OCO-2 Absorption Cross sections

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Keeyoon Sung       ... and others

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Agenda

1. Spectroscopy in OCO-2 retrievals
   • Parameter sources and computation
   • Validation and testing

2. Pending challenges
Why spectroscopy matters

- 0.25% OCO-2 Accuracy requirement requires 0.1% reference spectroscopic accuracy [Miller et al., 2005]
- This challenges measurement accuracy AND our understanding of the physics
- Many subtle physical effects come into play at this level [Miller et al., 2007]
  - Line Mixing ($O_2$, $CO_2$)
  - Speed Dependence ($CO_2$)
  - Dicke Narrowing ($O_2$)
- Getting it wrong can introduce airmass/regional biases

From Hartmann, J.-M., Tran, H., and Toon, G. C.: Influence of line mixing on the retrievals of atmospheric CO2 from spectra in the 1.6 and 2.1 μm regions, Atmos. Chem. Phys., 9, 7303-7312.
Table construction process

• Problem: Advanced spectroscopic models too slow for online use
• Solution: pre-computed lookup table for linear interpolation
• OCO-2 supercomputer computes cross sections at independent temperature and pressure levels (~1 month of CPU time)

Line and continuum parameters

OCO-2 cluster

HDF File: 71 pressure levels, 17 temperature levels
# Parameter sources

<table>
<thead>
<tr>
<th>ABSCO Tables</th>
<th>v3.3</th>
<th>v4.0</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>4850cm(^{-1}) CO(_2)</strong></td>
<td>Line shape</td>
<td>Voigt, Toth 2008</td>
</tr>
<tr>
<td>continuum</td>
<td></td>
<td>additional continuum</td>
</tr>
<tr>
<td><strong>6200cm(^{-1}) CO(_2)</strong></td>
<td>Line shape</td>
<td>SDV [Devi et al. 2007]</td>
</tr>
<tr>
<td>mixing</td>
<td>[Hartmann 2008]</td>
<td>Multi-spectrum [Devi et al. 2007]</td>
</tr>
<tr>
<td><strong>13200cm(^{-1}) O(_2)</strong></td>
<td>Line shape</td>
<td>Voigt [Tran 2006]</td>
</tr>
<tr>
<td>mixing</td>
<td>[Tran 2006]</td>
<td></td>
</tr>
<tr>
<td>rescaling</td>
<td></td>
<td>rescaled to match <em>a priori</em> surface pressure</td>
</tr>
</tbody>
</table>
ABSCO Evaluation

GOSAT soundings
- 1-3 bands, multiple absorbers
- Low spectral resolution
- Unconstrained atmosphere, aerosols, surface albedo

TCCON spectra
- 1-3 bands, multiple absorbers
- High spectral resolution
- Full atmospheric column
- Atmosphere conditions constrained at surface

Laboratory spectra
- 1 band, one absorber
- High spectral resolution
- Known laboratory conditions
- Mostly room temperature, low optical depth
Evaluation with lab spectra

1.6 μm band, path length 32.54m
optical path difference 75cm
Total cell pressure is 742 Torr
Sample is 9.03% air-broadened $^{16}\text{O}^{12}\text{C}^{16}\text{O}$

2 μm band, path length 29.3m
Optical path difference 112.5 cm
Total pressure 599.8 Torr
Sample: 4.95% air-broadened $^{16}\text{O}^{12}\text{C}^{16}\text{O}$
Evaluation with TCCON network data

TCCON retrieval for Park Falls 22 Dec. 2004
~12 airmasses

State of the art
First-order line mixing, Voigt shapes (HITRAN 2012?)

ABSCO v4.0
Nearest-neighbor line mixing
Speed dependent profile

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10/23/2012 OCO-2 ABSCO Overview
Evaluation with GOSAT data

Mean of soundings over TCCON stations

<table>
<thead>
<tr>
<th># Converged</th>
<th>Scatter v. TCCON</th>
<th>Correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>V+LM</td>
<td>V4.0</td>
<td></td>
</tr>
<tr>
<td>279 (65.6%)</td>
<td>300 (70.6%)</td>
<td></td>
</tr>
<tr>
<td>V+LM</td>
<td>V4.0</td>
<td></td>
</tr>
<tr>
<td>1.50 ppm</td>
<td>1.39 ppm</td>
<td></td>
</tr>
<tr>
<td>V+LM</td>
<td>V4.0</td>
<td></td>
</tr>
<tr>
<td>0.767</td>
<td>0.781</td>
<td></td>
</tr>
</tbody>
</table>

Graphs showing residuals and radiances for different data sets.
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Pending challenges

10hPa bias in surface pressure

Airmass bias in single-band CO$_2$ retrievals (especially in the 2.1 μm band)
The A Band surface pressure bias

- Errors currently addressed by rescaling cross sections to remove the empirical mean error
- Line mixing and Dicke narrowing may both play a role
- Future models will model these effects directly
Current challenges: H$_2$O broadening

Broadening by water (Sung 2009) appears significant

Change in SCO$_2$ cross sections

Worst-case fractional change in X$_{co2}$

Change due to H$_2$O broadening

Net effect

Single bands

Courtesy Fabiano Oyafuso, JPL
H$_2$O broadening of CO$_2$

Water broadening now implemented
- O$_2$ from Fanjoux
- CO$_2$ from [Sung 2009]

Single band results agree with an implementation in GFIT.

Changes X$_{CO2}$ by up to $\sim$0.4%, though residuals still dominated by other spectroscopic effects.

For L2, start with linear interpolation for the VMR interval from 0 to 5%?
Line-by-line residual inspections

Courtesy Yibo Jiang, Linda R. Brown
Improving H$_2$O intensities

Work in progress, courtesy Lorenzo Lodi and Jonathan Tennyson from UCL, Iouli Gordon from SAO, Yibo Jiang from JPL
# Moving to v4.1

<table>
<thead>
<tr>
<th>ABSCO Tables</th>
<th>V4.0</th>
<th>V4.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>4850 cm⁻¹ H₂O</td>
<td>Line parameters</td>
<td>HITRAN 2008</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4850 cm⁻¹ CO₂</td>
<td>Line shape</td>
<td>SDV [Benner/Devi]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Minor isotopes via Toth et al.</td>
</tr>
<tr>
<td></td>
<td>mixing</td>
<td>Multi-spectrum [Benner/Devi]</td>
</tr>
<tr>
<td>6200 cm⁻¹ CO₂</td>
<td>Line shape</td>
<td>SDV [Benner/Devi]</td>
</tr>
<tr>
<td></td>
<td>mixing</td>
<td>Multi-spectrum [Devi et al. 2007]</td>
</tr>
<tr>
<td>13200 cm⁻¹ O₂</td>
<td>Line shape</td>
<td>Voigt</td>
</tr>
<tr>
<td></td>
<td>mixing</td>
<td>First-order</td>
</tr>
<tr>
<td></td>
<td>rescaling</td>
<td>rescaled to match <em>a priori</em> surface pressure</td>
</tr>
</tbody>
</table>
Discussion

- Recent improvements are a step in the right direction
- Radiometric accuracies are not yet to the desired 0.1% level, and some systematic errors remain
- New measurements (CRDS) can better constrain line shapes
- Major priorities:
  - The A Band
  - $\text{H}_2\text{O}$ broadening (for which we’ll need accurate $\text{H}_2\text{O}$ retrievals)
Questions?