Satellite and Ground-based evaluation of 1.61 and 2.07 micron CO$_2$ absorption models for the OCO-2 mission

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1. Motivation
2. New CO$_2$ models for the 1.61 and 2.07 micron bands
3. Validation and testing method
   - Lab Spectra
   - Upward-looking FTS spectrometers
   - GOSAT orbital measurements
4. Pending challenges
The OCO-2 Mission

- Launch expected in late 2014
- Sounding spectrometer monitors three spectral regions
  - CO$_2$ in the 4850 cm$^{-1}$ (strong band)
  - CO$_2$ in the 6220 cm$^{-1}$ (weak band)
  - O$_2$ in the 13100 cm$^{-1}$ (A band)
- Will estimate dry air mole fraction ($X_{CO_2}$)
  - Provides unprecedented coverage to estimate regional-scale CO$_2$ sources and sinks (Crisp et al., 2012)
- High precision requirements
  - Goal ~ 0.3% (1 ppm out of 400)

This talk: Our process for evaluating spectroscopic models, illustrated for the two CO$_2$ bands
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.
New Models

Speed dependent profiles adjust pressure broadening to account for molecules having various speeds at collision

\[ \kappa(v) = \sum_{i=0}^{16} \frac{\nu_i e^{-\nu_i^2}}{\pi^{3/2} \alpha_D} \tan^{-1} \left\{ \frac{v - v_0 + \nu_i \alpha_D}{\alpha_L \left[ 1 + S \left( \nu_i^2 - 1.5 \right) \right] + H} \right\} \]

\[ \nu_i = -4 + \frac{i}{2} \]

Lorenz half width

We set Dicke narrowing to zero

<table>
<thead>
<tr>
<th>Spectral Region</th>
<th>Benchmark</th>
<th>Proposed</th>
</tr>
</thead>
<tbody>
<tr>
<td>4850 \text{cm}^{-1} \text{CO}_2</td>
<td>Line shape</td>
<td>Voigt profile [Toth 2008]</td>
</tr>
<tr>
<td>6200 \text{cm}^{-1} \text{CO}_2</td>
<td>Line shape</td>
<td>Voigt profile [Toth 2008]</td>
</tr>
<tr>
<td></td>
<td>Line mixing</td>
<td>ECS model [Lamouroux 2010]</td>
</tr>
</tbody>
</table>
Evaluation Methodology

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 of CO2 absorption models for the OCO-2 mission
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

Proposed model
Nearest-neighbor line mixing
Speed dependent profile

(Thompson et al., JQRST 2012)
Evaluation with TCCON network data

TCCON retrievals for Park Falls 22 Dec. 2004

Experience suggests that line mixing may account for most of the improvement (rather than the speed dependent profile).

This is consistent with the TCCON experiment.

Significant improvement at 2.07 microns

Modest improvement at 1.61 microns
Evaluation with GOSAT data

- Mean of soundings over TCCON stations
- Three-band retrieval using surface pressure to estimate Column-averaged dry mole fraction $X_{\text{co2}}$
- $O_2$ A Band parameters from (Tran et al., 2008)

(Thompson et al., JQRST 2012)
Evaluation with GOSAT data

Mean of soundings over TCCON stations, after zeroing out the mean bias

<table>
<thead>
<tr>
<th># Converged</th>
<th>Scatter v. TCCON</th>
<th>Correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benchmark</td>
<td>Proposed</td>
<td>Benchmark</td>
</tr>
<tr>
<td>279 (65.6%)</td>
<td>1.50 ppm</td>
<td>0.767</td>
</tr>
<tr>
<td>300 (70.6%)</td>
<td>1.39 ppm</td>
<td>0.781</td>
</tr>
</tbody>
</table>
Comments

• The new models seem a step in the right direction
  – Qualitatively similar improvements to three instruments and retrieval codes
• Radiometric accuracies are not yet to the desired 0.1% level
  – Some systematic errors remain
• New Cavity Ringdown Spectroscopy (CRDS) may help constrain line shapes
Some pending challenges

- Later upgrades have introduced H$_2$O foreign broadening of CO$_2$ (Sung et al. 2009), and O$_2$ (Vess et al. 2012).
- Significant uncertainties in continuum effects, especially the H$_2$O contribution.
- Intense focus on improving Oxygen A band spectroscopy:
  - Incorporating CRDS measurements in a multi-spectrum fit
  - Simultaneous retrieval of Galatry line profile with nearest-neighbor line mixing
  - Validation of models for Collision-Induced Absorption

Uncertainties in the H$_2$O continuum is large in CO$_2$ bands (Ptashnik et al. 2011; 2012)
Questions?