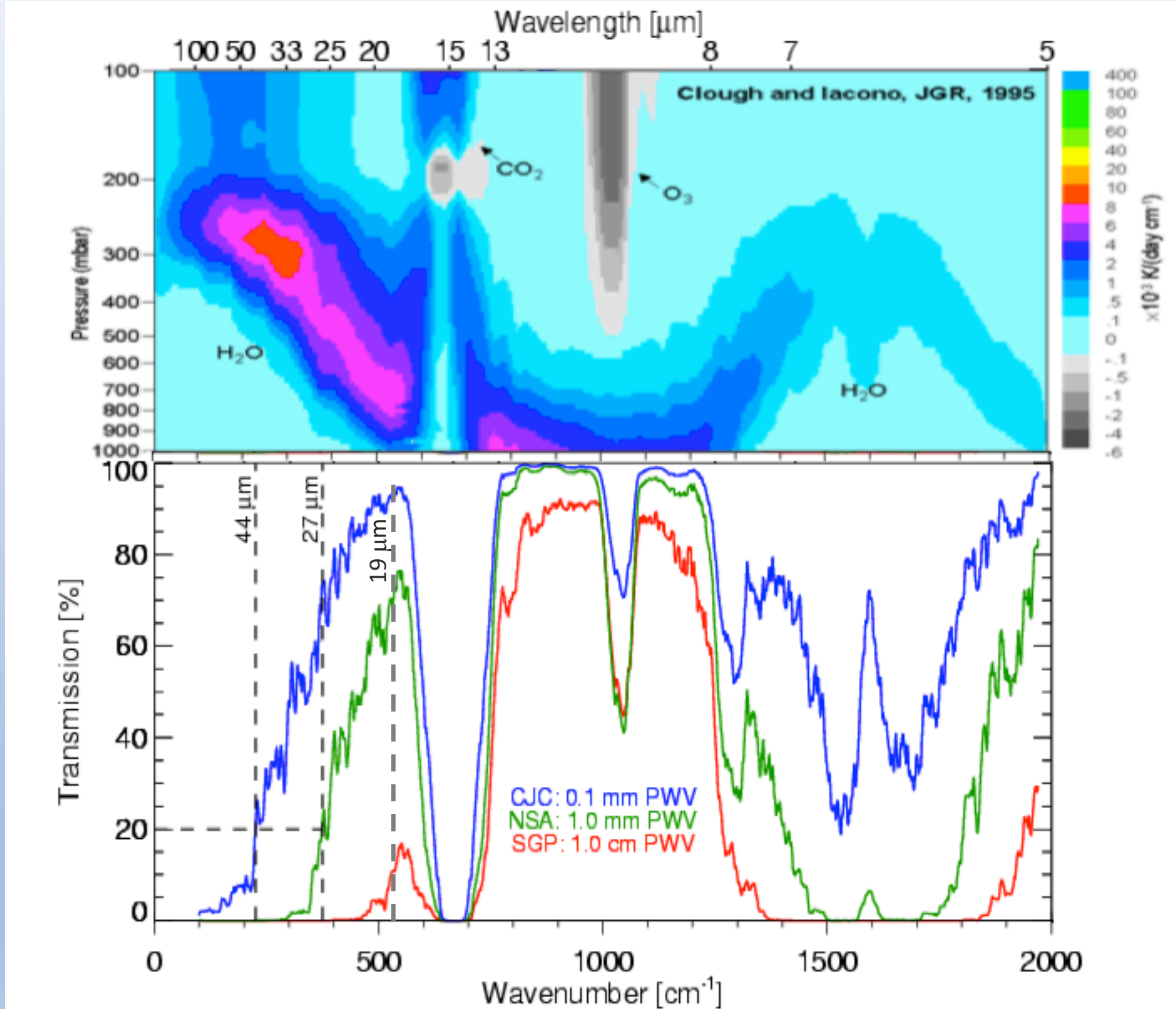
Spectral Cooling Rates (troposphere)

"Clough Plot"



As of ~10 years ago, had spectroscopic parameters been evaluated by field observations?

Dry locations needed to evaluate far-IR spectroscopy



Radiative Heating in Underexplored Bands Campaigns

Goal: Improve far-IR spectroscopy

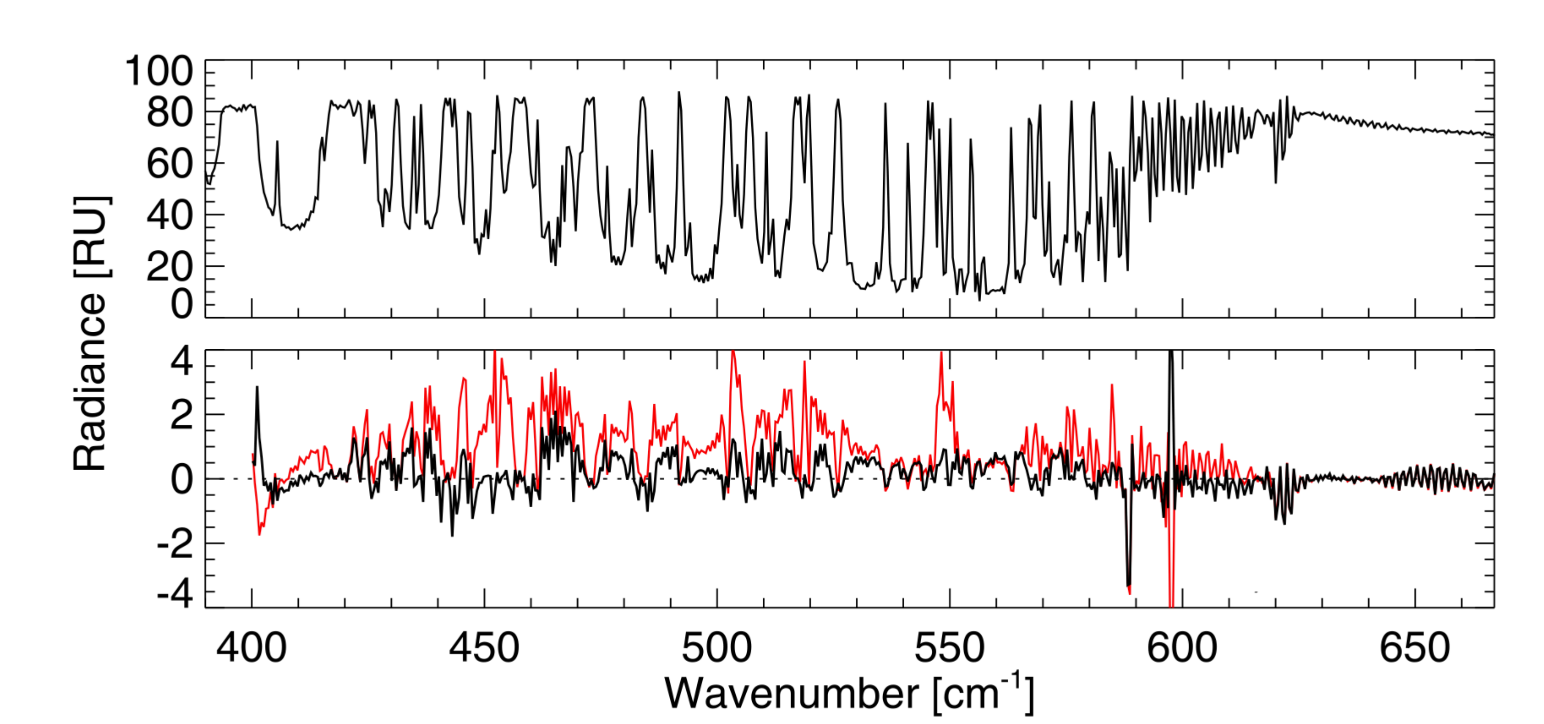
RHUBC-I

- ARM North Slope of Alaska Site, Barrow, AK
- February - March 2007, 70 radiosondes launched
- **Minimum PWV: 0.95 mm**
- 2 far-IR / IR interferometers
  - extended range AERI: > 400 cm^{-1}
- 3 sub-millimeter radiometers → determine PWV

RHUBC- I: Results

Spectroscopic modifications from RHUBC-I (Delamere et al., 2010)

- adjustments to water vapor foreign continuum
- foreign-broadened line widths for 42 H_2O lines were adjusted



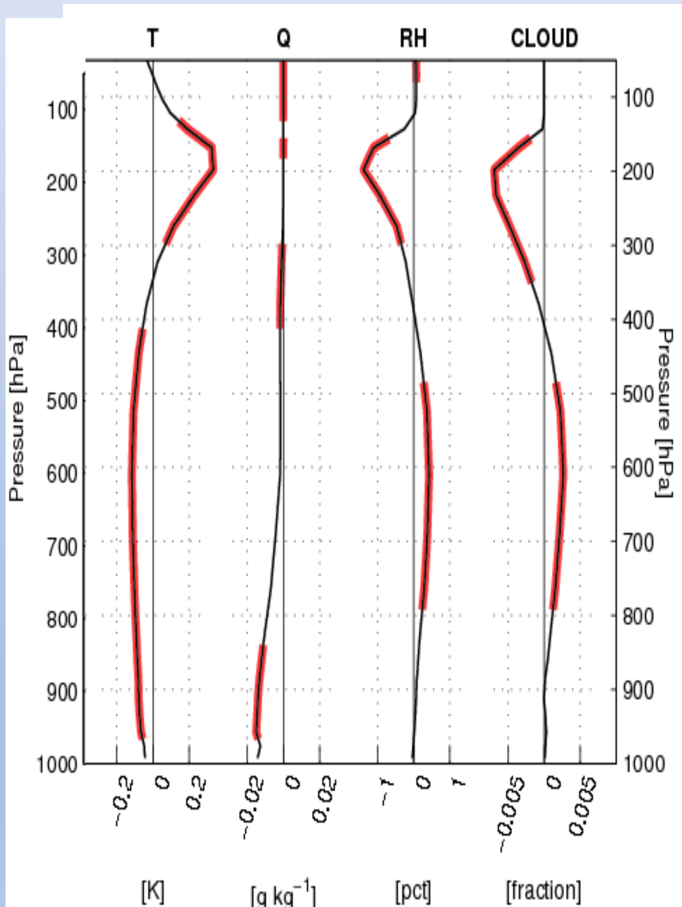
AERI_ER Measurements

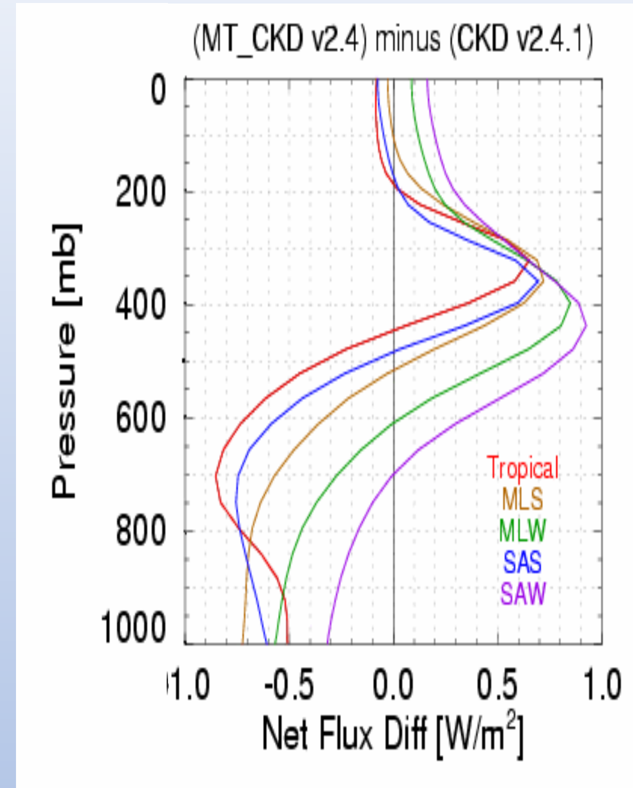
AERI_ER – LBLRTM residuals before RHUBC-I

Residuals after RHUBC-I

RHUBC- I: Results

Revised continuum and widths lead to significant changes in net flux





- ❖ RRTMG updated with revised continuum (MT_CKD_2.4)
- ❖ 20-yr simulation performed with CESM v1 (Turner et al., 2012)
  - statistically significant changes in temperature, humidity, and cloud fraction

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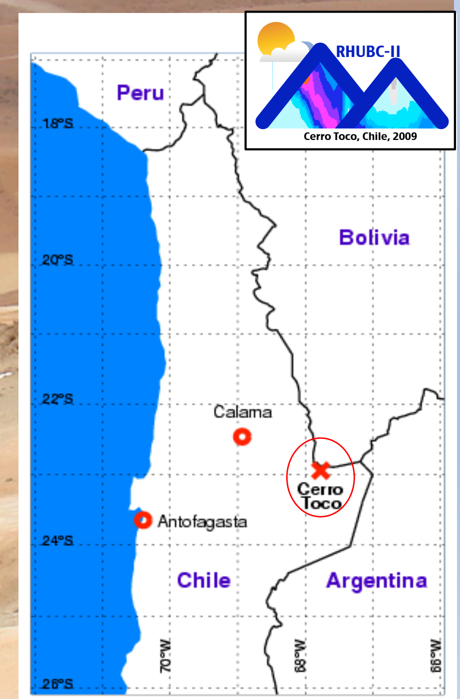
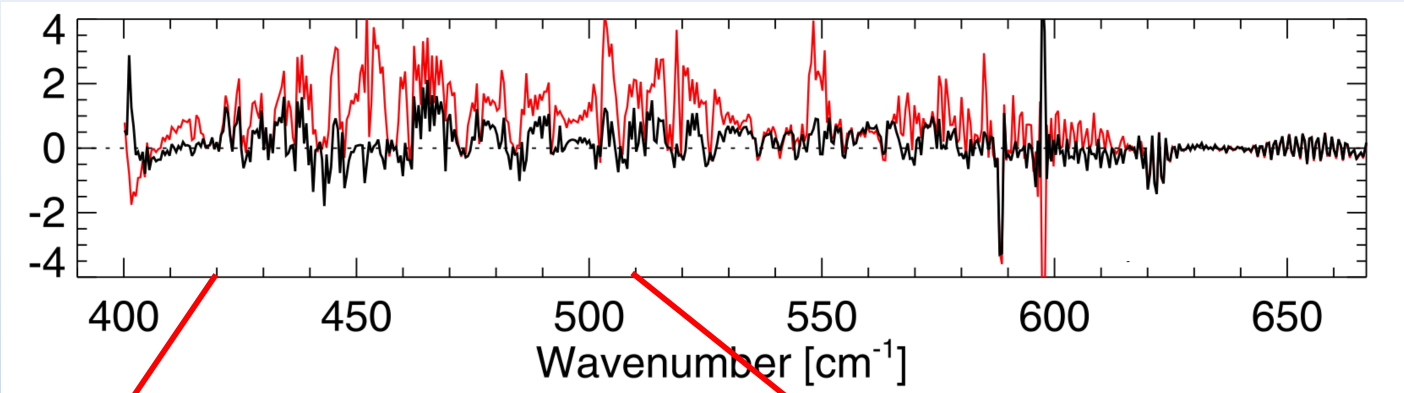
RHUBC-II

- Cerro Toco, Chile (23ºS, 68ºE, altitude - **5380 m**)
- August - October 2009, 144 radiosondes were launched
- **Minimum PWV: ~0.2 mm (5x drier than RHUBC-I)**
- Far-IR / IR interferometers
  - **REFIR-PAD – 100-1400 cm^{-1}**
  - **NASA FIRST – 100-1000 cm^{-1}**
- 183 GHz radiometer for determining H_2O

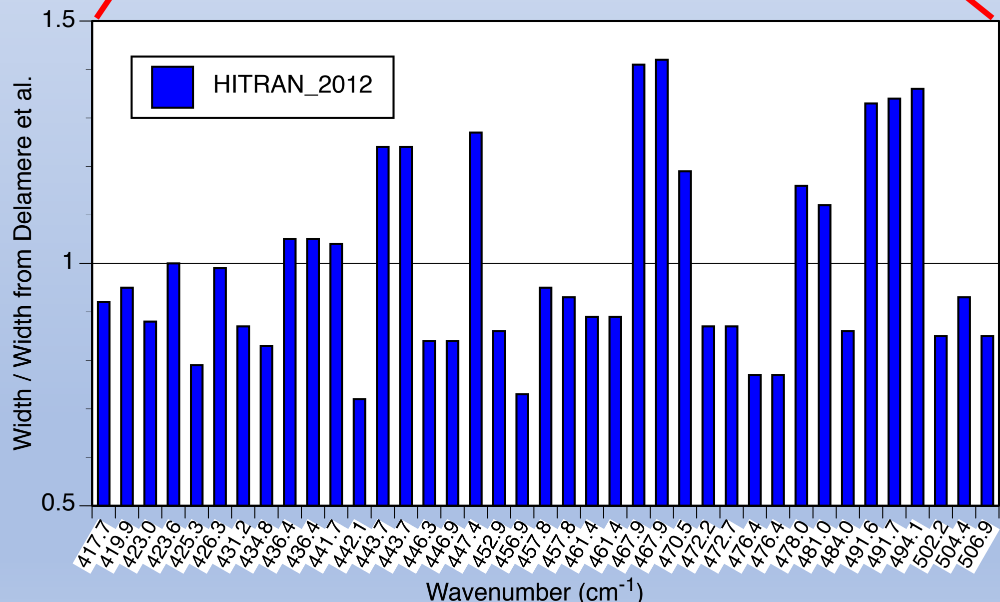


Impact of RHUBC- I Results on Line Databases **- Nothing**



AERI – LBLRTM residuals before RHUBC-I

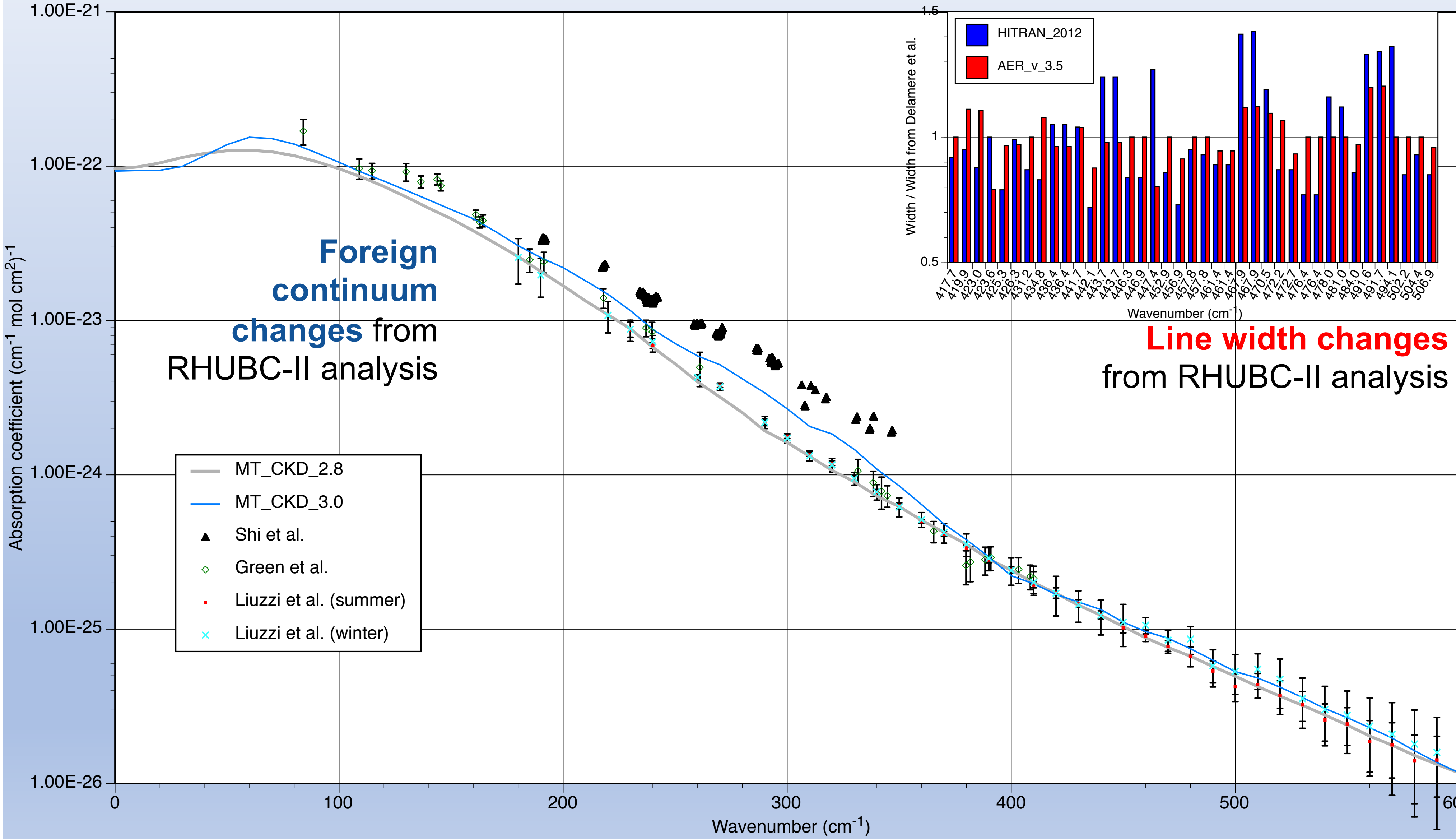
Residuals after RHUBC-I



HITRAN_2012 did not utilize the H_2O line widths from Delamere et al. (2010).

Ratios exceed HITRAN uncertainty codes.

RHUBC-II spectroscopic improvements

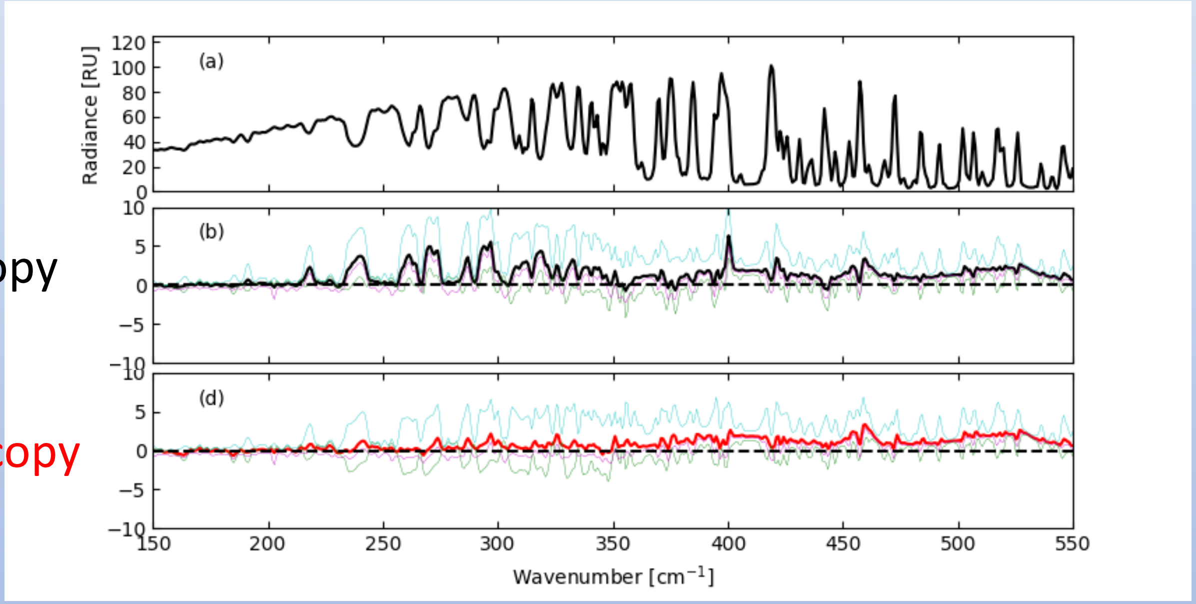


Evaluation with an independent instrument

Measurements by NASA FIRST instrument during RHUBC-II

Old spectroscopy

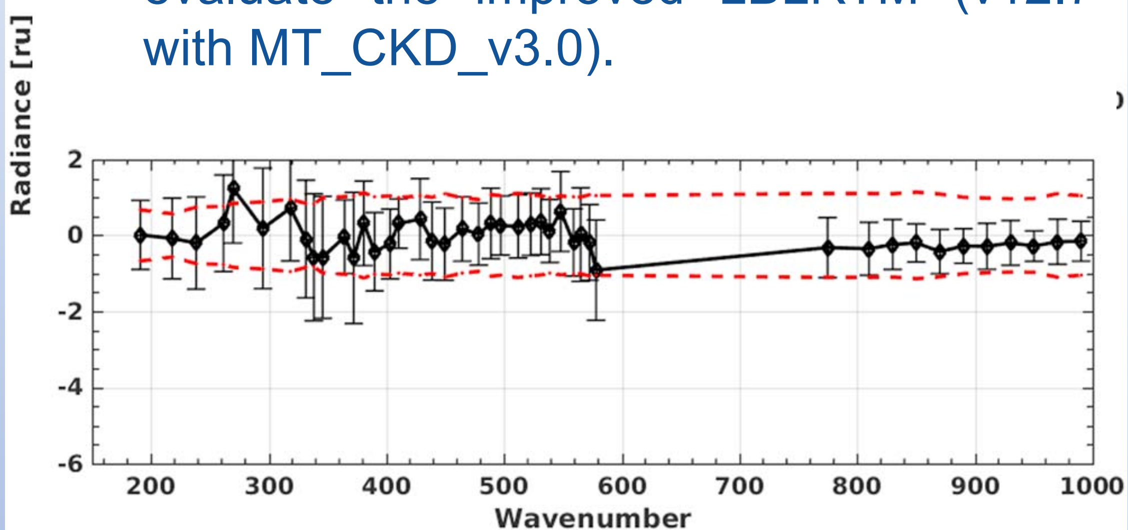
New spectroscopy



Significant improvement is seen.

Evaluation with an independent REFIR-PAD dataset

Rizzi et al. (2018) used REFIR-PAD measurements from Antarctica to evaluate the improved LBLRTM (v12.7 with MT_CKD_v3.0).



Winter cases from Rizzi et al. (2018)

"The new simulations show that residuals between 200 and 400 cm^{-1} are much reduced with respect to (previous results) and are now within the combined error estimates ... average residuals for austral winter days are remarkably close to zero"

Slide from Sung et al. on lab study of far-IR H_2O continuum

Effect of line widths on the observed CIA

Preliminary results

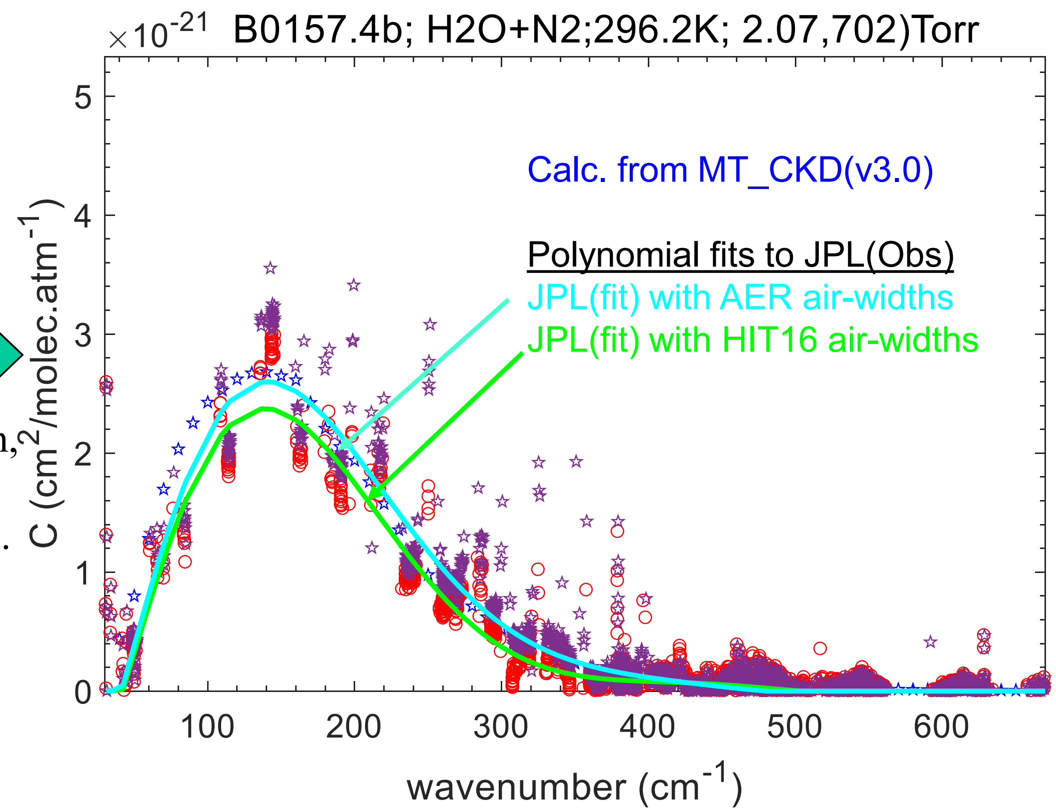
❑ B1057.4b spectrum

H_2O broadened by N_2 at 289 K
296.2 K , P=(2.7, 701.7) Torr

❑ CIA comparison

MT_CKD(v3.0) [water+air]
JPL(Obs) [water+N_2]
(1) used AER air-widths
(2) used HIT16 air-widths

For the resonance absorption simulation, the air-broadened widths were adjusted to be $\gamma_{N2} = \gamma_{air} \times 1.12$ and $\gamma_{O2} = \gamma_{N2} \times 0.50$.

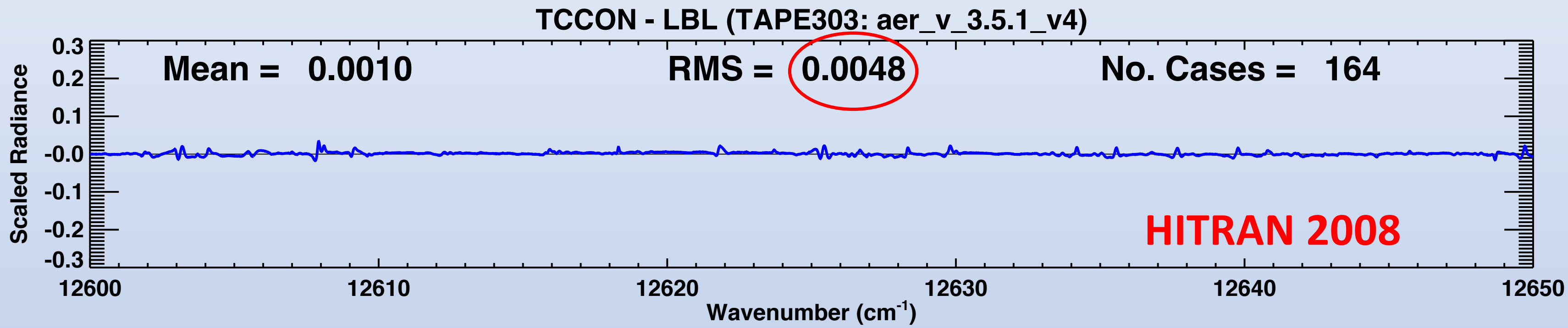


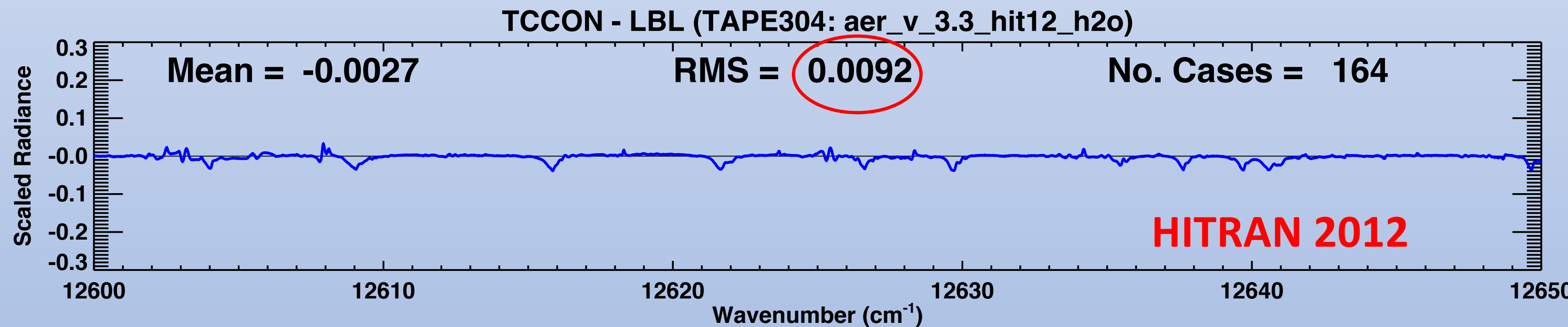
❑ New results at 296 K

(1) A better agreement bet. MT_CKD and JPL(Obs.)
(2) Still, JPL(obs) is lower in the region > ~120 cm^{-1}

Another example – near-IR water vapor widths

Plot: Average residuals between direct beam measurements from solar FTS in Lamont, OK (TCCON), and LBLRTM calculations with different line parameters





Based on this analysis, NIR and visible H_2O widths in the AER_v_3.6 H2O line file are:
< **6000 cm^{-1}** - HITRAN 2012; **6000-7925 cm^{-1}** - HITRAN 2012 *with Mikhailenko*;
7925-9395 cm^{-1} - HITRAN 2012 *with Regalia*; **9395-12000 cm^{-1}** - HITRAN 2012;
> **12000 cm^{-1}** : HITRAN 2008

plus **numerous widths** manually changed to improve residuals

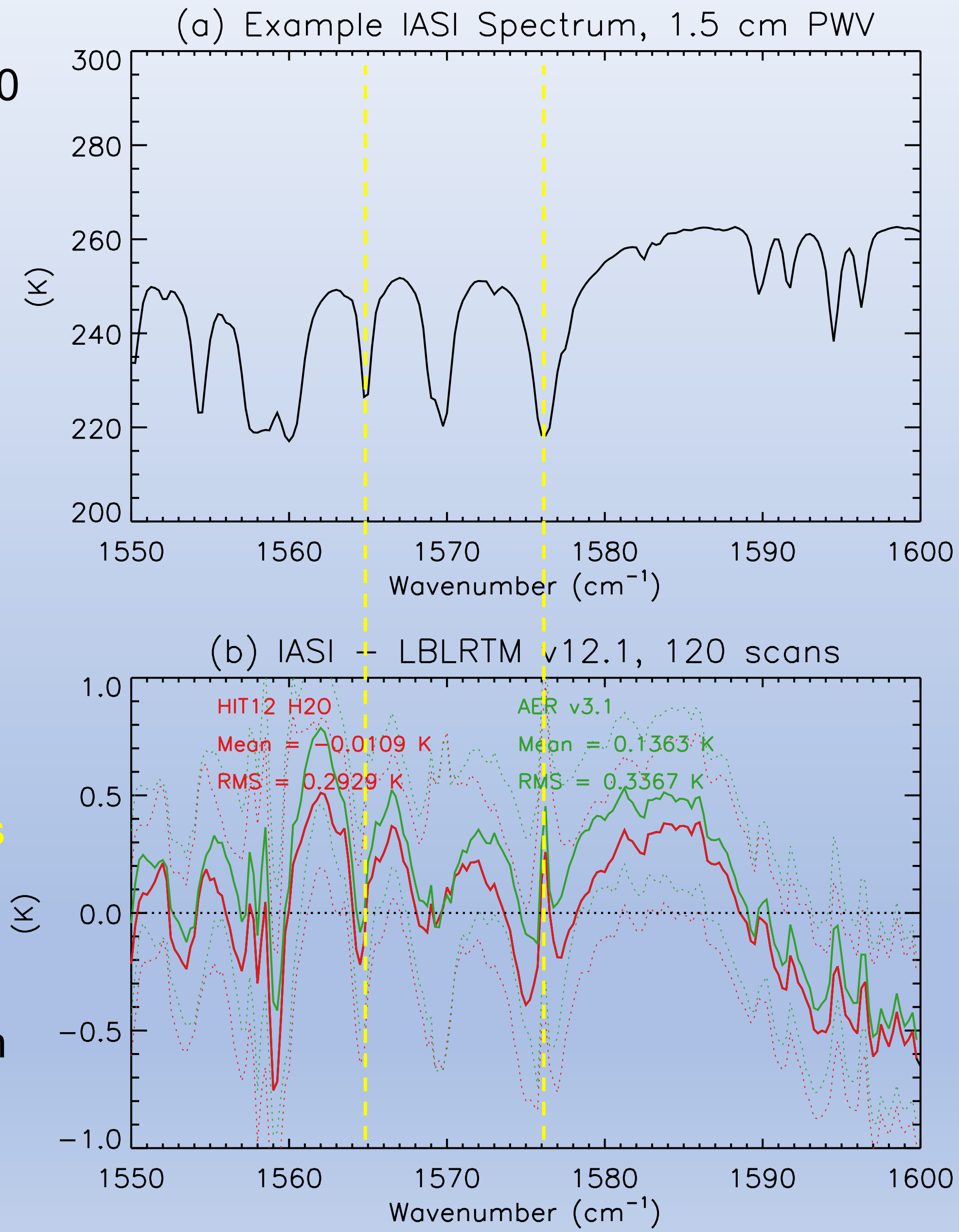
Infrared water vapor widths

Average brightness temperature for 120 IASI cases (courtesy M. Matricardi)

Average residuals between IASI and LBLRTM calculations

Dotted lines point out clear width errors

Note: Ongoing project at AER to improve infrared H_2O widths using both IASI and ground-based AERI measurements.



Main points

- Radiative closure experiments continue to play an important role in improving and validating spectroscopic input to radiative transfer calculations

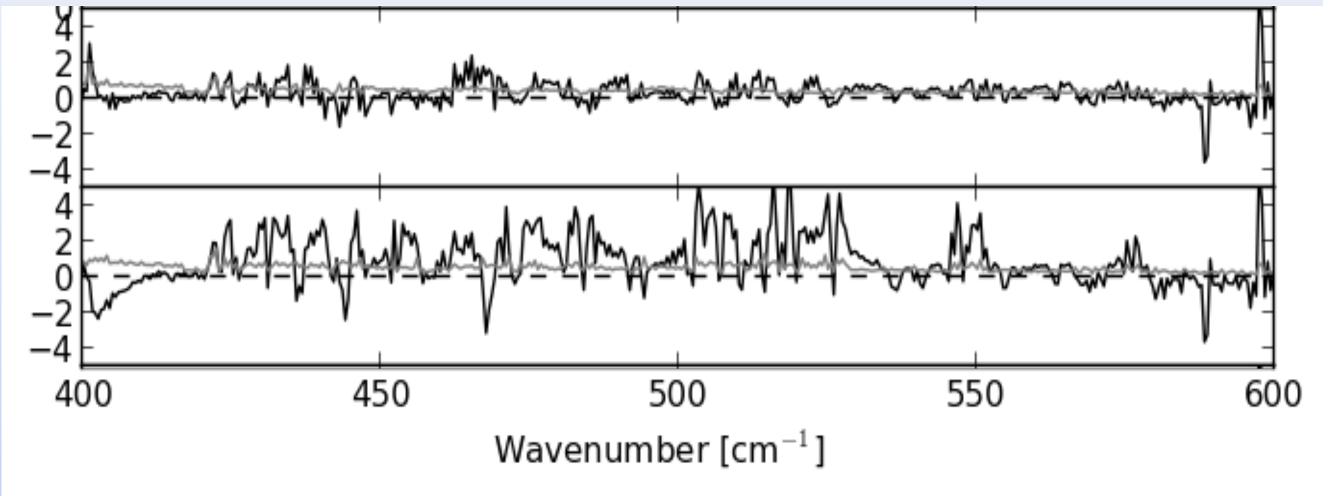
- Accurate water vapor continuum values derived from these closure studies can lead to improved retrieval products and, most likely, data assimilation.

- Line widths can also be improved from radiative closure studies and can impact the information obtained in microwindows between lines
  - line parameter databases should not be assumed to be improvements on previous versions or reflect atmospheric validation

Back-up slides

Impact of HITRAN widths on residuals

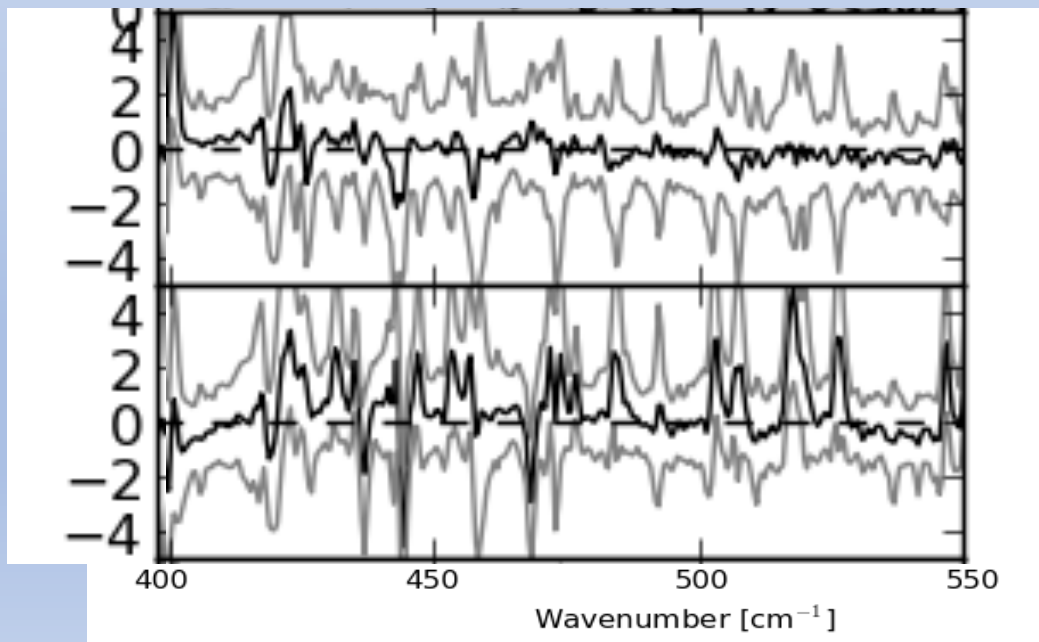
RHUBC-I



AERI – LBLRTM
residuals with
Delamere et al. widths

Residuals with
HITRAN_2012 widths

RHUBC-II



REFIR-PAD – LBLRTM
residuals with
Delamere et al. widths

Residuals with
HITRAN_2012 widths

RHUBC – II: Analysis

Effect of foreign continuum derived from RHUBC-II observations

(compared to previous version)