Improvements of CO$_2$ and O$_2$ transmission modeling with application to the ASCENDS mission

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Outline

- Introduction
- ASCENDS Program Overview
- Simulation framework for ASCENDS
- Improvements in transmission modeling
  - Accuracy of line-by-line spectral parameters
  - Alternative lineshapes
  - Line mixing
  - Collision-induced absorption
- Suggested use of multivariate data analysis (such as PCA) for the selection of optimum measurement wavelengths
- Conclusions and Future work
Introduction

- **ACTIVE SENSING OF CO2 EMISSIONS OVER NIGHTS, DAYS, AND SEASONS (ASCENDS)**
  - Recommended by NRC decadal survey as a Tier II NASA mission
  - < 0.5% accuracy (< 2ppm) in CO2 mixing ratio resolution is required

- NASA Langley Research Center (LaRC) is working on an **intensity modulated continuous wave (IMCW) laser absorption spectrometer** based remote sensing scheme for the detection of CO2 at 1.57 microns and O2 at 1.26 microns from space based platforms
  - Multiple wavelengths with differential absorption (DIAL) technique are utilized

- 1.26 micron band for O2 sensing is selected to obtain surface pressure
  - 1.26 micron band provides architectural and spectroscopic advantages
  - For our experiments two candidate wavelengths in this band will be utilized

- Nominally, wavelengths around 1.262 and 1.271 microns have been identified in initial tests
  - Lines in these two sub-bands are being further analyzed for sensitivity to environmental parameters
Active Sensing of CO2 Emissions over Nights, Days, & Seasons (ASCENDS) Mission
- To determine CO2 sources and sinks in the global carbon cycle-

**Mission Objectives**

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<tr>
<th>Requirements and Approach</th>
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<td>• ASCENDS is identified as a medium size mission in the NRC Decadal Survey is currently slated for 2019 launch</td>
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<td>• ASCENDS will deliver laser based remote sensing measurements of Global CO2 mixing ratios (XCO2) to a precision of 0.5 percent on horizontal scales of 100-km over land and 200-km over oceans and passive CO measurements for CO2 interpretation.</td>
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<td>• ASCENDS is the logical extension of OCO and GOSAT</td>
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<td>• NASA LaRC is partnered with ITT for ASCENDS experiments</td>
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<th>Benefits For Climate Science</th>
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<td>• Quantify global spatial distribution of atmospheric CO2 on scales of weather models</td>
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<tr>
<td>• Quantify global spatial distribution of terrestrial and oceanic sources and sinks of CO2 during day/night over all seasons.</td>
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<td>• Provide a scientific basis for future projections of CO2 sources and sinks through data-driven enhancements of Earth-system process modeling.</td>
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**NASA LaRC Role**

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<td>• NASA LaRC is conducting the Pre-Phase A studies to define science and mission requirements.</td>
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<td>• Potential major roles in implementation.</td>
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<td>• Science leadership</td>
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<td>• Active CO2, O2 and passive CO instrument design and build</td>
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<td>• Mission management</td>
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<td>• So far data have been collected from airborne instruments to verify the CO2 measurement capability of the laser based approach</td>
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ASCENDS Measurements

CO₂ column mixing ratio (XCO₂) measurement with Laser Absorption Spectrometer (LAS) technique requires the simultaneous measurement of the CO₂ column number density (CND); the O₂ column number density to converting the CND to XCO₂; and the path length of the measurement. A temperature profile measurement is also required to constrain the XCO₂ measurement. A column CO measurement over the same XCO₂ path is also recommended for interpreting sources and sinks of CO₂.

- **CO₂ Column measurement**
  - CO₂ Laser absorption spectrometer to resolve (or weight) the CO₂ altitude distribution, particularly across mid to lower troposphere
  - 1.57μm LAS only baseline or integrated 1.57μm + 2.0μm LAS option

- **Surface pressure measurement**
  - O₂ Laser Absorption Spectrometer operating at 1.26 / 1.27 μm to convert CO₂ number density to mixing ratio

- **Surface / cloud top altimeter**
  - Laser altimeter to measure CO₂ column length

- **Temperature sounder**
  - Six channel passive radiometer to provide temperature corrections

- **CO sensor**
  - Gas Filter Correlation Radiometers (at 2.3 & 4.6 μm) to separate biogenetic fluxes from biomass burning and fossil fuel combustion

- **Imager**
  - To provide cloud clearing for soundings
Overall ASCENDS modeling approach

Sources of data for simulations
- CALIPSO data
- 1) Experimental measurements
   2) Multi-spectrum fitting
   3) Line-by-line parameters for alternative lineshapes
   4) Additional effects and components
- GEOS-5
  (Goddard Modeling and assimilation Office)
- MODIS data

Lidar system parameters
- Aerosols attenuation
- Atmospheric absorption modeling for CO₂ and O₂
  - Alternative lineshape models, line-mixing, collision-induced absorption etc.
- Global atmospheric models
  - Total pressure, Temperature, Concentrations (CO₂, O₂, H₂O)

Surface reflectivity

Multivariate data analysis methods for selection of lines to sense CO₂ and O₂
Consideration of CO$_2$ and O$_2$
Transmission simulation errors

• Accuracy of line-by-line parameters
  - Line positions, intensities etc.

• Lineshape model accuracy
  - Including line-mixing and speed dependence

• Additional attenuation components
  - Collision-induced absorption

• Assumed O$_2$ pressure model approximation
  - Contribution due to non-linearity at higher altitudes
Effects of line-by-line parameters on simulations (CO$_2$ 1.57 μm band example)

CO$_2$ 1.57 μm band example line: Error ~ 0.7%

CO$_2$, 120km vertical path calculation (Voigt profile):

Differences primarily due to differences in line positions and intensities:

**HITRAN:**
Position: 6364.922030 cm$^{-1}$
Intensity: 1.370E-23

**Devi and Predoi-Cross et al.:**
Position: 6364.921972 cm$^{-1}$
Intensity: 1.3673E-23

A. Predoi-Cross et al, Can J. Phys, 87 (2009), pp 517-535
Need for improved transmission modeling for CO$_2$ and O$_2$

- Large uncertainties for some lines in HITRAN
- HITRAN data limited to Voigt lineshapes
- Voigt lineshapes accuracy $\sim 0.5$
- LBLRTM (Voigt profile)
- Accuracy of 0.3% required (NRC Decadal Survey):
  - More accurate line-by-line data
  - Experiments to extract accurate parameters
  - Alternative lineshapes (SDV, Galatry etc.)
  - Additional effects to be included (e.g. line mixing, collision induced absorption)
Alternative lineshapes

- Voigt profile
- HITRAN data may be used
- Nelkin-Ghatak (hard collisions)
- Galatry profile (soft collisions)
- Correlated Nelkin-Ghatak profile
- Correlated Galatry profile
- Rautian and Sobelman (hard and soft collisions)

Measurements required to obtain required simulation parameters
CO$_2$ and O$_2$ transmission modeling scheme

**CO$_2$ previously reported line-by-line parameters (non-HITRAN)**
- Speed dependent Voigt
- line-mixing
- temperature-dependence

**O$_2$ molecule line-by-line parameters**
- SDV, Galatry or other line shapes
- line-mixing, line narrowing etc.

**Multi-spectrum fitting techniques**

**O$_2$ molecule**
Experimental measurements planned (various pressures and temperatures)

**Line-by-line transmission modeling**
CO$_2$ (1.57 micron region)  
O$_2$ (1.26 - 1.27 micron region)

**Alternative lineshapes**
- Galatry, Rautian-Sobelman or other lineshape profiles  
- Line mixing, line narrowing etc.

**O$_2$ - Collision induced absorption**
HITRAN, additional attenuation contribution
Global atmospheric model

Adopting the Goddard atm. model and orbit sampling approach and extending to O₂ molecule

Variations of global $O_2$ concentration at higher altitudes (not ~ to Atm. pressure) lead to insignificant OD differences ($< 0.001 \%$), “fixed ppmv” for $O_2$ at all altitudes may be used.
Global variations of O$_2$ and CO$_2$ transmission

1) Need to establish optimum measurement wavelengths for CO$_2$ and O$_2$ sensing:
   - High sensitivity to CO$_2$, O$_2$ concentrations
   - Low sensitivity to variations in temperature and pressure

2) Large number of datasets with varying Pressure / Temperature / CO$_2$ and O$_2$ concentrations.

3) Complex relation between Temperature / Pressure / gas concentrations and spectral line features

4) Multivariate data analysis methods (such as PCA etc.) to establish optimum CO$_2$ and O$_2$ wavelengths

Sample O$_2$ line calculation (120 km vertical path) at selected points along the modeled satellite path with varying atm. model parameters.
Collision-induced absorption for O₂
Additional collision-induced absorption contribution, ~ 3%

Example calculation:
1 km horizontal path
Calculation for one set of HITRAN CIA cross-sectional data (single Total pressure / Temperature combination)
Total pressure: 751.7 Torr
Temperature: 295K

HITRAN line-by-line Calculation for O₂
HITRAN line-by-line smoothed to 0.5 cm⁻¹ (black)
HITRAN collision-induced absorption data for O₂ (red)

Additional continuum attenuation component to add to the total contribution
## Magnitude of errors in transmission simulations, steps for reduction

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<th>Source of error</th>
<th>Estimated contribution</th>
<th>Suggested error reduction methods</th>
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<tr>
<td>Uncertainties in the line-by-line parameters (HITRAN vs. latest experimental data)</td>
<td>0.5% – 1%</td>
<td>Careful measurements (varying temperatures and pressures) with successive multi-spectrum fitting</td>
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<tr>
<td>Voigt lineshape profile accuracy limitations</td>
<td>~0.5%</td>
<td>Implementation of alternative lineshapes providing higher precision. Laboratory measurements to obtain additional parameters required.</td>
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<tr>
<td>Collision-induced absorption continuum contribution (O$_2$ 1.26 / 1.27 μm)</td>
<td>~3%</td>
<td>To be included in the model (may be corrected for experimentally)</td>
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<tr>
<td>Errors in O$_2$ modeling due to non-linearity of O$_2$ ppmv at higher altitudes</td>
<td>&lt;0.001%</td>
<td>Negligible</td>
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Conclusions and Future work

- Need for high precision experimental data to implement alternative lineshapes
  - No data available for O$_2$ 1.26 – 1.27 μm band
  - Data exists for CO$_2$ 1.57 μm band but selection of optimum lineshape is necessary
- Merging CO$_2$ and O$_2$ transmission models into the complete modeling framework (instrument parameters, aerosols, surface reflectivity etc.)
- Evaluation of multivariate analysis methods for the selection of lines
- Comparison of simulations with field measurements

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