Radiance computations for Planetary Atmospheres under Non-Equilibrium Conditions

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ABSTRACT

Atmospheric characterization through an analysis of remotely obtained spectral data requires rapid and robust radiation transport algorithms. This paper reviews the capabilities of SAMM2, a high-fidelity background radiance and transmission code. SAMM2 incorporates all of the major components necessary for background scene generation at all altitudes: climatology, solar irradiance, molecular chemical kinetics and molecular spectroscopic data. It is capable of accurately predicting atmospheric radiances and transmittances under both low-altitude local thermodynamic equilibrium conditions as well as upper-altitude non-equilibrium conditions. SAMM2 provides comprehensive coverage in the .4 to 40 micron (250 to 25,000 wavenumber) wavelength region for arbitrary lines-of-sight. The capabilities of SAMM2 are demonstrated by computing radiance and transmission values for the atmospheres of Mars and Titan.

1. INTRODUCTION

Characterization of planetary atmospheres generally involves the remote collection of spectral information followed by an inference of the combinations of constituents responsible for the observed spectra. The accuracy of the characterized atmosphere depends critically on the sophistication of the underlying radiation transport (RT) algorithm and atmospheric chemistry modeling and implies the need for high-fidelity models. Conversely, there currently exists a substantial collection of satellite programs actively accumulating new data regarding atmospheres of planets and satellites within the solar system. Given the limited resources available for processing this data, the speed of computation may become a critical issue under certain circumstances. These competing goals point to the need for an algorithm which allows a user-specified level of fidelity.

The U.S. Air Force funded several efforts to model radiance and transmission in the Earth's atmosphere. One of these codes is MODTRAN [1], which was developed by the U.S. Air Force to compute radiance and transmission in Earth's lower atmosphere. In this context, the lower atmosphere is defined as that in which molecular collisions comprise the dominant relaxation process and the distribution of energies of atmospheric molecules can be thought of as having a well-defined temperature. This is the local thermodynamic equilibrium (LTE) regime which, in the Earth's atmosphere, extends from the ground to no higher than 50km. For other planetary atmospheres, the extent of the LTE regime will be a function of its atmospheric density with this regime more localized for thin atmospheres such as Mars and extending higher for high-density atmospheres such as Neptune or Saturn's moon Titan. Separately, SHARC [2], the Strategic High-Fidelity Radiance code was developed by the U.S. Air Force to rapidly compute infrared radiance and transmission in Earth's upper atmosphere. In this context, the upper atmosphere is defined as that in which the dominant relaxation process is radiative emission. The lifetime of an internal excited state of a molecule is shorter than the collisional relaxation time in the non-LTE regime, which in the Earth's atmosphere extends as far down as 50km to the edge of the atmosphere.

This paper deals with the successor to SHARC. This code, referred to as SAMM2 [2] (SHARC and MODTRAN Merged, version 2), provides a seamless unification of the capabilities contained in both SHARC and MODTRAN. Specifically, it contains algorithms which have been designed to be applicable through both the LTE and non-LTE regimes. When appropriate, designs contained in either SHARC (aurora, chemical kinetics, climatology) or MODTRAN (aerosols, clouds, multiple scattering) were reused. When the existing designs could not span both LTE and non-LTE regimes, most notably the radiation transport (RT) models, new algorithms were constructed. SAMM2 has been designed to be easily extensible. It is this extensibility which allows SAMM2 to be used for analysis of planetary atmospheres other than the Earth.

2. MODEL DESCRIPTION

In the following section, we will outline the significant features of the SAMM2 radiance code. Additionally, we will specify the user inputs necessary to use SAMM2 for astronomical observations and use two target systems as concrete examples. The first system will be the Martian atmosphere [4]. This atmosphere is substantially thinner than the Earth and provides an excellent illustration of the important of including non-LTE physics. The second system will be Saturn's moon Titan [5] which has an atmosphere that is substantially colder and denser than the Earth. Taken together, these substantially differing atmospheres outline the utility of SAMM2 as a unified modeling tool for planetary atmospheric characterization and demonstrates the substantial operational range of this general-purpose code.

2.1 Climatology

The observed radiance will always be strongly dependent upon the details of the climate along the line-of-sight (LOS). The SAMM2 code makes no assumptions regarding planetary climate conditions and all appropriate details must be supplied by the user. SAMM2 obtains the user-specified description of the climatology through the input of atmospheric profiles. These altitude-dependent profiles provide temperature, pressure and molecular constituent details. At its simplest, a planet's climate can be described through the use of a single time-averaged atmospheric profile. Alternatively, a more detailed description can be constructed through the inclusion of multiple atmospheric profiles. Each profile would have a volumetric region of applicability in addition to necessary atmospheric information. In this way, a complex collection of local atmospheric conditions can be assembled into a consistent description of a planetary climate.

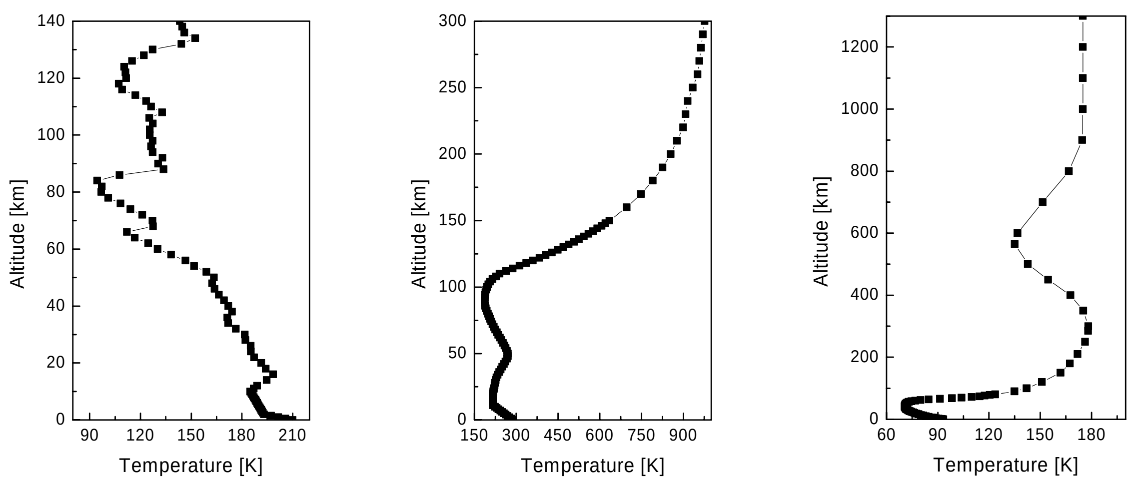

Fig. 1. Atmospheric temperature profiles of Mars (left), the Earth (center), and Titan (right).

These conditions must clearly be specific to the target planet of interest. To that end, SAMM2 often utilizes the SHARC/SAMM Atmospheric Generator (SAG) [6], a more sophisticated tool for automatically generating position-dependent atmospheric information for Earth modeling. An equivalent tool does not currently exist for other planetary atmospheres. However, the file format which SAG uses to communicate with SAMM2 is simple to create. Data output from planet-specific models such as NASA's Global Reference Atmospheric Models [7] can be fit into the SAG atmospheric format in a straight-forward manner. For the examples shown here, we have taken atmospheric profiles which are publicly available and transformed them into the SAMM2 atmospheric data format. We have used recent results from the Planetary Data Subsystem's (PDS) Mars Pathfinder mission data [8] to provide a description of the Mars atmosphere and we have used an engineering atmosphere model published by Yelle *et al.* [9] to provide a description of Titan's atmosphere. An illustration of the temperature profiles of these models is shown in Fig. 1 along with a temperature profile of the Earth obtained from the U.S. Standard Atmosphere. An illustration of the particle density profile for each atmosphere is shown in Fig. 2.

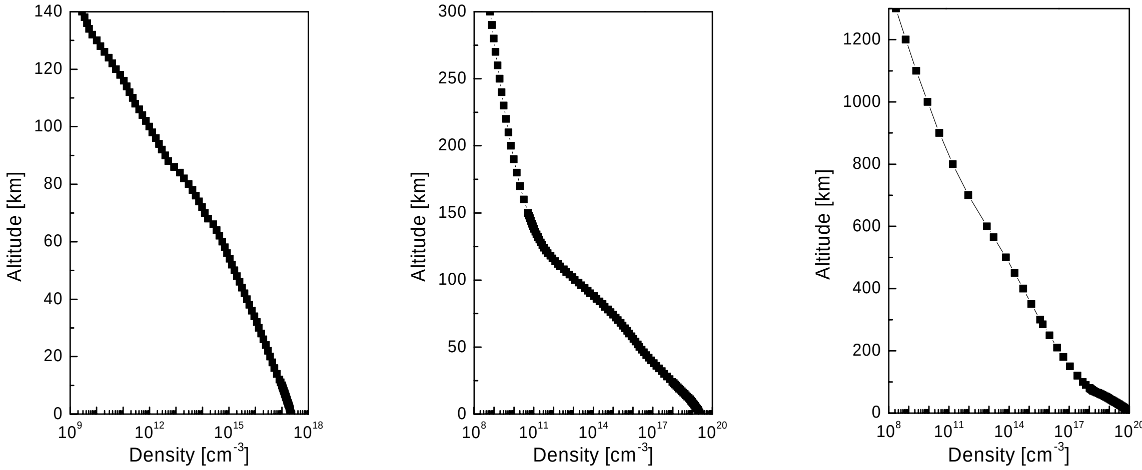

Fig. 2. Atmospheric molecular density profiles for Mars (left), the Earth (center), and Titan (right).

In addition to supplying atmospheric constituent profiles, local weather events can also be included in a SAMM2 calculation. Specifically, SAMM2 provides for the inclusion of both cloud and aerosol profiles of user-specified properties and extent. As with atmospheric constituent modeling, the available tools are most developed for modeling the Earth atmosphere. However, also as with atmospheric constituent modeling, the file format necessary to introduce weather processes such as cirrus-like clouds in the Martian atmosphere [10] or aerosol properties such as tholin near Titan's surface [11] are straight-forward. More complex would be the inclusion of exotic weather phenomena such as auroras [12] as seen on Earth or weather phenomena such as elves, sprites, and blue jets.

2.2 Chemistry

Once the planetary climate has been constructed, SAMM2 next determines the altitude-dependent excited state distribution of the internal states of all atmospheric radiators. This step marks the most significant algorithm enhancement as compared to traditional LTE computations. Specifically, under LTE conditions this step is unnecessary as the Maxwell-Boltzmann distribution defined by the local temperature determines the excited state population distribution. SAMM2 is a vibrationally non-LTE code and is applicable when a thermal distribution of excited states cannot be assumed. In these instances, the excited state molecular population distributions must be determined through chemical kinetics computations which includes upwelling and downwelling molecular radiance, collisional processes, and external photon sources (solar, lunar, and celestial). These computations presume molecular states are in rotational equilibrium while making no such assumptions regarding molecular vibrational and electronic excitations. The resultant steady-state populations of excited states will be used for radiance calculations.

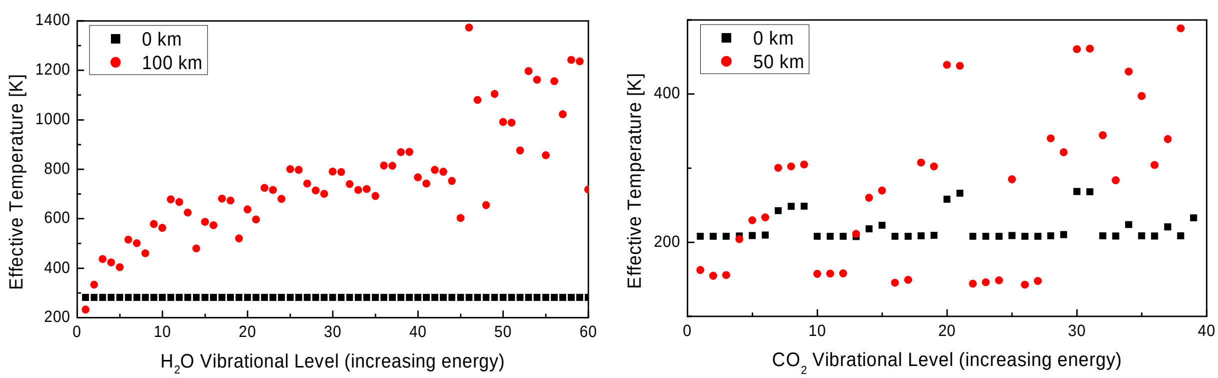

Fig. 3. Excited state population distributions of water for the Earth (left) atmosphere and carbon dioxide for the Martian (right) atmospheres.

An example of the results of several chemical kinetics computations are shown in Fig. 3. They illustrate the daytime distribution of effective vibrational temperatures relative to the ground state for a sequence of energetically increasing molecular bands at varying altitudes. This illustration shows both the flexibility of a fully vibrationally non-LTE chemical kinetics treatment as well as the necessity for such a model. At the lowest altitude in both atmospheres, shown as black data points in both plots, the effective vibrational temperatures are nearly constant and equal to the local temperature. Consequently, the excited state profile takes on the usual Planck Function distribution. This is precisely the behavior which would be expected and the same result would have been obtained under the LTE assumption. It is an important result because it shows that the non-LTE the approach taken in SAMM2 reduces to the expected LTE result under the appropriate atmospheric conditions. Consequently, SAMM2 can be used for pure LTE and pure non-LTE applications as well as applications which span both the LTE and non-LTE regimes.

At higher altitudes we see significant deviations from LTE behavior in Fig. 3. For these higher altitudes, shown as red data points in both plots, the effective vibrational temperatures of the internal states of the molecules deviate substantially from the local temperature. Recognizing that the molecular vibrational temperatures can no longer be set equal to the layer temperature, some models such as NEQAIR [13] have applied a two temperature approach. In this approach, an effective vibrational temperature distinct from the layer temperature is used to represent the vibrational temperature for all internal molecular states. Eventually, even this approximation will break down. At the highest altitudes, we find effective vibrational temperatures can vary substantially from one state to the next. The distributions shown by the red data points in Fig. 3 lie far outside the LTE limit and cannot be described by a single molecular vibrational temperature. We note this non-LTE behavior is a universal behavior of all atmospheres as a result of the lower atmospheric densities in the upper altitude with the altitude defining the onset of non-LTE conditions is a function of the density of the atmosphere in question and the details of the atmospheric chemistry.

Under most conditions, very little needs to be updated for accurate atmospheric chemistry modeling of planetary atmospheres. The primary constituents of both Mars and Titan atmospheres, the two example systems considered here, are also found in the Earth atmosphere. Consequently, the necessary atmospheric chemistry, namely reaction rate coefficients for rotational, vibrational and electronic transitions, is available for use with no further inputs from the user. In the upper ionosphere of Titan, more exotic hydrocarbons are formed [14], some of which are not usually found in any appreciable quantity in the Earth's atmosphere. To explicitly include them as non-LTE atmospheric species, it would be necessary to construct appropriate reaction chemistry profiles. This will generally not be the case and, instead, the user will only need to supply the appropriate celestial information. Specifically, the user will need to supply an irradiance profile for the dominant external photon sources. This will most likely be the sun, but can be lunar or planetary and celestial irradiance source at night time.

2.3 Geometry

Once an atmosphere is specified, SAMM2 is able to take a set of user-specified coordinates and compute the appropriate LOS for the specified path. This LOS computation takes into account the effects of refraction due to atmospheric constituents. The default geometry specifications within SAMM2 should be sufficient for all planetary atmospheres and only one modification will need to be made. SAMM2 requires a planetary radial model in order to accurately compute the LOS for a non-nadir viewing path.. This model may be as simple as defining the average radius of Mars or Titan in our example cases or it may be a more sophisticated model which specifies a latitude- and longitude-dependent planetary radius. For the example cases shown here, we will assume the equatorial radius of Mars is 3,402 km and the equatorial radius of Titan is 2,575 km.

2.4 Spectroscopy

Information related to atmospheric molecular spectroscopy is provided to SAMM2 through the use of the HITRAN database [15]. This actively maintained database has compiled decades of atmospheric spectral line information into a single reference source. It contains highly accurate measurements of molecular transition frequencies and their associated oscillator strengths. For cases in which spectroscopic data is unavailable or spectral lines are so closely packed that they cannot be individually resolved, molecular cross-section information is provided as a substitute. This database provides spectral information for the full range of atmospheric species which will be encountered both in the Earth atmosphere and within the example atmospheres of Mars and Titan. Additionally, the modifications necessary to transform standard HITRAN data into a form readily usable for non-LTE applications has been well documented [16]. These modifications have been directly incorporated into SAMM2 and will require no additional modifications to support additional planetary atmospheres.

At runtime this spectroscopic information, which is referenced to a standard temperature and pressure, is modified to take into account the details of the local atmospheric conditions. Specifically, modifications are needed to compensate for the finite temperatures and pressures of planetary atmospheres. The Voigt lineshape [17] is an appropriate form to take into account both temperature and pressure broadening under the assumption that the two quantities are independent variables. This line shape function at a frequency ν relative to a line center position ν_0 can formally be expressed as a convolution of the Doppler-broadened and pressure-broadened (Lorentz) line shapes:

$$f_{Voigt}(\nu - \nu_0) = \int f_{Lorentz}(\nu' - \nu_0) \cdot f_{Doppler}(\nu - \nu') \cdot d\nu'$$

2.5 Radiation Transport

The determination of radiance and transmission values for an arbitrary LOS through a planetary atmosphere is by far the most computationally intensive step in this model. The approach taken in SAMM2 is to provide the direct solution of the RT equations. As a result, no additional changes are required by the user for use with planetary atmospheres other than the Earth. SAMM2 provides multiple RT algorithms to choose from at runtime. These algorithms provide the user with the ability to specify the appropriate level of fidelity and speed of computation for a particular application. In order of decreasing fidelity, the first algorithm is a non-LTE line-by-line algorithm (QBL), the second is a non-LTE correlated-*k* algorithm and the third algorithm is a non-LTE band model.

These algorithms achieve part of their computational efficiency through separating line shape contributions into three distinct regions: (1) line centers, (2) line tails and (3) continuum contributions. Line center contributions are defined as the portion of all lines whose transition frequencies lie within a given spectral interval $\Delta\nu$. As line centers are the dominant source of observed radiance, they are treated with the highest level of accuracy within all algorithms. The treatment of line centers differs markedly between these algorithms and will be described later in this section. The second region, referred to as "line tail" contributions, represents the spectral absorption line contributions of lines whose centers are not located within the interval $\Delta\nu$. Line tails maintain a temperature and molecular density dependence, but are treated with a lower level of fidelity than line centers. Any non-LTE behavior of the line tails will be disregarded. This treatment provides for a substantial increase in computational speed for these RT algorithms and results in a relatively minor loss of accuracy. The third and final region is referred to as "continuum" contributions and represents any absorption features not accurately described by a line shape profile. These contributions usually arise from molecular collisions and are the least important. Continuum contributions will have most temperature-dependent behavior ignored.

The highest-accuracy model available to the user is the non-LTE line-by-line QBL model [3]. This algorithm computes radiance and transmission values at a native resolution of 0.001 cm^{-1} and the results can be down-sampled to a coarser spectral interval as specified by the user. In addition to the previously mentioned separation of spectral lines into line centers, line tails and continuum contribution, this algorithm makes use of two important techniques to increase computational efficiency. The first technique is to take each HITRAN spectral line and forces the line center position to appear precisely at a grid point. This small shift does not diminish the fidelity of the QBL algorithm. At its most extreme, this shift will move a spectral line ±0.0005 cm^{-1} from the line center position reported on the HITRAN database and is well within the measurement uncertainty of all but the most highly resolved spectral lines. This small spectral shift allows the second time-saving technique employed by the QBL algorithm. Namely, the explicit computation of the Voigt line shape profile at runtime is substituted by an off-line creation of a Voigt profile database. Runtime determination of the appropriate Voigt profile requires only a multi-dimensional interpolation over the appropriate line shape parameters. The extent of this database is large enough to encompass line shape profiles which will be encountered both within the Earth atmosphere and the atmospheres of Mars and Titan. No modifications to this database will be needed.

This line-by-line approach produces highly accurate results at the cost of longer computational times. For instances where the user is willing to trade line-by-line accuracy for a factor-of-100 speed increase, a non-LTE correlated-*k* algorithm is included in SAMM2. Correlated-*k* algorithms substitute the integration of absorption coefficients in frequency space with an equivalent integration in cumulative probability space [18]. There are two advantages to such an approach. The first advantage is that, in this space, the absorption coefficient becomes a slowly varying function cumulative probability, allowing for a significantly coarser integration step. The second advantage is that this transformation maintains spectral correlation between layers and the integration is effectively monochromatic. The type of correlated-*k* algorithm implemented in SAMM2 is related to concepts described by Goody *et al.* [19].

This approach substitutes the true cumulative probability space distribution with a statistical representation of the *k*-distribution. These statistical representations are computed off-line prior to computation for a range of Doppler and Lorentz widths and line densities and the resulting database of *k*-distributions is interpolated upon at runtime [20]. This correlated-*k* algorithm is able to make use of the same techniques for computing line tail and continuum contributions as the QBL algorithm, leaving the line center computations as the unique step in this algorithm.

A non-LTE band model will be available for instances where additional efficiency gains beyond the non-LTE correlated-*k* algorithm are needed. Like the QBL and non-LTE correlated-*k* algorithm, this model will separate each spectral line into a line center, line tail, and continuum contribution. The non-LTE band model will use the highly efficient line tail and continuum methods already outlined while line center contributions are treated substantially differently. Computations can no longer be considered monochromatic as radiance and transmission values for each band model interval, typically on the order of 1 cm^{-1}, is computed using a single set of values. Values in this interval are modeled as a distribution of two distinct collections of lines, each with their own average strength and line density. This two distribution method is better able to capture the non-LTE physics than a typical band model approach which constructs a single distribution based on all lines whose centers lie in a spectral interval. The resulting model is appreciably faster than the non-LTE correlated-*k* algorithm, but with this speed increase will come a reduction in the fidelity of the final radiance and transmission values.

Given the significant computational time involved in radiation transport step, efforts are currently underway to provide the user with additional runtime RT options. These algorithms would have full access to the results of the chemical kinetic computations performed in SAMM2 prior to the RT computation step. The inclusion of third-party RT algorithms could provide additional, and possibly faster, means to solve for non-LTE radiance and transmission.

3. RESULTS

We will examine the results of radiance and transmission calculations using various RT algorithms available in SAMM2. The first example will examine the Titan atmosphere. This atmosphere contains a thick aerosol layer which substantially diminishes visibility near the surface. The chosen 100km line-of-sight extended down to 200km above Titan's surface. This LOS avoids the naturally occurring opacity of Titan's surface. The transmission signal from this path is shown in Fig. 4. As expected, the transmission signal is dominated by the infrared methane bands in addition to the molecular nitrogen continuum feature. The RT algorithms within SAMM2 are in good agreement. As a comparison, an Earth atmosphere computation was performed considering only methane and nitrogen as atmospheric radiators. This 50km Earth path shows transmission loss due to the same methane bands. However, the overall transmission loss is substantially less, given the less dense atmosphere on Earth.

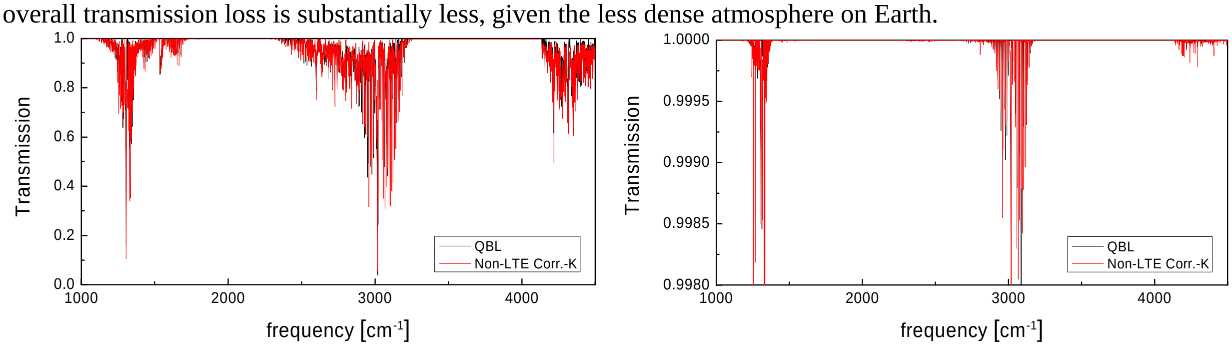

Fig. 4. Upper altitude transmission spectra of Titan using multiple RT algorithms (left) and an upper altitude transmission spectra of Earth using multiple RT algorithms and considering only methane and nitrogen (right).

The second example examines the Martian atmosphere. This atmosphere is substantially thinner than Titan and will not generate opaque infrared spectra. This daytime calculation consists of a down-looking path beginning at the top of the Martian atmosphere and extending to 10 km above the surface. We focus specifically on the radiance in the vicinity of the so-called 10 μm hot bands in the Martian atmosphere. Like the majority of the Martian spectrum, carbon dioxide is responsible for these two bands, centered at 960 cm^{-1} and 1063 cm^{-1}. In Fig. 5, an illustration of radiance in this region is shown with the results degraded to a 4 cm^{-1} resolution, a resolution finer than the Mars Thermal Emission Spectrometer native resolution [21]. This compares favorably to previously published results [22] showing the presence of these bands in the upper atmosphere.

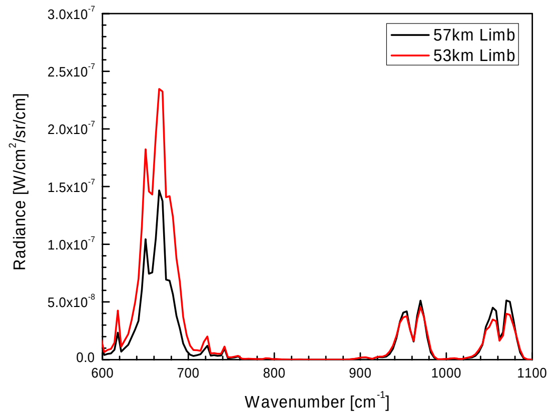

Fig. 5. Radiance for the Martian atmosphere in the vicinity of the 10μm hot bands.

4. CONCLUSIONS

We have provided an overview of SAMM2, a high-fidelity radiance code which operates at all altitudes. Though SAMM2 was originally created with Earth applications in mind, its modeling capabilities are robust and SAMM2 can be used for modeling other planetary atmospheres. We have demonstrated how SAMM2 can provide radiance calculations for planetary atmospheres using the proper combination of user inputs. These inputs fall into three categories:

- Climatology – The user must supply the appropriate atmospheric information, including temperatures and particle densities. Additionally, the user must provide weather information such as cloud and aerosol properties.
- Chemistry – The appropriate incident solar irradiance for the top of the atmosphere of the planet of interest must be provided.
- Geometry – An appropriate model of the planet radius must be supplied.

With these inputs, SAMM2 is capable of generating atmospheric radiance and transmission values for a range of planetary atmospheres as has been demonstrated with Mars and Saturn's moon Titan as examples.

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