Analysis of oxygen spectral lines in the 1.27 micron band for the ASCENDS mission

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ASCENDS Related NPP and IIP awards

- NASA Postdoctoral Program (NPP) award:
  - Topic: "Design and Optimization of the Laser Absorption Spectrometer Based Measurements for the ASCENDS Mission"
  - Improvements of line-by-line modeling accuracy (for CO_2 and O_2)
  - Experiments to obtain additional line-by-line parameters for advanced lineshape models
  - Modeling framework for ASCENDS
  - Development and optimization of the retrieval algorithm
- Recently ESTO awarded NASA Langley ACES (ASCENDS CarbonHawk Experiment Simulator) IIP
  - PI: Narasimha Prasad
  - IIP just started. The current work will be infused into ASCENDS effort at NASA LaRC

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

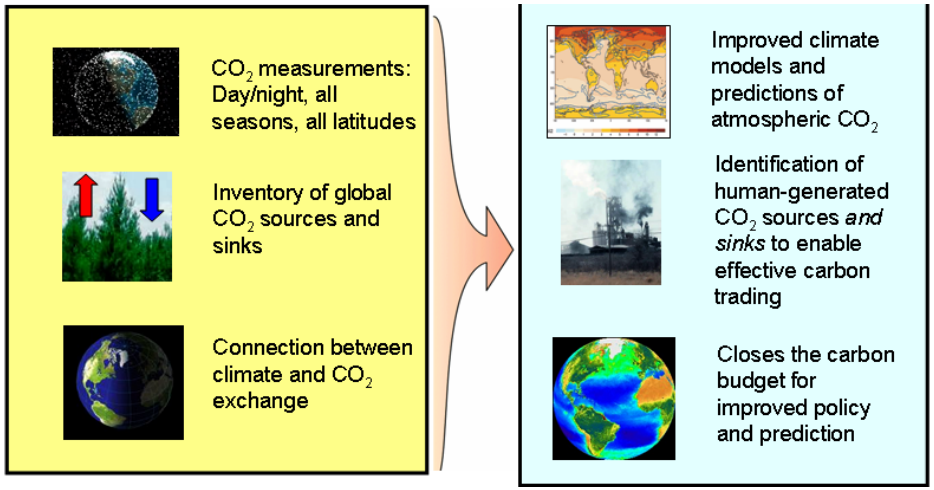
Introduction

- **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 CO_2 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 CO_2 at 1.57 microns and O_2 at 1.26 microns from space based platforms
  - Multiple wavelengths with differential absorption (DIAL) technique are utilized
- 1.26 micron band for O_2 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



Benefits For Climate Science

- Quantify global spatial distribution of atmospheric CO_2 on scales of weather models
- Quantify global spatial distribution of terrestrial and oceanic sources and sinks of CO_2 during day/night over all seasons.
- Provide a scientific basis for future projections of CO_2 sources and sinks through data-driven enhancements of Earth-system process modeling.

Requirements and Approach

- **ASCENDS is identified as a medium size mission in the NRC Decadal Survey is currently slated for 2019 launch**
- **ASCENDS will deliver laser based remote sensing measurements of Global CO_2 mixing ratios (XCO_2) 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 CO_2 interpretation.**
- **ASCENDS is the logical extension of OCO and GOSAT**
- **NASA LaRC is partnered with ITT for ASCENDS experiments**

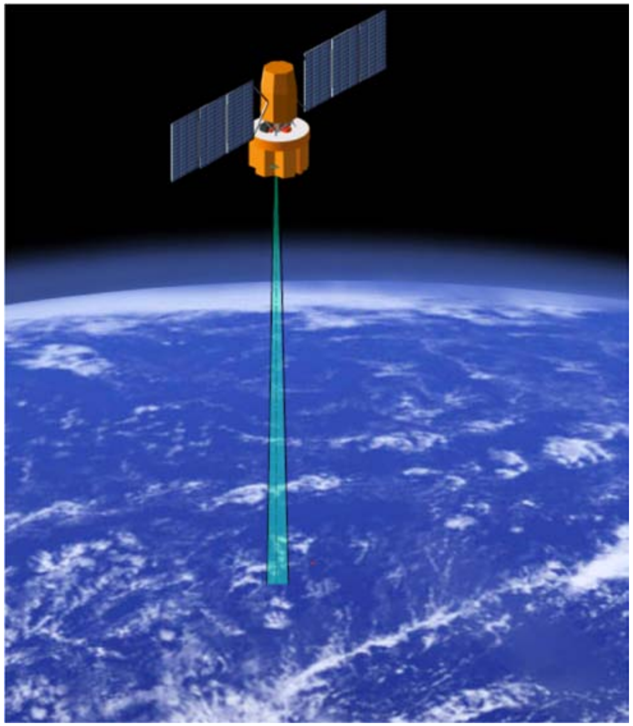
NASA LaRC Role

- **NASA LaRC is conducting the Pre-Phase A studies to define science and mission requirements.**
  - **Potential major roles in implementation.**
  - **Science leadership**
  - **Active CO_2, O_2 and passive CO instrument design and build**
  - **Mission management**
- **So far data have been collected from airborne instruments to verify the CO_2 measurement capability of the laser based approach**

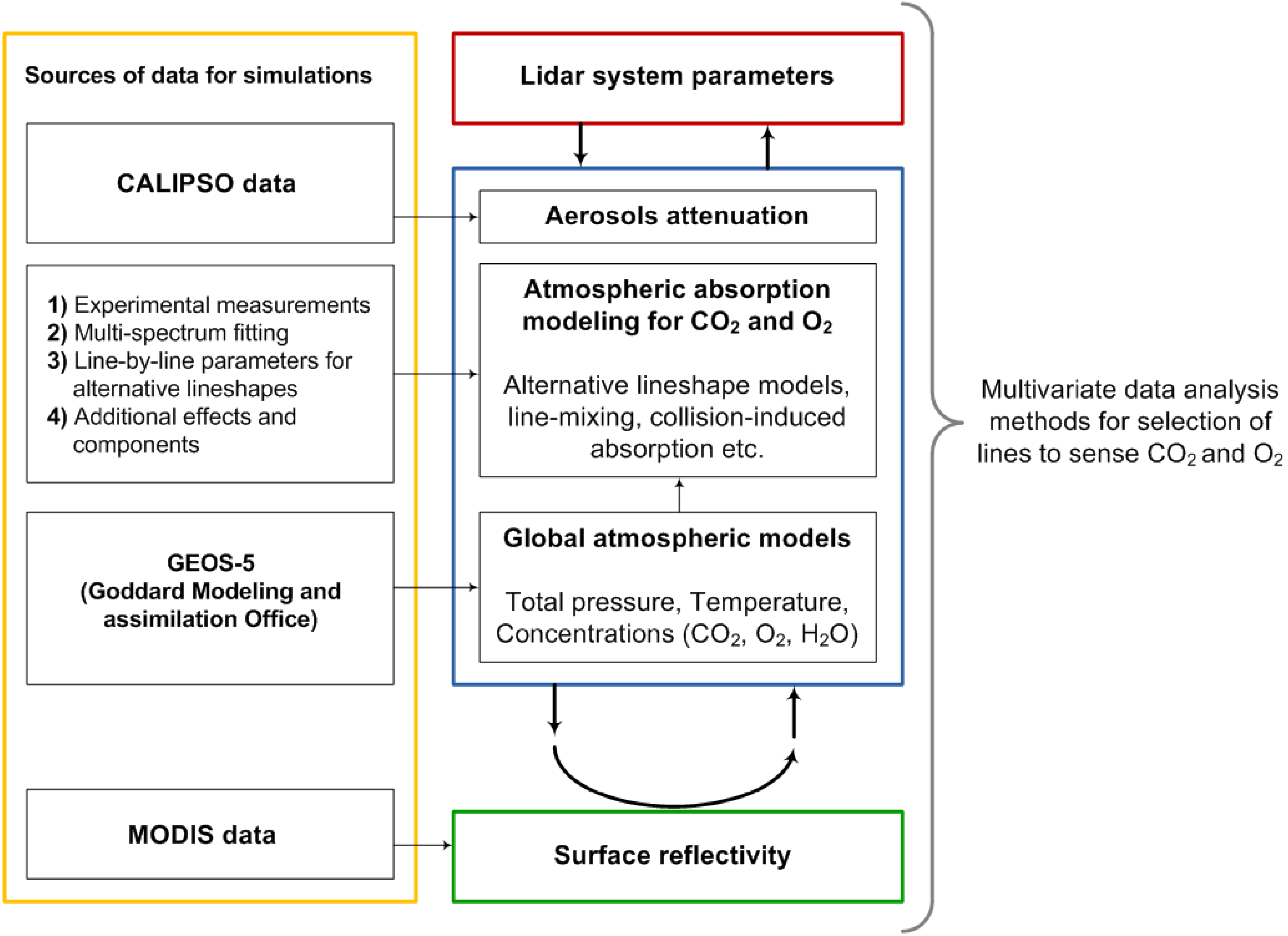
ASCENDS Measurements

CO_2 column mixing ratio (XCO_2) measurement with Laser Absorption Spectrometer (LAS) technique requires the simultaneous measurement of the CO_2 column number density (CND); the O_2 column number density to converting the CND to XCO_2; and the path length of the measurement. A temperature profile measurement is also required to constrain the XCO_2 measurement. A column CO measurement over the same XCO_2 path is also recommended for interpreting sources and sinks of CO_2

- CO_2 Column measurement
  - CO_2 Laser absorption spectrometer to resolve (or weight) the CO_2 altitude distribution, particularly across mid to lower troposphere
  - 1.57μm LAS only baseline or integrated 1.57μm + 2.0μm LAS option
- Surface pressure measurement
  - O_2 Laser Absorption Spectrometer operating at 1.26 / 1.27 μm to convert CO_2 number density to mixing ratio
- Surface / cloud top altimeter
  - Laser altimeter to measure CO_2 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

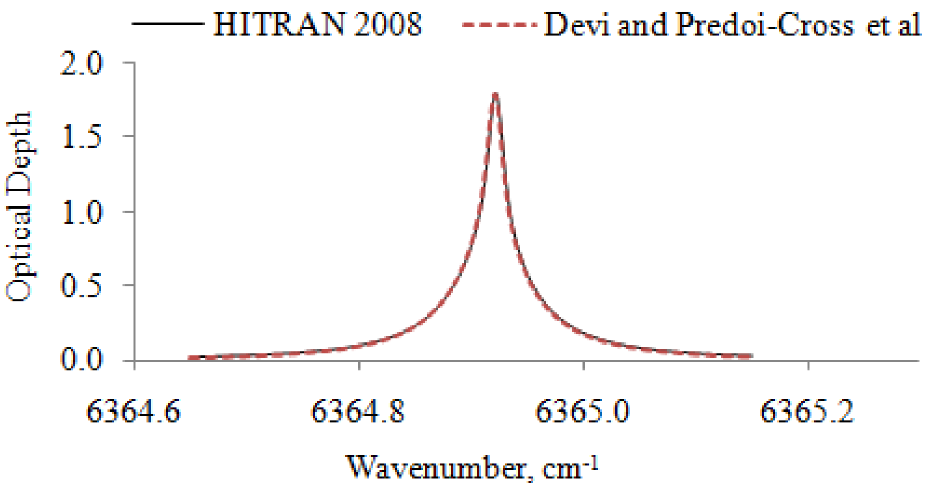


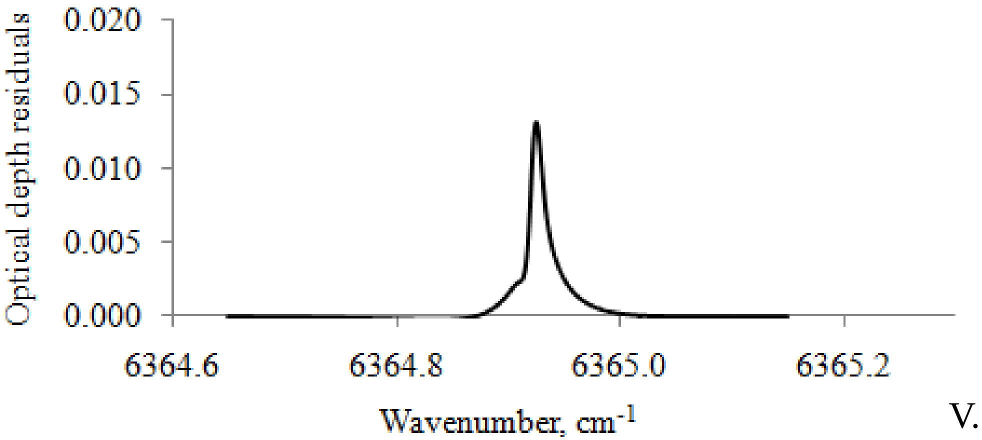
Consideration of CO_2 and O_2 Transmission simulation errors

- 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

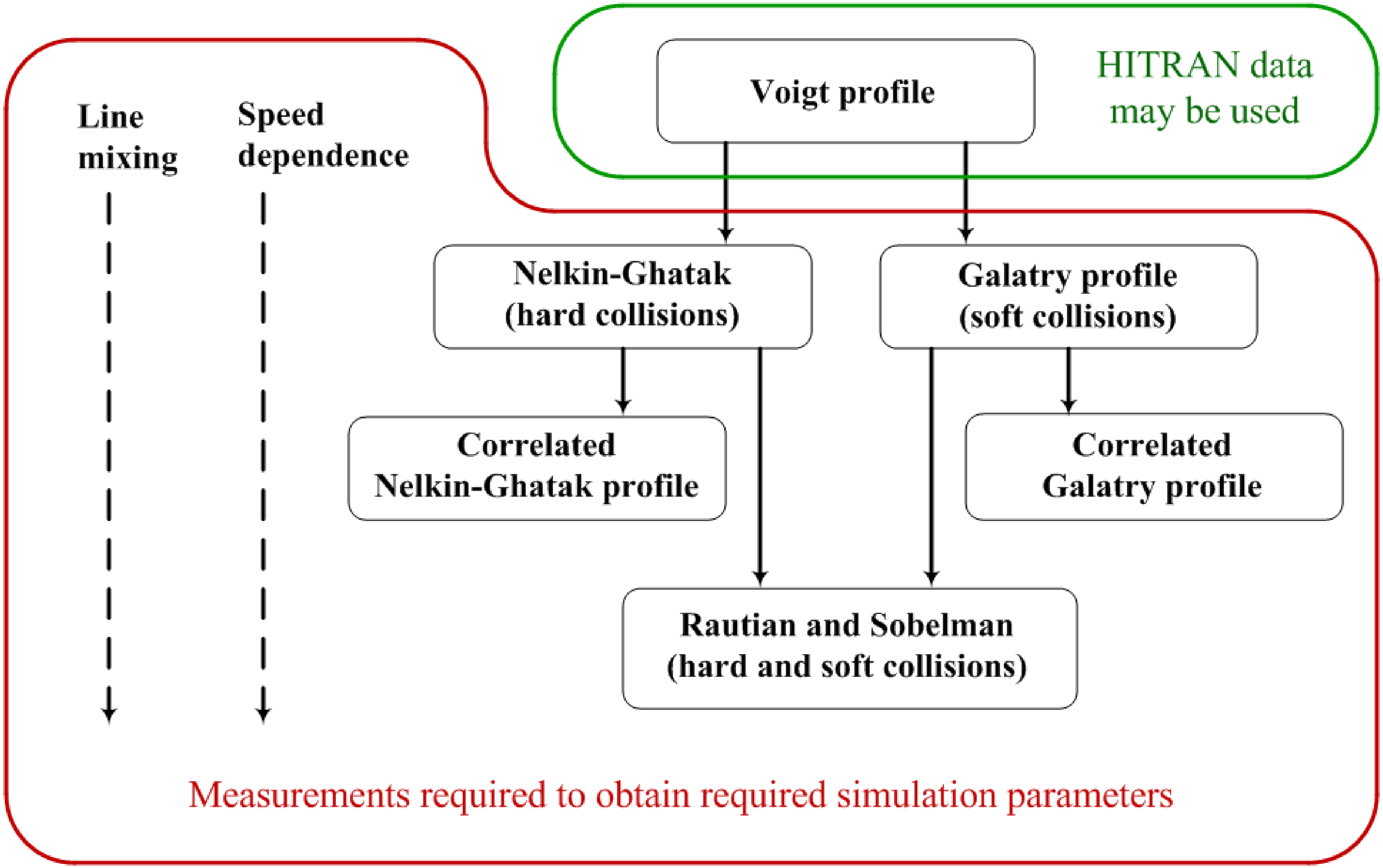
Devi and Predoi-Cross et al.:
Position: 6364.921972 cm-1
Intensity: 1.3673E-23

V. Malathy Devi et al, J Mol Spec, 242 (2007), pp. 90-117
A. Predoi-Cross et al, Can J. Phys, 87 (2009), pp 517-535

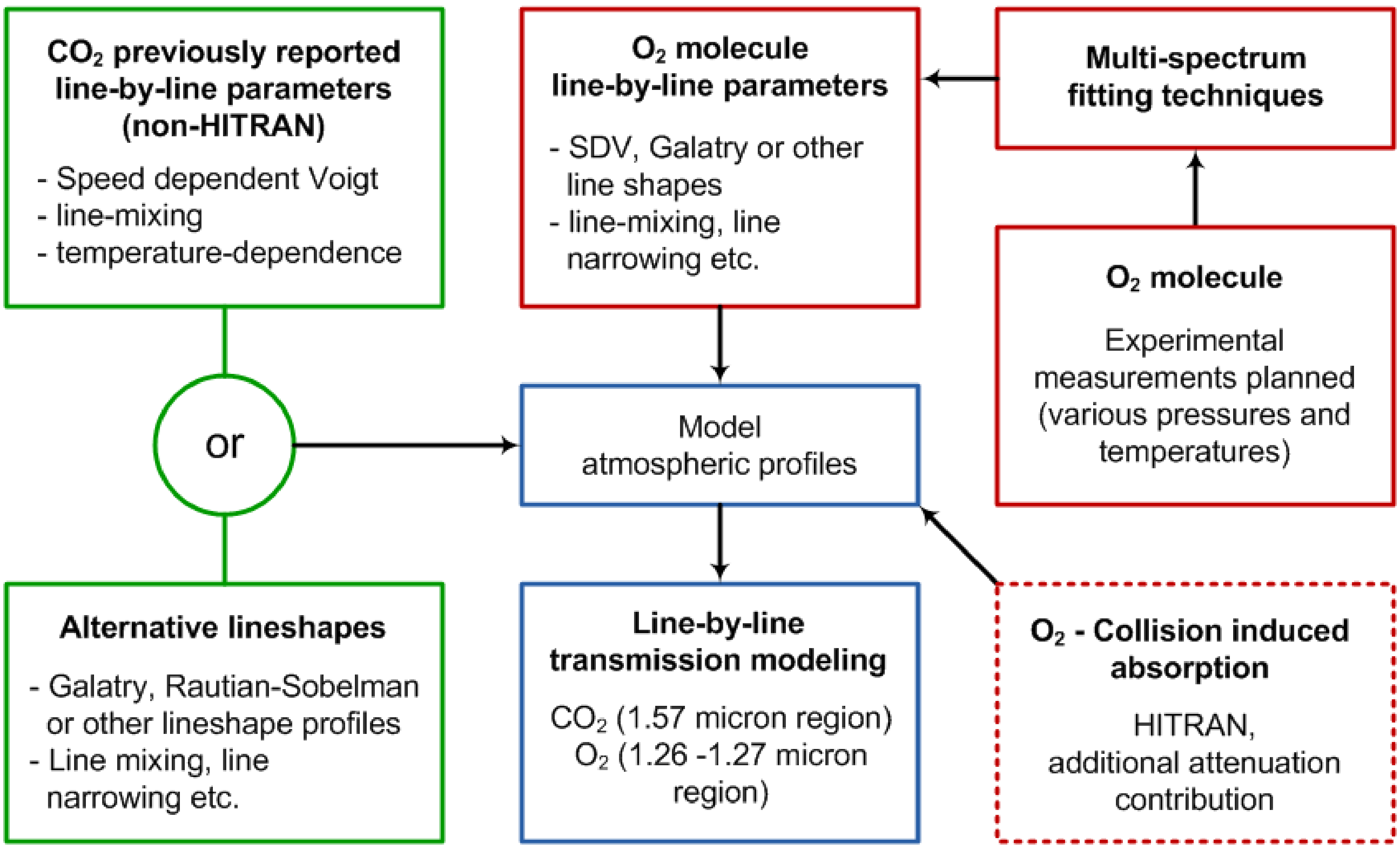
Need for improved transmission modeling for CO_2 and O_2

- Large uncertainties for some lines in HITRAN
- HITRAN data limited to Voigt lineshapes
- Voigt lineshapes accuracy ~ 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

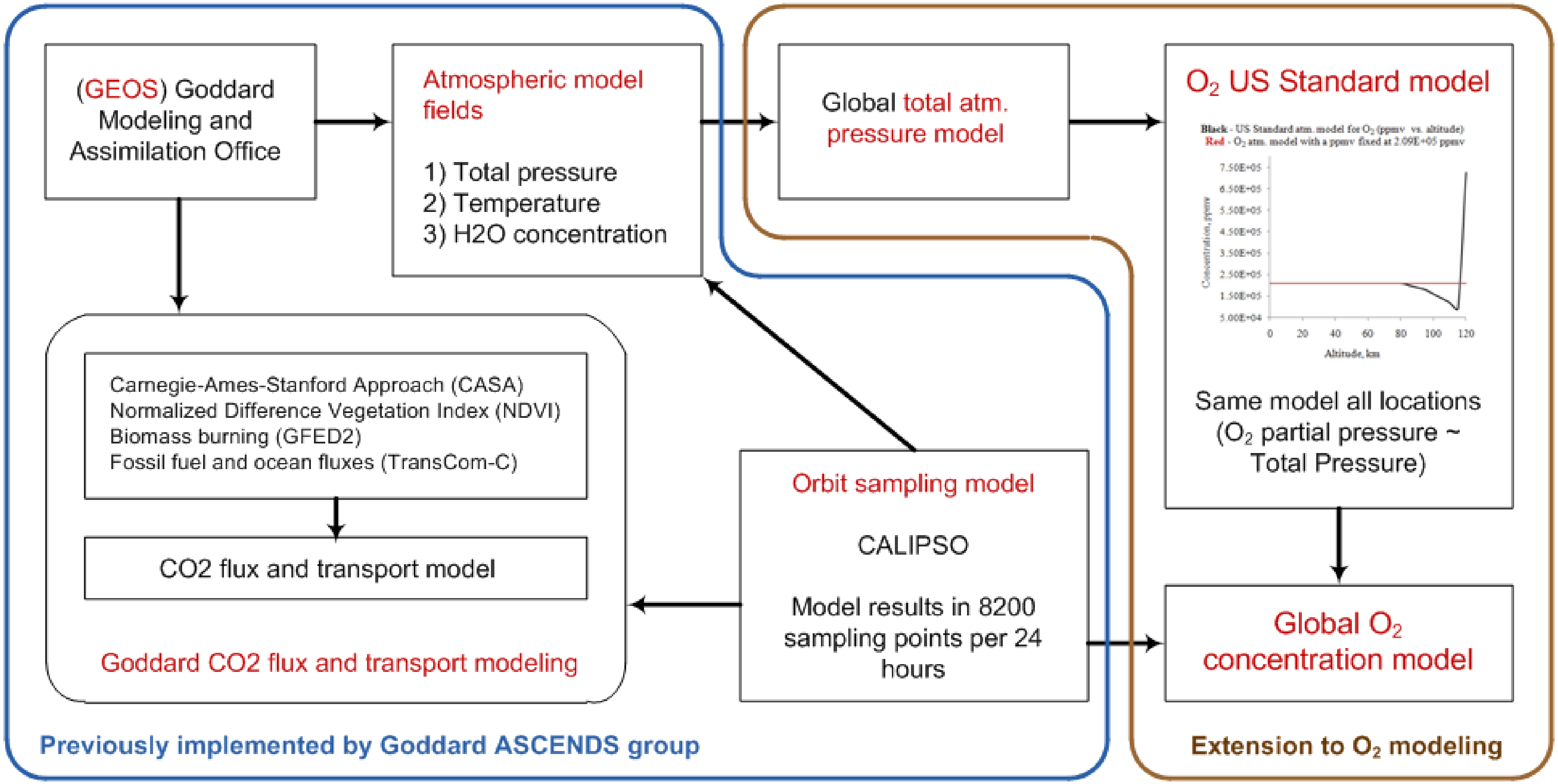


CO_2 and O_2 transmission modeling scheme



Global atmospheric model

Adopting the Goddard atm. model and orbit sampling approach and extending to O_2 molecule

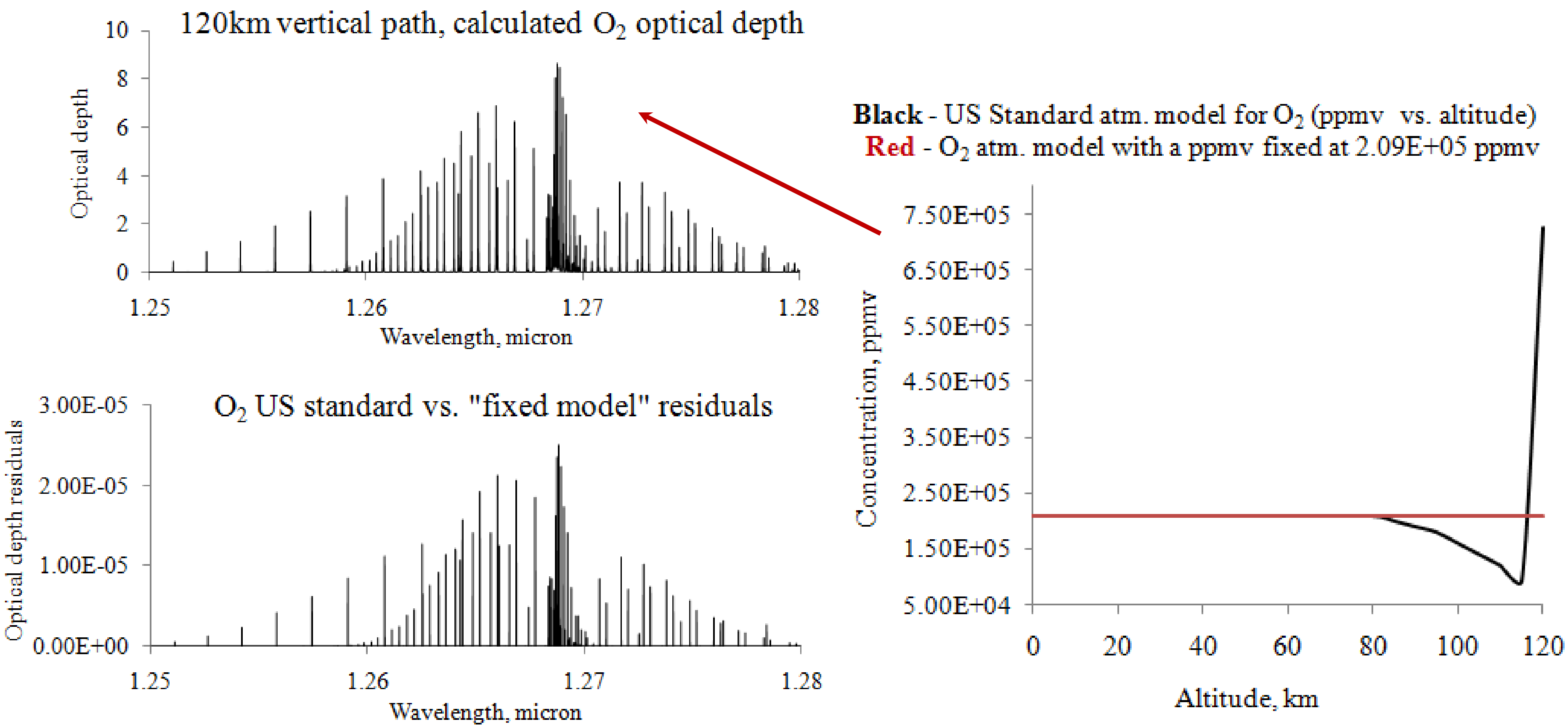


1) S. R. Kawa et al, “Simulation studies for a space-based CO_2 lidar mission”, Tellus (2010), 62B, 759-769

2) S. R. Kawa et al., “Global CO2 transport simulations using metheorological data from the NASA data assimilation system”, J. Geophys. Res., **109**, 2004, D18312

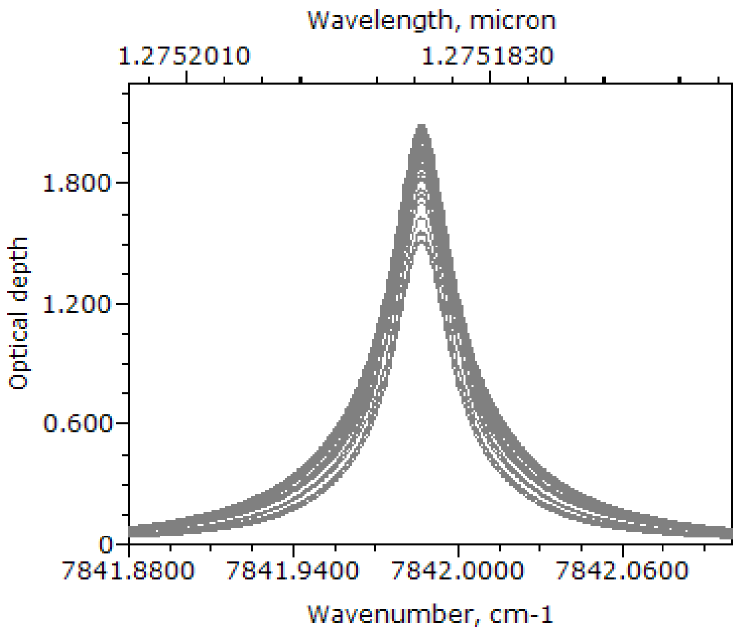
O_2 atm. model vs. altitude

(Negligible non-linearity error contribution, < 0.001 %)



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



Sample O_2 line calculation (120 km vertical path) at selected points along the modeled satellite path with varying atm. model parameters.

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

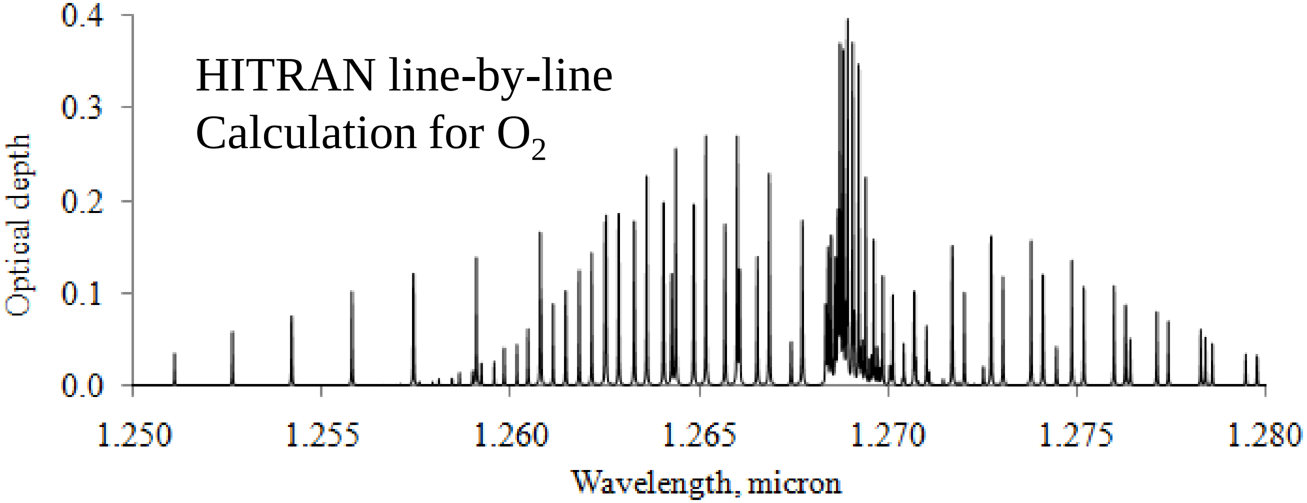
2) Large number of datasets with varying Pressure / Temperature / CO_2 and O_2 concentrations.

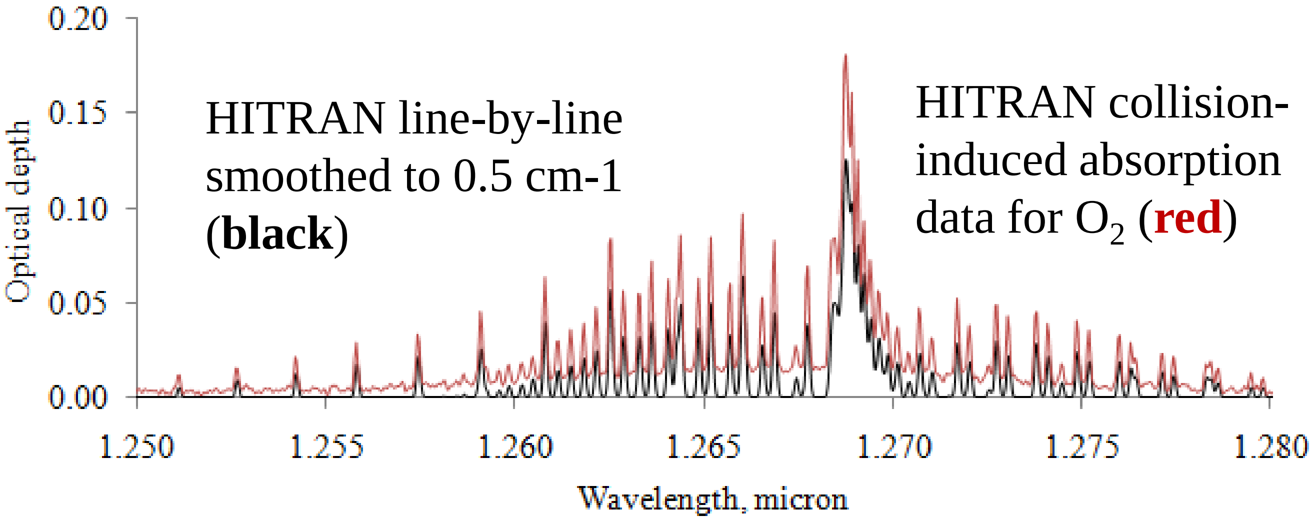
3) Complex relation between Temperature / Pressure / gas concentrations and spectral line features

4) Multivariate data analysis methods (such as PCA etc.) to establish optimum CO_2 and O_2 wavelengths

Collision-induced absorption for O_2

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

Additional continuum attenuation component to add to the total contribution

Magnitude of errors in transmission simulations, steps for reduction

Source of error	Estimated contribution	Suggested error reduction methods
Uncertainties in the line-by-line parameters (HITRAN vs. latest experimental data)	0.5 % – 1 %	Careful measurements (varying temperatures and pressures) with successive multi-spectrum fitting
Voigt lineshape profile accuracy limitations	~ 0.5 %	Implementation of alternative lineshapes providing higher precision. Laboratory measurements to obtain additional parameters required.
Collision-induced absorption continuum contribution (O_2 1.26 / 1.27 μm)	~3%	To be included in the model (may be corrected for experimentally)
Errors in O_2 modeling due to non-linearity of O_2 ppmv at higher altitudes	< 0.001%	Negligible

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
- Further analysis to further quantify errors
- Comparison of simulations with field measurements

Acknowledgements

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