Improvements of CO_2 and O_2 transmission modeling for ASCENDS mission applications

Denis Pliutau, and Narasimha S. Prasad
NASA Langley Research Center
Mail code 468
Hampton, VA 23681, USA
narasimha.s.prasad@nasa.gov

1. Introduction

The National Research Council's (NRC) Decadal Survey (DS) of Earth Science and Applications from Space has identified the Active Sensing of CO_2 Emissions over Nights, Days, and Seasons (ASCENDS) as an important atmospheric science mission. The CO_2 mixing ratio needs to be measured to a precision of 0.5 percent of background or better (slightly less than 2 ppm) at 100-km horizontal resolution overland and 200-km resolution over oceans. To meet this goal, the ASCENDS mission requires simultaneous laser remote sensing of CO_2 and O_2 in order to convert CO_2 column number densities to average column CO_2 mixing ratios (XCO_2). As such, the CO_2 column number density and the O_2 column number density will be used to derive the average XCO_2 column. NASA Langley Research Center (LaRC), working with its partners, is developing CO_2 and O_2 lidar technology in the 1.57-μm and 1.26-1.27-μm bands to be used for XCO_2 measurements.

The optimal selection of laser wavelengths for the sensing of CO_2 and O_2 and the development of the XCO_2 retrieval algorithm require accurate transmission modelling studies. Traditionally, calculations of this kind have been based on the use of the HITRAN database and are carried out using various line-by-line software simulation programs such as the LBLRTM.[1, 2]

ASCENDS groups at both NASA LaRC and Goddard Space Flight Center (GSFC) have carried out simulation studies to estimate the potential capabilities of their measurement approach for the sensing of CO_2.[3,4] These studies were bases on the use of the LBLRTM program with updated atmospheric model parameters (Pressure, Temperature and molecular concentrations as a function of altitude). Such approach is based on the use of the HITRAN database and as such has some accuracy limitations. Currently, the HITRAN database does not provide parameters required for modeling of spectral line shapes more accurate than Voigt. To achieve the accuracy set forth for the ASCENDS mission, the use of more sophisticated line shape models and consequently knowledge of additional spectral parameters unavailable in HITRAN is required.

In this paper we describe our ongoing modeling efforts as well as an improved modeling approach to enhance the accuracy of CO_2 and O_2 line-by-line transmission simulations by incorporating more advanced speed dependent Voigt (SDV) modelling and utilizing additional data such as the collision induced absorption cross-sections for the O_2 molecule and updated atmospheric profile models.

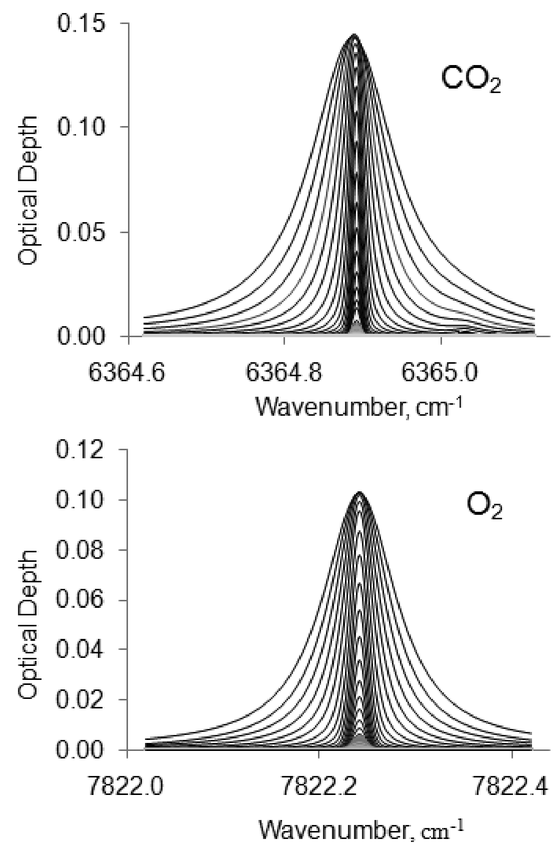

Fig. 1 Calculated changes in CO_2 and O_2 absorption lines as a function of altitude.

2. CO_2 and O_2 transmission modeling

Our current CO_2 and O_2 transmission modeling efforts include the selection of the optimum laser wavelengths in the 1.57 and 1.26-1.27 micron bands by investigating the behaviour of absorption lines in these bands as a function of altitude. For example, Fig. 1 shows calculations for selected lines of CO_2 and O_2 molecules for different layers in the vertical 120km path geometry composed of 60 layers. Modified US Standard atmospheric model is used to produce a 120km averaged CO_2 concentration of 393ppm.

3. Accuracy improvements of transmission calculations

Several groups have done extensive measurements for the CO_2 molecule bands near 1.57 micron which provide more accurate and complete data than that currently available in the HITRAN database. Examples are recent studies carried out by Devi et al. and Predoi-Cross et al which, in addition to the standard line-by-line data, provide pressure shift temperature dependence and speed dependent Voigt coefficients, as well as line-mixing parameters.[5,6] We have used their results for line-by-line transmission modelling in the CO_2 band near 6348 cm^{-1} instead of the HITRAN database parameters to improve the accuracy of our CO_2 transmission simulations. For example, Fig. 2 shows a vertical path calculation for a CO_2 line near 6364.92 cm^{-1} carried out for a vertical path of 120km with 60 layers using modified US Standard model with proportionally increased concentration of the CO_2 gas to produce a column averaged concentration of 393ppm. As can be seen, a comparison is made of the calculation carried out using HITRAN 2008 with that based on the Devi and Predoi-Cross data (Voigt profile is used, no speed dependence, line mixing and temperature dependence of line shifts is included). As can be seen, the differences in the spectral parameters alone result in residuals which exceed the required accuracy set forth for the ASCENDS mission measurements.

Experimental measurements are planned at carefully controlled temperature and pressure conditions to determine line-by-line parameters for the O_2 molecule in the 1.26-1.27 micron band using least squares multi-spectrum fitting techniques. These studies will make it possible to extend the speed dependent Voigt or similar modeling approach to the O_2 molecule.

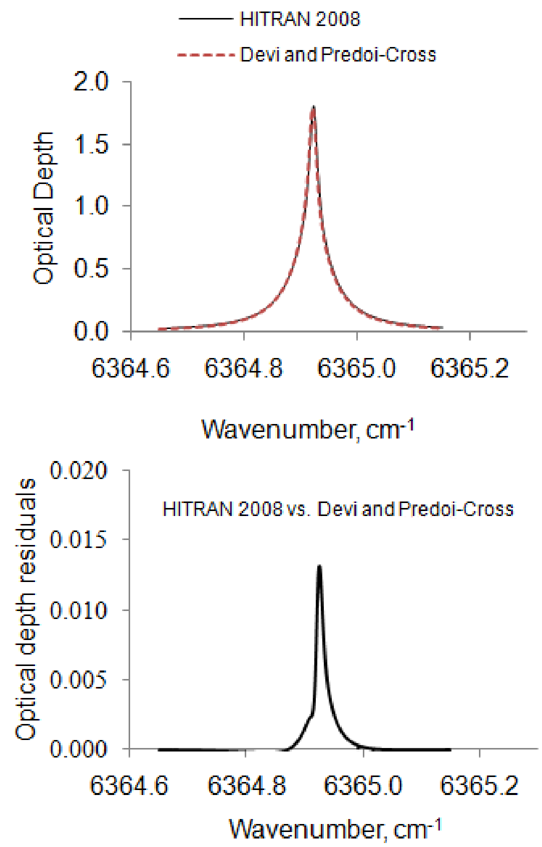

Fig. 2 Comparison of calculations for a single CO_2 line near 6364.92 cm^{-1} using the data from the HITRAN 2008 and that from Devi and Predoi-Cross (5, 6).

4. Summary of the modeling approach

A summary of our modelling method is presented in the figure below. As can be seen, previously reported data is used for speed dependent Voigt line-by-line transmission modelling for the CO_2 molecule. The same approach will be extended onto the O_2 line-by-line simulations after the required spectral parameters have been determined through experiments and least squares multispectrum fitting techniques. It is important to point out that the atmospheric models have to be modified accordingly to take into account the increased level of CO_2 concentrations. In addition, we may supplement our O_2 transmission simulations with collision induced absorption data soon to be included in the HITRAN database (from: Dennis K. Killinger, Laurence S. Rothman, private communication).

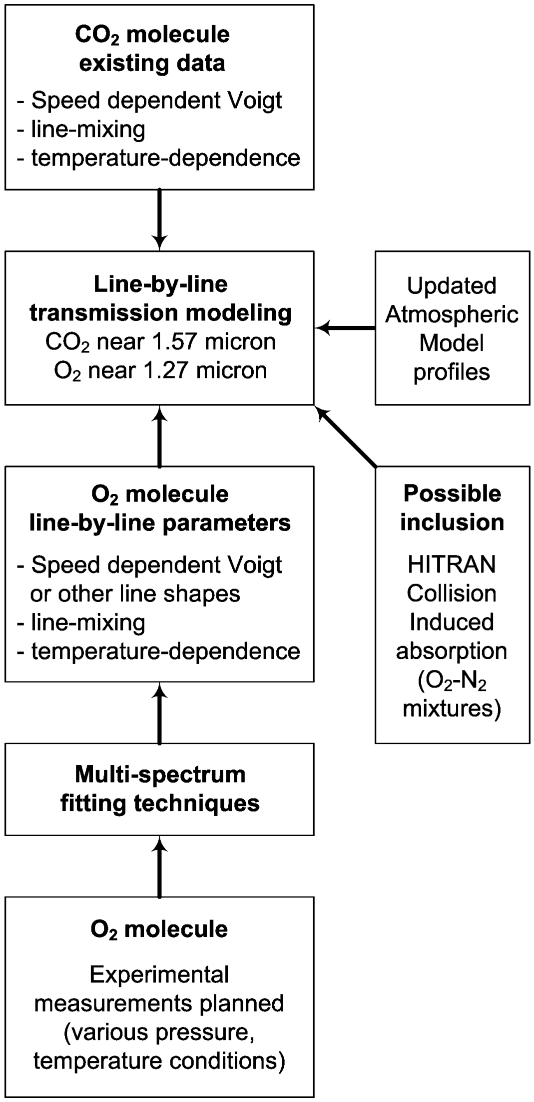

Fig. 3 Summary of the modeling approach being implemented for the modeling of CO_2 and O_2 atmospheric transmission.

5. Conclusion

Toward this end we have carried out preliminary simulation studies for the optimum selection of laser wavelengths for CO_2 and O_2 sensing. Our current work includes modification of our calculations by including the newest and more accurate data. A new speed dependent Voigt line-by-line modeling approach based on new data is being implemented to provide improved accuracy of CO_2 transmission calculations. Laboratory measurements are planned to obtain the required spectral parameters for O_2 non-Voigt line-by-line transmission modelling.

Our improved method involves more accurate CO_2 and O_2 calculations combined with updated atmospheric models and O_2 collision-induced absorption contributions. Eventually this method will be used in the development and optimization of the XCO_2 retrieval algorithm through comparison with laboratory and field measurements and refinement of our simulations.
A more detailed description of our work and additional results will be presented at the meeting.

6. Acknowledgements

This research was supported in part by an appointment to the NASA Postdoctoral Program at the Langley Research Center, administered by Oak Ridge Associated Universities through a contract with NASA.

7. References

1. L. S. Rothman et al., “The HITRAN 2008 molecular spectroscopic database”, JQSRT, **110**, 533-572, (2009).

2. Clough S. A., et al., “Atmospheric radiative transfer modeling: a summary of the AER codes”, JQSRT, **91**, 233-244, (2005).

3. T. Scott Zaccheo et al., “End-to-end testbed for rapid analysis of laser remote sensing data and application to flight data in preparation for ASCENDS”, AMS 2009.

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

5. V. Malathy Devi et al., “Line-mixing and speed dependence in CO_2 at 6348cm^{-1}: Positions, intensities, and air- and self-broadening derived with constrained multispectrum analysis”, J. Mol. Spec., **242**, 90-117, (2007).

6. A. Predoi-Cross et al., “Temperature dependences for air-broadened Lorentz half-width and pressure shift coefficients in the 30013←00001 and 30012←00001 bands of CO_2 near 1600 nm”, Can. J. Phys., **87**, 517-535, (2009).