Validation of H₂O line and continuum spectroscopic parameters in the far infrared wave number range

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Outline

- **Consistency**
  - Using data from ECOWAR-COBRA campaign (March 2007)
    - I-BEST
    - REFIR-PAD
      - LBLRTM 11.3
      - LBLRTM 11.3+ECOWAR
      - LBLRTM 12.0

- **Closure experiment**
  - $\sigma$-IASI
  - Results

- **Conclusions**
Validation of line and continuum spectroscopic parameters with measurements of atmospheric emitted spectral radiance from far to mid infrared wave number range

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The work is mainly based on

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Water vapor continuum
Ozone
Carbon dioxide

Abstract

The latest release of a high-resolution transmission molecular absorption database along with two improved models of water vapor continuum absorption are used to check their impact on the improvement of state-of-art radiative transfer. Radiative transfer performance has been assessed using high mountains atmospheric emitted spectral downwelling radiance observations in the 360–1200 cm\(^{-1}\) spectral regions. These high mountains observations are particularly suited to check the behavior and performance in the water vapor rotation band. In addition, they also have allowed us to gain insight into understanding the quality of recent new compilation of lines and related treatment for the \(v_2\) CO\(_2\) band and the \(O_3\) band at 9.6 \(\mu\)m. Comparisons are made between forward calculations of atmospheric transmission spectra and spectral radiances measured using two ground-based Fourier transform instruments. The results demonstrate that water vapor absorption largely benefits from the recent improvement in the related continuum (both self and foreign). In addition, ozone absorption is very accurately reproduced and, although to a less extent, this is also the case of CO\(_2\) absorption in the long wave \(v_2\) band.

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The key instruments
- REFIR and I-BEST, FTS instruments developed in our laboratories in order to sense properly the Far Infrared portion of atmospheric radiance
- 10-100 μm with a sampling rate finer than 0.5 cm$^{-1}$
New water vapor continuum absorption coefficients

- Water vapor foreign-broadened continuum coefficients for the range 240 to 590 cm\(^{-1}\) as derived from our analysis and comparison with two versions of MT_CKD model, Burch's (1974) and Tobin data (1999).

REFIR and I-BEST have provided basic contributions to the science of water vapour spectroscopy: \(\text{H}_2\text{O}\) rotation band.

*The Atmosphere is less opaque than model*

CAVIAR (Continuum Absorption by Visible and IR radiation and Atmospheric Relevance)

TAFTS (Tropospheric Airborne Fourier Transform Spectrometer)

- Foreign-broadened water vapour continuum in the far-infrared pure rotation band between (85–420 cm\(^{-1}\))
Instrumental set-up

- **REFIR/PAD**
  - Developed at IFAC/CNR in Florence

- **I-BEST**
  - Detector MCT
  - Detector DTGS

**REFIR/PAD** developed and operates at our laboratory since 2001
The 15 of March 2007, I-BEST and REFIR were at Cervinia station 2000 m a.s.l.
REFIR was hosted in the lidar container.
Ancillary Information

- 16 I-BEST spectra  
  2'16" Long
- 8 REFIR Spectra  
  5'10" Long
- Recorded the 15 of March 2007, between 15:00 and 23:00 GMT
- Three Radiosondes, RS92k (started @ 15:20, 18:35, 21:01)
- These data have never been used in the previous study
Colocated I-BEST and REFIR observations

- An example of REFIR and I-BEST (detector MCT) simultaneous spectra,
- The spectral coverage extends from 260 to 1800 cm\(^{-1}\)
## Synoptic table of spectral parameter used

<table>
<thead>
<tr>
<th>Name</th>
<th>LBLRTM Version</th>
<th>Continua MT_CKD</th>
<th>Released</th>
<th>Changes</th>
<th>Line File</th>
<th>Based on</th>
<th>Changes</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.3</td>
<td>V11.3</td>
<td>V2.1</td>
<td>Nov 2007</td>
<td></td>
<td>aer_v2.1</td>
<td>HIT04+</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EC</td>
<td>V11.3</td>
<td>V2.1 modified</td>
<td>Jun 2008</td>
<td>Foreign in [240-590] cm⁻¹</td>
<td>aer_v2.1</td>
<td>HIT04+</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[2]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. Rothman et al. (2009), JQSRT, doi:10.1016/j.jqsrt.2009.02.01
Methodology

Spectral radiance \quad Forward model

\[ r = F(s; v) \]

spectral parameters \quad atmospheric state vector \ T, W

- To take into account both local environment and eventual bias introduced by Radiosonde (and/or) Interpolation we tuned PWVs for each spectrum and for each spectroscopic issues.
- In this case we assume fixed spectral parameter and we move only water vapor PWV.

- Taylor expansion with respect to a initial guess (denoted with 0 pedix)

\[ r = r_0 + K_q(q - q_0) + \text{higher order terms} \]

- Inverted using least square method using the spectral range \([360-600] \text{ cm}^{-1}\)
Both EC and 12.0 outperform the 11.3 one,

There are regions where EC fits better than 12.0 the spectra (495 & 530) cm\(^{-1}\) and regions where 12.0 fits better EC (505 & 550) cm\(^{-1}\)
Both EC and 12.0 outperform the 11.3 one,

- There are regions where EC fits better than 12.0 the spectra (465, 495 & 530) cm\(^{-1}\) and regions where 12.0 fits better than EC (505 & 550) cm\(^{-1}\).
Both EC and 12.0 outperform the 11.3 one, and they fit the window @ 406 cm$^{-1}$

EC fits better than 12.0 the spectra @ 380 & 435 cm$^{-1}$ while 12.0 fits better than EC around 450 cm$^{-1}$

<table>
<thead>
<tr>
<th>Name</th>
<th>Bias (R.U.)</th>
<th>RMS (R.U.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.3</td>
<td>-0.38</td>
<td>1.10</td>
</tr>
<tr>
<td>EC</td>
<td>-0.02</td>
<td>0.60</td>
</tr>
<tr>
<td>12.0</td>
<td>0.08</td>
<td>0.59</td>
</tr>
</tbody>
</table>
Comparing residuals with radiometric noise

- The mean residuals are larger than the radiometric noise.
  - In the CO2 band (Temperature profile)
  - In the Ozone band (Ozone Profile)
  - In H2O rotational band (Water Vapour profile)
- It is crucial to perform a closure experiment.
Flow charts

\[ \chi^2_{th} = N_{ch} + 2 \sqrt{2} N_{ch} \]
σ-IASI is a line-by-line radiative transfer model designed for fast computation of spectral radiance and its derivatives (Jacobian) with respect to a given set of geophysical parameters.

- It adopts a grid of 63 pressure levels [1050.00-0.005 hPa].
- It is Based on look-up table of monochromatic optical depth + an interpolation procedure.
- The OD look-up-table has been built starting from LBLRTM 12.0 (HITRAN08 spectral database, aer_v3.0)
- Continuum MT_CDK 2.5.2

- It is a FORTRAN90 Code running on LINUX and Windows platform with Intel Compiler.
Comparing residuals with radiometric noise

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Closure Profiles

- First guess profiles come from the tuning described before for the 12.0.
- The Retrieved profiles, in green, fit better the observations but systematic features still appears.
No sensitive improvements with the retrieved profiles.
The RMS slightly decrease for I-BEST due the better performance between [490 - 530] cm\(^{-1}\)
For REFIR RMS slightly increase due to the worse performance @ 370 & 420 cm\(^{-1}\)
Closure profile Consistency @ 15 micron

- Both bias and RMS reduce with Retrieved profiles
- But the residuals around 600 and 740 cm\(^{-1}\) are greater than the radiometric error.
The bias line in magenta is obtained using LBLRTM 9.4, without the Hartmann model for the CO$_2$ line coupling

No sensitive changes in the atmospheric window
The Residual is almost confined in the error bar.
Closure profile Consistency @ 9.6 micron

- Retrieved profile fit very well observation in the Ozone band.
- Residual is in the error band that for I-BEST is very low (~0.3 mW/m^2-cm^-1-sr).

<table>
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<tr>
<th>Name</th>
<th>Bias (R.U.)</th>
<th>RMS (R.U.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.0</td>
<td>1.0</td>
<td>1.3</td>
</tr>
<tr>
<td>Retr</td>
<td>0.06</td>
<td>0.3</td>
</tr>
<tr>
<td>12.0</td>
<td>0.5</td>
<td>0.9</td>
</tr>
<tr>
<td>Retr</td>
<td>-0.2</td>
<td>0.6</td>
</tr>
</tbody>
</table>
Conclusions

**Consistency**
- Water vapor Foreign continuum parameters retrieved from ECOWAR/COBRA campaign represent a breakthrough with respect to MT_CKD 2.1
- They are in agreement with coefficient derived during CAVIAR campaign with TAFTS instrument.
- **LBLRTMv12.0** and **EC** show the same consistency with the Observations in the Rotational Water Vapor Band

**Closure**
- The quality of Ozone spectral parameters is very good.
- There are still problems in the $\nu_2$ CO2 band around 610 and 740 cm$^{-1}$.
  - Larger in the LW portion (Uninvestigated from satellite)!
- There are still problems in the Water Vapor Rotational band.
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Further Job for Us!
REFIR (Radiation Explorer in the Far InfraRed)

- REFIR-PAD clear sky spectrum and related NESR
I-BEST FTS
ABB-BOMEM MR104
Spectral Range 5-40 μm, Sampling rate 0.393 cm⁻¹
Detectors:
- Uncooled Pyroelectr
- Cooled MCT
Operated at Difa/Unibas Laboratory since 2001
More details in
doi:10.1364/AO.47.003

VAISALA RS-92K
Radio-sounding Unit
I-BEST Radiometric Noise

- **Detector MCT**
  - HBB T = 50°C,
  - Meas. time 2'18''
  - 60 Spectra
  - sigma scale is 10 time smaller than mean scale

- **Detector DTGS**

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2012 HITRAN/ASA Workshop, Reims, France, August 28-30, Guido Masiello
Methodology

Spectral radiance \( r = F(s; \nu) \)

Forward model

**spectral parameters** \( \mathbf{c} \) \( \mathbf{c} \) is part of the set of spectroscopic parameters.

After Taylor expansion with respect to a initial guess (denoted with 0 pedix)

**continuum coeff. Jacobian** \( \mathbf{K}_c \)

**\( T \) and \( W \) Jacobians**

\[
\mathbf{r} = \mathbf{r}_0 + \mathbf{K}_c (\mathbf{c} - \mathbf{c}_0) + \mathbf{K}_T (\mathbf{T} - \mathbf{T}_0) + \mathbf{K}_q (\mathbf{q} - \mathbf{q}_0) + \text{higher order terms}
\]

\[
\mathbf{K}_c = \left( \frac{\partial F}{\partial c_1(\sigma_i)}, \ldots, \frac{\partial F}{\partial c_L(\sigma_i)} \right)
\]

Inverted using least square method

**\( H_2O \) Foreign Continuum** coefficients vector \( \mathbf{c} \) is part of the set of spectroscopic parameters.
Observed-Calculated Residual

- Observed radiance (upper panel) and observed minus calculated (lower panel).

Calculations are shown using
- $H04^+$, mt$	extunderscore$ckd 2.1
- $H04^+$, ecowar, i.e. continuum coeff. determined from the 3 case studies analyzed in the ECOWAR/COBRA campaign.
- Light gray area indicated 3 sigma interval.
- This consistency sensitively improves using new continuum coefficients
Colocated i-BEST and REFIR observations

- This is an example of comparison between REFIR and I-BEST simultaneous observations.
- I-BEST was operated in MCT mode
- The bottom panels shows the difference between spectra (blue) compared with the sum of the radiometric noises.
Fitting Local Environment: Temperature

- Using the raw radiosonde profile, in the CO$_2$ Q-branch at 15 μm, the computed spectrum shows a “cold” bias of 1.5 K.
- In this range the atmosphere is very opaque (τ ~ 0)
  - → downwelling radiance is sensitive to the temperature of atmospheric layers very close to the instrument.
- The instruments are in the van and it may heats the air close to it.

- The cold bias is sensitively reduced
- The intense spike at 667 cm$^{-1}$ is due to the emission of CO$_2$ inside the instruments.
Fitting Local Environment: Water Vapor

- The Columnar Amount retrieved for the two Instruments and for the three spectral parameter choices.
- The Retrieved PWVs are in +/- 10% with respect to the Raodiosonde.
- 12.0 Sees less water vapor than others
  - 12.0 says that the atmosphere is more opaque!
Radiative Fluxes

- EC and 12.0 show the same consistency with observed data.
- But the atmosphere modeled by 12.0 is more opaque than EC model.
- This fact has climatological implication.

Radiative fluxes (Down, Up and Net) computed for U.S.Std. atmosphere (left)
- Difference introduced by new coefficients (right)
  - The new coefficients produce a net flux 0.65 W/m² higher @500 hPa.
  - This change is equivalent to that of subtracting ≈ 30 ppmv of CO₂ into the atmosphere.