Application of MODTRAN® to Planetary Atmospheres

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ABSTRACT

At last year's AMOS conference we described modifications made to MODTRAN5® in order to make it more generally applicable to arbitrary planetary atmospheres. It was then used to compare to a wide variety of spectral data for Neptune, spanning the UV through far-IR spectral regime, ~0.4-200 μm. At this year's meeting, we describe our continuing efforts along these lines, and apply an upgraded version to Saturn, providing similar data comparisons over a broad wavelength region. The primary upgrades include an input option to automatically generate the pressure-altitude profile from the hydrostatic equation, development of a molecular band model parameter database based on the isotopic abundances of Saturn, and the addition of continua spectral data, such as H_2-CH_4 and CH_4-CH_4 dimer absorption coefficients. Clouds and haze, which are highly variable and play a dominant role in the radiation transfer in Saturn's atmosphere, provide a good test of MODTRAN®'s capability to treat these complications.

1. INTRODUCTION

The accelerating development pace of new sensors and ground-based and space-based large optical platforms means that the pace of discovery of new extra-solar planets will continue to explode and provide an enormous quantity of planetary spectra, covering a very broad spectral domain. Additionally, these assets will also be trained on the planets in our solar system. This drives a need for new and/or improved radiation-transfer (RT) models capable of handling the quantity and spectral breadth of such data. At last year's AMOS conference, we demonstrated that MODTRAN5®, which is an extensively used and well validated RT code for terrestrial applications, could be modified for general application to arbitrary planetary atmospheres [1,2]. This modified version was then used to compare to a wide variety of spectral data for Neptune, spanning the UV through far-IR spectral domain, ~0.4-200 μm. At this year's meeting, we present our continuing efforts to generalize MODTRAN®, and we highlight this upgraded version by comparing to similar spectral data for Saturn.

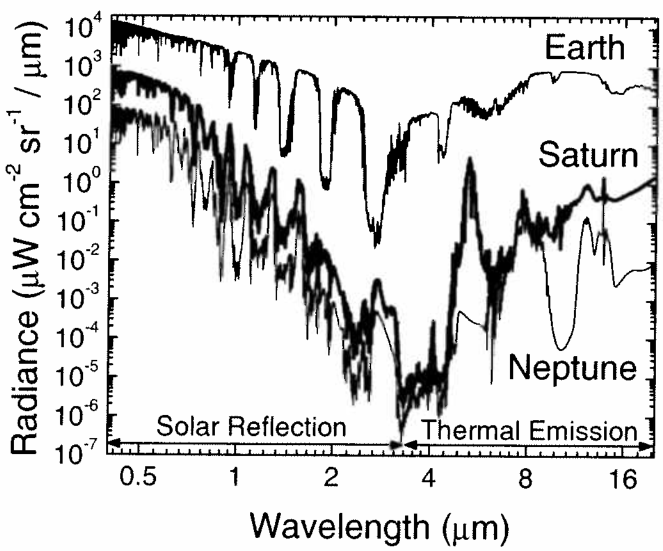

Fig. 1. Examples of modified MODTRAN® clear sky calculations of the remotely viewed spectral signatures of the Earth, Saturn and Neptune for a nadir line of sight.

Fig. 1. highlights the nature of the challenge by comparing planetary spectra for Earth, Saturn, and Neptune. Neptune and Saturn's radiances are much lower than Earth's because they are much colder, ~100 K vs. ~300 K, and

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much further away from the sun. Of more interest are the large differences in the detailed spectral structure. The primary emission-absorption features for Earth are due to H_2O and CO_2. In contrast, on Neptune and Saturn they are due to CH_4 and H_2. The central issue in generalizing MODTRAN® for planetary applications is the incorporation of new spectral data bases for the much wider variety of molecular species, clouds, and aerosols encountered on other planets and moons.

2. MODTRAN® OVERVIEW

MODTRAN® is the product of a long standing and continuing collaboration, starting in 1987, between Spectral Sciences, Inc. and the Air Force Research Laboratory. The exact number of regular users is not well established, but conservative estimates place it at well over 2,000. The code is well validated and a yearly technical conference is held to discuss problems, progress, and applications. Its key attributes are summarized below:

- 1D Atmospheric Radiative Transfer Model
- IR / Vis / UV Transmittances, Radiances and Fluxes
  - 1-50,000 cm^{-1} or 0.2-10^4 μm
- Band model and *k*-distribution RT approaches
- 0.1, 1.0, 5.0 & 15.0 cm^{-1} resolution molecular band models
  - Based on HITRAN line parameter data base [3,4]
- Stratified Molecular / Aerosol / Cloud Atmosphere
  - Standard and User-Specified data bases
- DISORT 2^N-Stream Solar and Thermal Scattering
- Spherical Refractive Geometry
- Surface emission & reflectance with BRDF
- Assumes LTE (Local Thermodynamic Equilibrium)

3. CODE MODIFICATIONS

The primary changes to the code for its application to the outer planets were implemented previously for application to Neptune [1]. This involved adding a variety of different spectral data bases appropriate for the species encountered in atmospheres of the outer planets and moons (e.g., Neptune, Saturn, Uranus, Jupiter, and Titan). Additional changes were made to the MODTRAN® source code to extend its temperature range down to 30K and to properly compute the extra-terrestrial Rayleigh cross-sections.

The new modifications implemented for Saturn are summarized below:

- Created band model parameters using Saturn's isotopic abundance for deuterium
- Incorporated H_2-CH_4 and CH_4-CH_4 collision-induced continua [5,6]
- Defined cloud and aerosol parameters for three Saturn cloud/haze layers [7]
- Added planet mass and air molecular weight inputs for use in solving the hydrostatic equation

The isotopic abundance of deuterium on Saturn is ~8.7×10^{-5} [8], about a factor of 6 less than the terrestrial value. Currently, the MODTRAN® spectral band model parameters are generated for fixed values of the molecular isotopic abundances. Changing the abundances requires re-generation of the band model parameters; however, in future versions of the planetary code, the flexibility to change abundances on-the-fly is an envisioned upgrade.

H_2-CH_4 and CH_4-CH_4 collision-induced absorption is evident in some planetary atmosphere long-wave signatures [9]. However, these contributions are much weaker than the collision induced absorption from H_2-H_2 and H_2-He absorption because of the lower abundance of CH_4 (~0.4%) compared to H_2 (~90%) and He (~10%). Although we have added these continua in MODTRAN®, their absorption is not appreciable in any of the data comparisons presented here.

Hazes and clouds are common occurrences for the outer planets due to the extremely cold temperatures and moderate pressures encountered in the tropopause and lower stratosphere. Ammonia and hydrocarbon species, such as CH_4 and C_2H_6, readily condense under these conditions. MODTRAN®5 models arbitrary aerosol haze profiles, with the flexibility to change spectral properties (aerosol type) at each altitude level or to assign fixed spectral optical properties within selected altitude regions. The technical challenge is in specifying the scattering and absorption optical data for the haze and cloud particles. In the case of Saturn, there are three identified cloud/haze layers for which approximate optical properties have been estimated. We utilize both the 1995 and 1999 characterization of these cloud layers at 36°S latitude from Pérez-Hoyos *et al.* [7]. Because of the variation in solar illumination with latitude during Saturn's 29.4 year orbital period, as shown in Fig. 2, the stratospheric and upper tropospheric haze layers change quantitatively over this time interval.

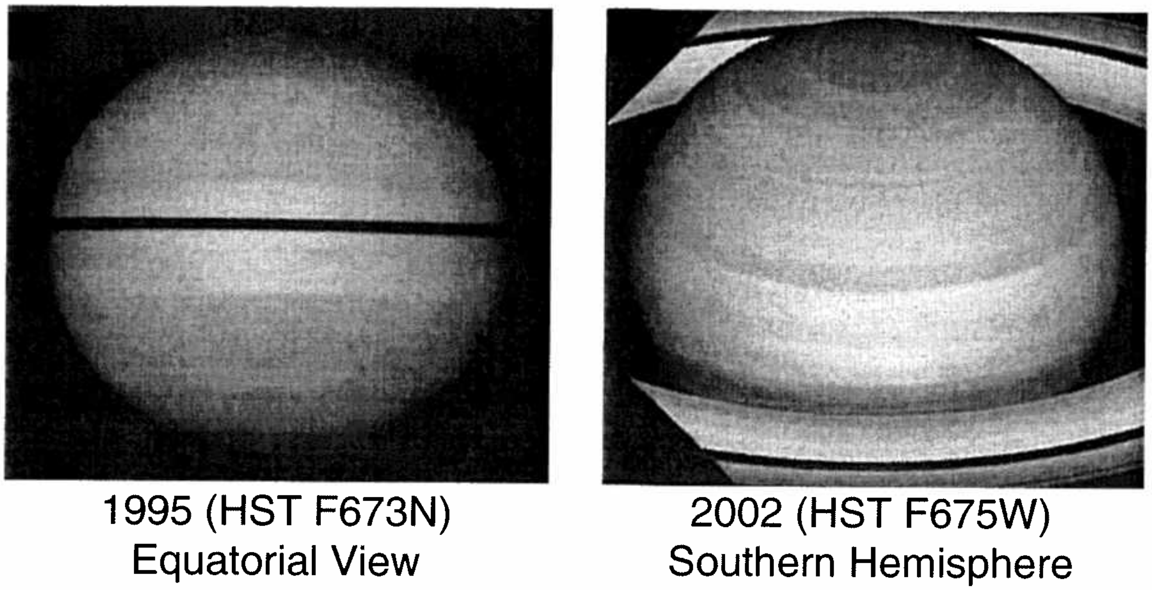

Fig. 2. Hubble Space Telescope images of Saturn at equinox (left) and solstice (right) [7].

The optically thin stratospheric haze (located between 10 to 1 mbar) contains condense hydrocarbons, and is modeled as a Mie cloud layer using an index of refraction appropriate for condense methane ($m_r = 1.5$, $m_i = 0.001$). Although the particles are modeled as spheres with a 0.2 μm mean radius, they are believed to be irregularly shaped crystals. As a result, neither the shape of the spectral extinction curve predicted by Mie theory nor the Angstrom Law parameterizations provide a reasonable fit to observations. Pérez-Hoyos *et al.* simply define a vertical optical depth at a series of Near-IR, visible and UV spectral points using HST filter data; at longer wavelengths, the stratospheric cloud is assumed transparent.

The 1995 upper troposphere cloud (500 to 80 mbar) at 36°S was given an optical depth of 20 below 588nm, increasing to 25 at 673nm before dropping to 18 at 890 nm and 8.8 at 953nm [7]. With the increased solar exposure, the 1999 upper tropospheric cloud (350 to 75 mbar) at the same latitude has about half the optical opacity - a constant optical depth of 9 below 814 nm and a value of 7.7 at 1042 nm. The visible spectral region single scatter albedo generally increases with wavelength from ~0.84 to ~0.995 for both upper tropospheric clouds; beyond 1 um, a single scattering albedo of 1 is assumed. The scattering phase function is approximated with a relatively flat double Henyey-Greenstein parameterization; the forward peak to minimum ratio is less than 100 within the Vis/Near-IR spectral region.

The optically thick lower tropospheric cloud, with cloud top near ~1.4bar, was modeled with a spectrally constant optical depth, $\tau > 100$, isotropic scattering, and a scattering albedo of 1. Fig. 3 illustrates the cloud structure and the specific parameterization for all three cloud/haze layers.

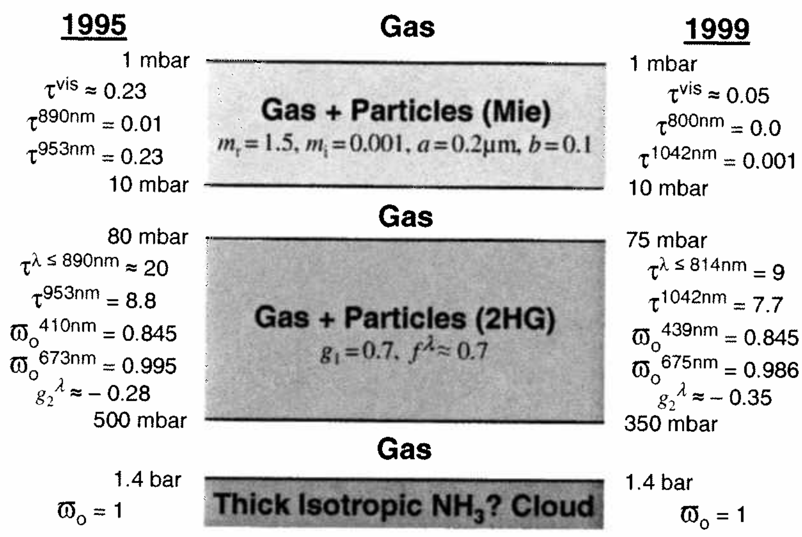

Fig. 3. Pérez-Hoyos *et al.* [7] characterization of Saturn's cloud and haze layers at 36°S. The parameters listed include optical depth τ, single scattering albedo ϖ_o, double Henyey-Greenstein data g_1, g_2 and *f*, index of refraction (m_r, m_i), and Hansen and Travis particle size distribution parameters, *a* and *b*.

4. APPLICATION TO SATURN

We have performed a number of comparisons between MODTRAN® modified for planetary applications and observational data for Saturn over a broad wavelength region, spanning the visible through far infrared spectral domains. These calculations are based on the reference atmosphere temperature and species concentration profiles depicted in Fig. 4 (T and CH_4 from [9]; He from [10]; C_2H_6 and C_2H_2 from [11]; PH_3 from [12]; and NH_3 from [13]. Before discussing the comparisons, it is helpful to first consider the individual spectral contributions to a vertical LOS (Line-Of-Sight) transmission spectrum as shown in Fig. 5. The dominant role of CH_4 is clearly evident, where it is seen that CH_4 alone would prevent one from viewing deeper than about 10 bar for much of the ~0.8-9.0 μm region. Similarly, the H_2 collision induced absorption features prevent seeing deeper than ~1 bar beyond 10 μm. One can probe deeper into the atmosphere in the visible and near infrared regions, penetrating into the lower tropospheric cloud at 1.3 bar. The IR bands of PH_3 and NH_3 are strongly absorbing just above the lower tropospheric cloud. The absorptions due to the trace species, C_2H_6 and C_2H_2 are much weaker and these species are only observed in the stratosphere, below ~10 mbar.

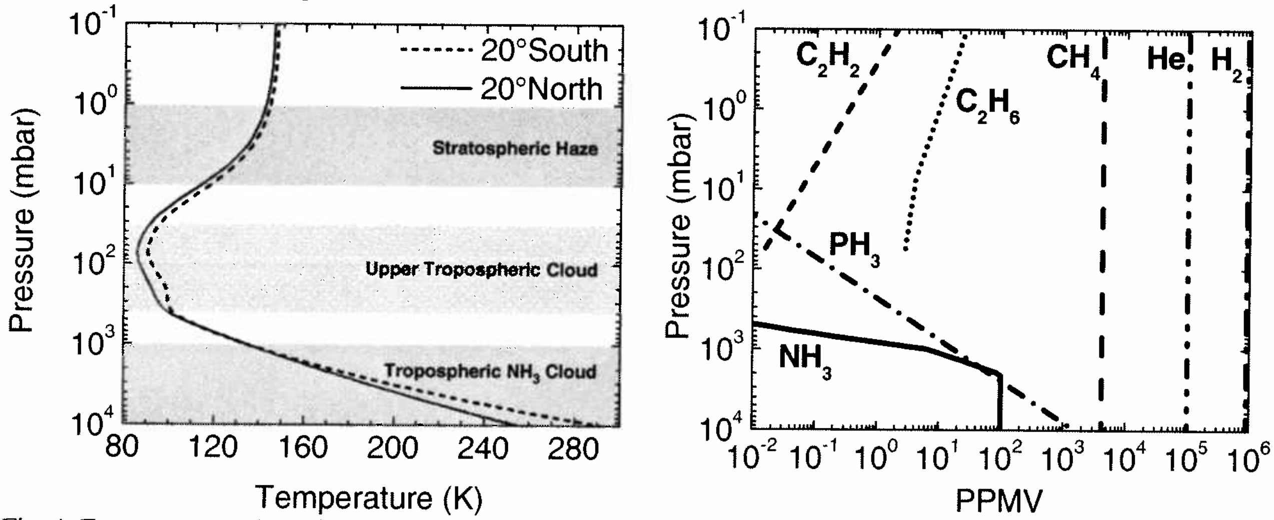

Fig. 4. Temperature and species concentration profiles for Saturn. The 20°N temperature profile is ~5K colder than the 20°S profile in the upper troposphere. The approximate pressure-altitude ranges for the previously retrieved haze and cloud layers are also indicated.

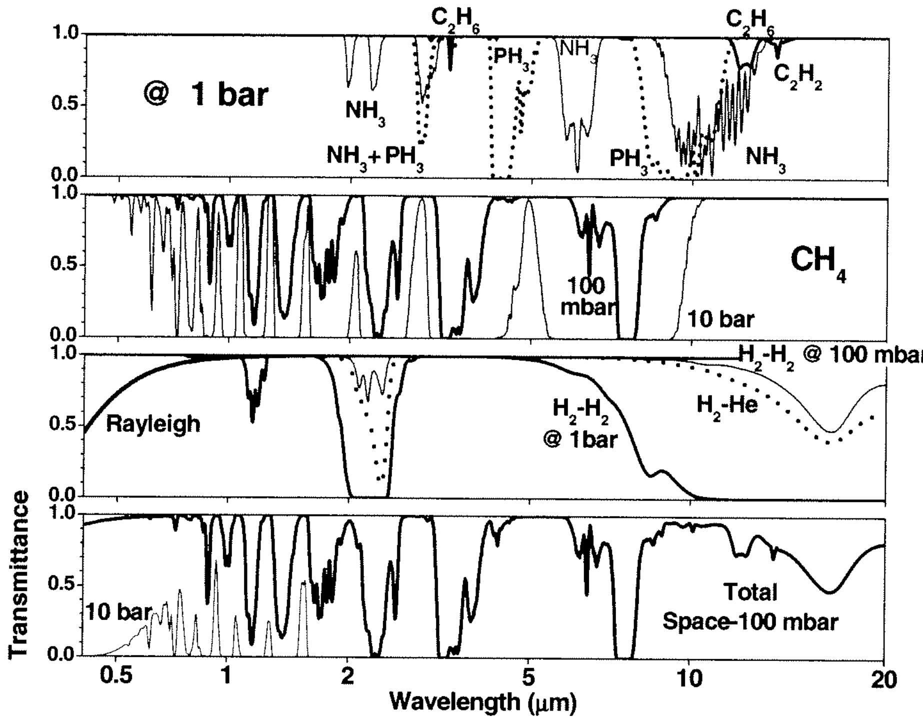

Fig. 5. Species spectral transmission components at 0.1% resolution for a nadir path from Space to 100 mbar. The top panel shows NH_3, PH_3, C_2H_6, and C_2H_2. The panel below shows CH_4 only (thick line). The next panel down illustrates H_2-He and H_2-H_2, (thick lines) as well as Rayleigh scattering (dashed line). The bottom panel shows the total for the three panels above (thick line). Also shown are the effects of higher pressure (thin lines) on the total, the H_2-H_2 collision induced absorption, and the CH_4 transmission components.

A comparison for the long wavelength to far-IR spectral region, ~14.3-50 μm (200-700 cm^{-1}), is shown in Fig. 6 [8]. This is a region dominated by emission of NH_3 (< 300cm^{-1}) and H_2. The reference 20°N temperature profile was shifted -3K to match the minimum temperature of the retrieved profile [8] for this 28-42°N IRIS data with a mean emission angle of 32.9°. Given this and noting that the NH_3 reference profile was also taken from [8], an excellent match to the data results. However, our goal here, and in the other comparisons, is not to adjust all available parameters to achieve an ultimate fit to the data, but rather to demonstrate that the modified MODTRAN® can produce good results across a very broad wavelength regime.

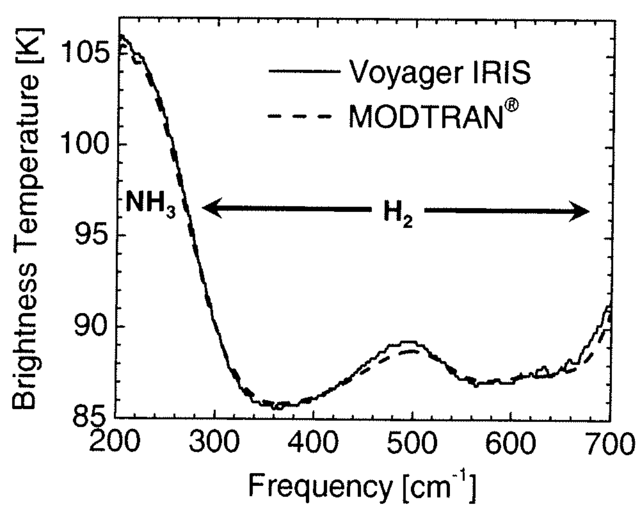

Fig. 6. Comparison of modified MODTRAN® calculations to long wavelength IR data for Saturn at 4.3 cm^{-1} spectral resolution [8]. The calculations are based on the reference 20°N temperature and species profiles shown in Fig. 4.

The next two comparisons focus on long-wave IR data at moderate spectral resolution, as shown in Fig. 7. Fig. 7a features the 12.2 μm C_2H_6 band and the 13.7 μm C_2H_2 band, while spectral emission from the 7.7 μm CH_4 band is illustrated in Fig. 7b [11]. The effective emission angle for these 40°N to 40°S observations is 24°. Although the reference C_2H_6 and C_2H_2 profiles were taken from [11], no adjustments were made to the reference 20°N temperature profile. Initially the CH_4 / CH_3D comparison was performed with the planetary atmosphere band model data developed last year [1] using terrestrial isotopic abundances. As noted above, the deuterium abundance on Saturn is more than a factor of 6 less. As a result, the CH_3D Q-branch emission centered at 1297 cm^{-1} was ~50% too large. New band model parameter data were generated specifically for Saturn to produce the fit of Fig. 7b.

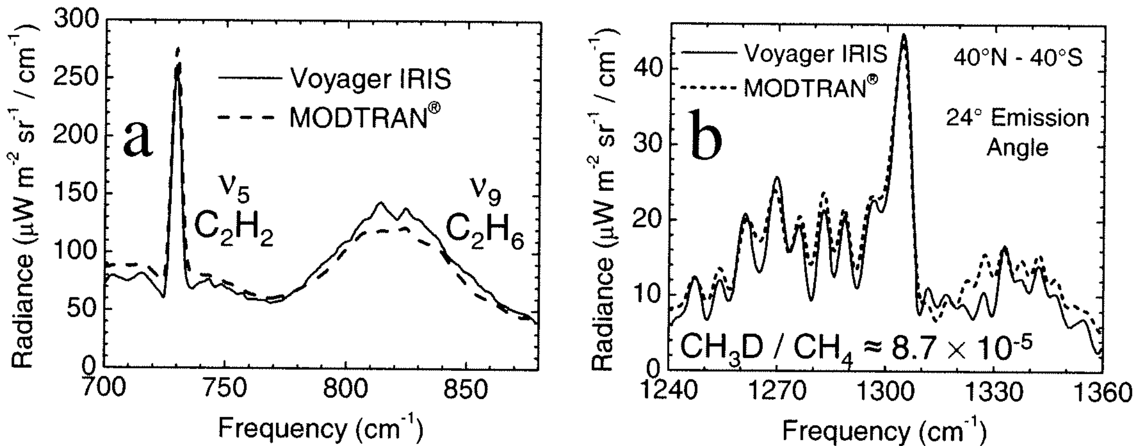

Fig. 7 Comparisons of modified MODTRAN® calculations to IRIS long wavelength IR data for Saturn [11]. The 13.7 μm ν_5 acetylene band and the 12.2 μm ν_9 ethane bands are shown in (a), while (b) contains the 7.7 μm ν_4 methane band.

As we progress into the mid-wave IR, solar scatter becomes the dominate radiance source in Saturn mid-day spectra. This is the case for the high spectral resolution data comparison [12] in Fig. 8. In this 2.89 to 2.90 μm bandpass, PH_3 and CH_3D molecular absorption lines attenuate the direct solar scatter from the lower tropospheric cloud.. The illustrated NIRSPEC sensor data, recorded from the Keck II telescope, is shown with regions of strong telluric absorption excluded. For calibration of the measured data, similar spectra were obtained of the G2V star HD 32092 [12]. The measurements focused on a 40°S swatch of ~44° latitude width and centered at the center meridian. For this calculation alone, we adopted the modeling assumption of [12] and replaced the lower tropospheric molecular and particulate profiles with a Lambertian surface at 460 mbar. The stratospheric and upper tropospheric haze was also assumed to be transparent in this region. The spectral albedo from Fig. 5a of [12] is ~0.42 in this spectral region. Using these parameters, the MODTRAN® predictions are too high by ~25%; the MODTRAN® result has been scaled by 0.75 in Fig. 8.

At this juncture, we are trying to resolve the ~25% discrepancy between the MODTRAN® calculations and those reported previously. Atmospheric scatter is insignificant in this clear sky, i.e., particle free, simulation. In addition, the cold Saturn atmosphere has a very small thermal radiance at 2.9 μm. As a result, the radiance signal is simply the product of four terms:

- the top-of-atmosphere (TOA) solar irradiance (~0.33 W m^{-2} / μm),
- the cosine of the solar zenith (0.88 – 0.96),
- the surface reflectance (~0.42) over pi steradians, and
- the sun-to-surface-to-TOA transmittance

Between molecular absorption lines, e.g., at 2.8943 μm, the 0.004% spectral resolution L-shaped path transmittance approaches 0.9. Thus, this product is ~ 0.036 W m^{-2} sr^{-1} / μm, considerably more than the measured value of 0.028 W m^{-2} sr^{-1} / μm. We suspect that the discrepancy arises either from a calibration error or model input assumption. However, it is noted that MODTRAN® is capturing the primary spectral structure.

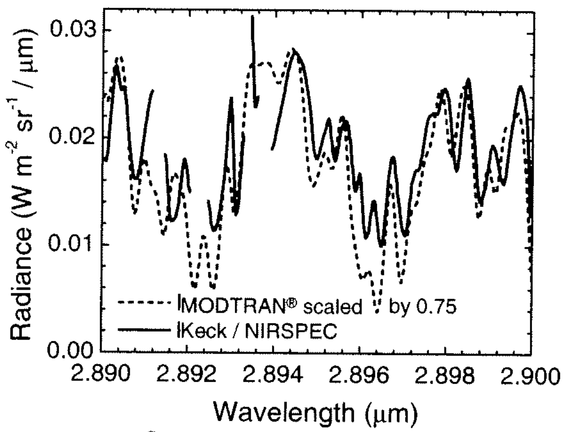

Fig. 8. Comparison of modified MODTRAN® calculations to high spectral resolution mid-wavelength IR data for Saturn [12]. The MODTRAN® results have been scaled by 0.75.

The final spectral comparison [14] covers the visible-near infrared spectral region and is shown in Fig. 9. For the MODTRAN® calculations, the integration over the whole disk was approximated by a 60° surface to sensor zenith angle, an air mass of 2. Multiple scattering was computed using 8-stream DISORT with MODTRAN®'s correlated-*k* method. All three cloud layers were defined according to [7] using their 1995 36°S characterization. At five spectral hinge points (467, 588, 673, 890 and 953 nm), the single scattering albedo for both the stratospheric and upper tropospheric cloud were lowered slightly (up to 1.2%) to match the continuum albedo levels. Although the CH_4 mixing ratio was set at 0.42%, the amount of methane absorption is clearly under-predicted. Since MODTRAN employs the short-wave absorption data from [14], the results indicate that the methane column has been under-estimated. This could result for one of two reasons. Either the 2 air mass approximation for the whole disk average is too low (the geometric includes long limb paths around the edges) or the cloud top heights are too high, which prematurely ends the effective methane path.

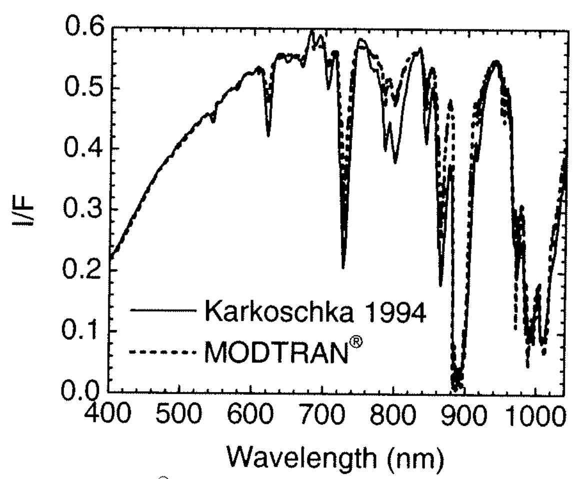

Fig. 9. Comparison of modified MODTRAN® calculations to observations of Saturn's geometric albedo over the visible-near IR wavelength region.

One last comparison was performed examining the longitudinal variation from 1999 HST measurements [7]. Fig. 10 shows the results for calculations at 36°S. There is essentially perfect agreement for two of the bands, and a few percent discrepancies for the other two bands. These results are extremely sensitive to the scattering phase function value at the solar scattering angle, which is near 175° for these calculation. It would not be surprising if these differences arose from short-wave Mie calculation inconsistencies between those used to define the stratospheric haze [7] and those performed by us to specify MODTRAN® inputs. It is also possible that the differences between scatter models (DISORT vs. doubling methods) and/or atmospheric layering produced the small residuals.

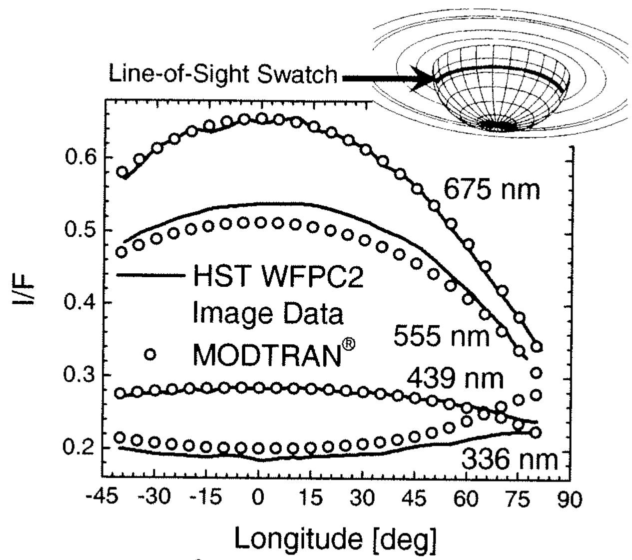

Fig. 10. Comparison of modified MODTRAN® calculations to observations of Saturn's longitudinal variations [7].

5. CONCLUSIONS AND FUTURE EFFORTS

The primary conclusions include:

- We are continuing development of a MODTRAN™5 prototype for application to planetary atmospheres.
- The initial data comparisons for Saturn, like those for Neptune, appear reasonable over a very broad wavelength regime.

Future efforts include:

- Adding more species and extending to higher temperature
- Improving the CH_4 spectral data base
- Including new cloud and haze models
- Adding generalized stellar source and geometry models
- Validating against other codes and more data (e.g., Jupiter, Titan,...)
- We anticipate releasing an initial prototype in late 2008.

6. ACKNOWLEDGEMENTS

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