BTRAM: An Interactive Atmospheric Radiative Transfer Model

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ABSTRACT

The Blue Sky Transmission and Radiance Atmospheric Model (BTRAM) was developed in an effort to create a radiative transfer model that was both fast and fully customisable by the user. A number of earlier radiative transfer models, such as FASCODE and MODTRAN, offer powerful simulation capabilities, but have interfaces that make it difficult to tailor the model to the specific needs of a user. BTRAM, developed in the Interactive Data Language (IDL®) [5], provides users with a straightforward interface that allows the efficient calculation of radiative transfer through custom atmospheric profiles or gas cells, from submillimetre to visible wavelengths, all at variable resolution. BTRAM also allows the user to convolve simulated spectra with custom instrumental line shapes, providing a more realistic simulation of instrumental performance.

This paper discusses the radiative transfer calculations used in the BTRAM code and presents applications of BTRAM simulated spectra from the far-infrared/submillimetre through to the visible spectral region.

Keywords: Radiative transfer, spectroscopy, infrared, submillimetre, visible

1 INTRODUCTION

An essential first step in the design of remote sensing instrumentation is to predict the spectral radiance incident on the spectrometer/radiometer. Computer simulations, known as radiative transfer models (RTMs), provide valuable information for both the prediction of instrument performance and the analysis of remote sensing data [12].

From an astronomical perspective, atmospheric water vapour is the principal source of opacity at submillimetre wavelengths where many objects emit most of their energy. Although high altitude observatories (such as the James Clerk Maxwell Telescope (JCMT) in Hawaii and the Atacama Large Millimeter Array (ALMA) in Chile) are located above most of the water vapour in the atmosphere, there still exists sufficient water vapour above them to render such observations difficult if not impossible. Moreover, since water vapour is not distributed uniformly through the atmosphere, but varies both spatially and temporally, interpretation of measurements becomes challenging.

To study the variations in atmospheric water vapour content, expressed in precipitable water vapour (PWV), we have developed an infrared radiometer (IRMA) [7], which measures atmospheric emission in the 20 μm spectral region, over a carefully selected band known to contain almost exclusively rotational transitions of water vapour. To convert atmospheric radiance measurements at 20 μm into PWV requires a flexible RTM capable of site-specific atmospheric modeling. Among the numerous RTMs currently used in the field, the Fast Atmospheric Signature Code (FASCODE) [2] developed by the United States Air Force in the 1970's, is one of the most widely employed. FASCODE is a complex RTM, written in Fortran, which allows users to simulate a wide range of observing geometries through any of the six atmospheric models (Tropical, Mid-latitude (Summer), Mid-latitude (Winter), Subarctic (Summer), Subarctic (Winter), and US Standard 1976) included with the code. The program also includes a module which allows users to simulate radiative transfer through an atmosphere containing a variety of aerosols. While FASCODE has found wide use in the community, it is a large, unwieldy program that lacks a simple user-interface. Due to its size, FASCODE is a difficult program to customise, as modifications may have unintended and potentially far-reaching effects. A serious limitation to FASCODE is that the included atmospheric profiles are of a

general nature and not site-specific. Since there is no simple way to alter these atmospheric profiles, users must laboriously create their own profiles as text files, to then be ingested by the main program.

The desire for a user-friendly RTM, that simplifies the inclusion of site-specific atmospheric profiles, and the requirement of compact code to allow for ease of maintenance and modification, provided the impetus for the development a new layer-by-layer, line-by-line RTM called BTRAM. This paper presents an overview of the algorithms used in the RTM to produce the spectra and illustrates the utility of BTRAM in three applications spanning far-infrared to visible wavelengths.

2 BTRAM BACKGROUND

2.1 Radiative Transfer

The transfer of energy in the form of electromagnetic radiation depends on the absorption, emission and scattering processes in the medium through which the radiation propagates. The equation of radiative transfer describes these interactions mathematically, and has broad application in subjects including electro-optics, material science, astrophysics, atmospheric science, and remote sensing. The equation describing the processes of transmission is known as the radiative transfer equation (RTE) and is given here [4]:

$$I(\sigma) = I_0(\sigma)\, e^{-\tau(\sigma)} + B(\sigma,T)(1 - e^{-\tau(\sigma)}), \qquad (1)$$

where $I_0(\sigma)$ is the spectral intensity of the radiation entering the propagating medium, σ is the opacity of the medium, and $B(\sigma,T)$ is the Planck blackbody equation at the temperature, T, of the medium. In Equation (1), $I_0(\sigma)\, e^{-\tau(\sigma)}$ describes the transmission of the input radiation through the medium and $B(\sigma,T)(1 - e^{-\tau(\sigma)})$ represents the emission of the medium. Analytic solutions to the RTE exist for simple cases, but for more realistic media numerical methods are required.

When performing radiative transfer calculations for atmospheric simulations, it is standard practice to approximate the atmosphere as a series of homogeneous, plane parallel layers. A simple, 3 layer atmosphere is illustrated in Figure 1. In this figure, an external astronomical source provides an initial spectral intensity that enters the top layer of the atmosphere. The radiative transfer equation in the top layer in Figure 1 gives the spectral intensity of the radiation exiting the top layer. This process is repeated for each subsequent layer until the intensity exiting the bottom of the atmosphere is calculated. This process illustrates the layer-by-layer nature of most atmospheric radiative transfer programs.

One of the main steps in the RTM computation involves calculating the spectral opacity, τ, of the layer at each frequency or wavelength. While this may be a complicated calculation if the layer parameters are allowed to vary, it reduces to a simple calculation if homogeneous layers are used:

$$\tau = k_\sigma\, n_{av}\, dz, \qquad (2)$$

where k_σ is the absorption coefficient at wavenumber σ, n_{av} is the average number density of the absorbing species in the layer, and dz is the thickness of the layer. We choose to express the frequency in wavenumber, the natural unit for a Fourier transform spectrometer. When only a single spectral line is present, the absorption coefficient, k_σ, is given by:

$$k_\sigma = S\, f(\sigma - \sigma_0), \qquad (3)$$

where $f(\sigma - \sigma_0)$ is a normalised line shape (Doppler, Lorentz, Voigt, etc.) and S is the line strength tabulated in molecular databases (e.g., HITRAN [9-11], GEISA, JPL). If more than one spectral line is present, the total absorption coefficient at a given frequency is simply the sum of the contributions made by each individual spectral line, i.e.:

$$k_{\sigma total} = \sum_{i=0} (k_{\sigma i}). \qquad (4)$$
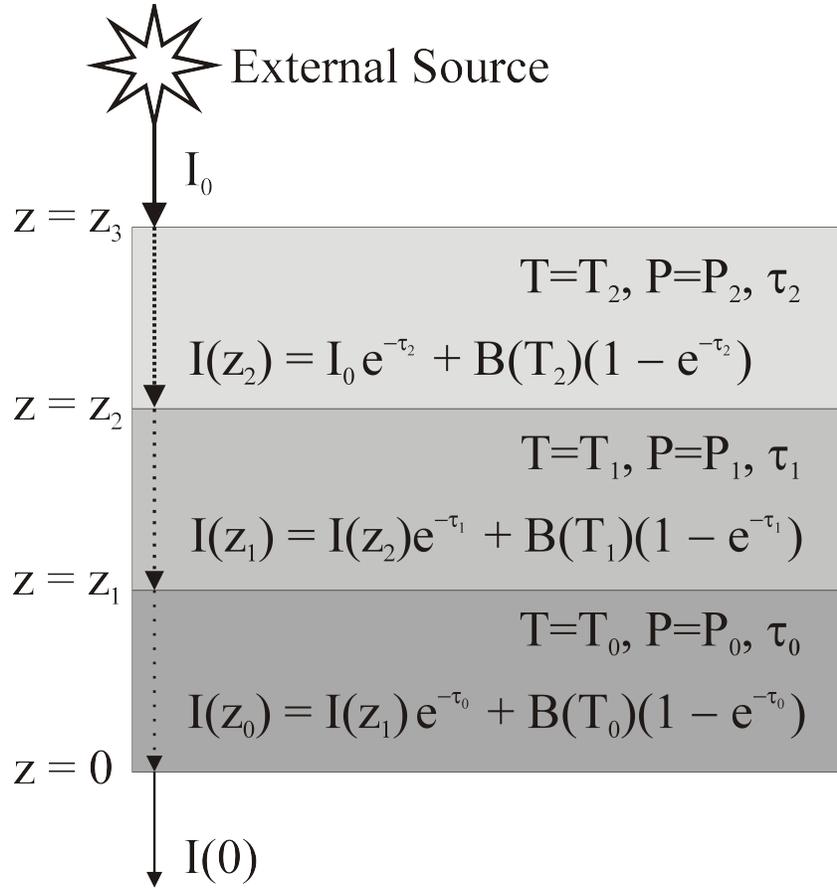
Figure 1. Radiative transfer through a three layer atmosphere showing how the spectral intensity exiting the bottom layer, $I(0)$, is related to the source intensity incident on the top layer, I_0. Each atmospheric layer is homogeneous in temperature, pressure, and molecular density.

BTRAM uses the 2008 version of the HITRAN database [9], the most recent update to the catalogue. Using the GUI, users can select up to 39 molecular species to include in gas-cell simulations. In basic atmospheric simulations, only the molecules which have well defined mixing ratio profiles in the FASCODE atmospheric models, and which contribute significantly to the opacity (H_2O, CO_2, O_3, N_2O, CO, CH_4, and O_2), are included. However, BTRAM has been designed so that the number of usable molecular species can be easily expanded to all 39 HITRAN species if the appropriate mixing ratio profiles are added to the atmospheric models.

Since the original impetus for developing BTRAM was to accurately model the opacity due to atmospheric water vapour from high altitude sites, it was important to account for the strong line wing effects known to occur with water vapour. BTRAM accounts for this increased wing opacity by using the treatment proposed by Clough et. al. [3], which employs an empirical analytical representation for the water vapour continuum.

2.2 Radiative Transfer Model Development

As mentioned earlier, the development of BTRAM was based on the desire to create an RTM that was more user-friendly, maintainable and customisable than FASCODE. The Interactive Data Language, IDL®, a fourth-generation computer language, was chosen as the platform for development since it offered several advantages over FORTRAN, notably: compact coding, simple syntax, advanced array calculation routines, and powerful data visualisation capabilities.

The main advantage of using IDL to code BTRAM was its ability to perform efficient array calculations. Since the spectral regions being modeled can potentially contain thousands of spectral lines, using program loops to calculate the cumulative contributions to opacity for each line, at each frequency, and in each layer can result in poor performance. Since IDL stores the spectral line information in a memory-mapped database, radiative transfer calculations are performed efficiently over these arrays of lines.

Since BTRAM was intended to model electromagnetic spectra originating in space and passing through the Earth's atmosphere, a design constraint limiting the observing geometries to "space-to-ground" and horizontal gas cells was introduced. The space-to-ground option allows a user to simulate observations through a column of atmosphere extending from space to the ground along any zenith angle. The atmosphere through which an observation is made is modeled as a number of separate layers, each internally homogeneous in terms of pressure, temperature, and molecular density with effective values determined from the parameters' values at the layer boundaries. The gas cell geometry is a single such layer, with pressure, temperature, molecular densities, and cell length as specified by the user.

User-friendliness was another goal considered in the development of BTRAM. IDL has extensive graphical user interface (GUI) features which provide the user with an intuitive way to interact with BTRAM. The GUI allows users to create model atmospheres and gas cells according to their own specifications. In addition, users can select one of the 6 atmospheric profiles used in FASCODE (Tropical, Mid-latitude (Summer), Mid-latitude (Winter), Subarctic (Summer), Subarctic (Winter), and US Standard 1976) as well as several custom profiles including Antarctica, Mauna Kea (Hawaii), Antofagasta (Chile) and Chajnantor (Chile).

Once the appropriate input parameters have been selected (e.g., base pressure and temperature, lapse rate, water vapour scale height, atmospheric profiles, etc.) BTRAM creates a multi-layer atmosphere model using an automatic layering function to generate layer boundaries between the user-specified minimum and maximum altitudes (layers are 0.25 km thick for altitudes from 0 to 4 km, 0.5 km thick for altitudes from 4 to 12 km, 2 km thick for altitudes from 12 to 30 km, and 4 km thick for altitudes from 30 km to 54 km). BTRAM approximates the atmosphere as a series of homogeneous layers whose characteristics are determined by averaging the atmospheric parameters calculated at each layer's upper and lower boundaries.

A laboratory gas cell is modeled by selecting individual gases at their desired partial pressures, and the temperature and length of the cell. The model includes a blackbody source placed at the entrance to the cell. Emission due to the cell contents alone can be simulated by setting the blackbody temperature to zero. An atmosphere-type gas cell can also be modeled using the input atmospheric parameters. In this case, the molecular distribution in the cell is determined from the molecular mixing ratios from any of the atmospheric model profiles described above.

The output from BTRAM takes the form of transmittance, emittance or opacity as a function of either frequency or wavelength. Once a spectrum has been generated it may be convolved with an instrumental line shape (e.g., triangle, Gaussian, and sinc) to produce a more realistic simulation of instrumental performance.

3 APPLICATIONS

BTRAM was initially developed to produce site-specific data in the far-infrared and submillimetre region of the electromagnetic spectrum. Over the last few years our group has been involved in a series of experiments to determine the amount of water vapour in the atmosphere using a wide range of instrumentation from high resolution optical spectrometers to infrared radiometers, covering 3 orders of magnitude in wavelength. The following sections illustrate the utility of BTRAM in three specific wavelength regimes.

3.1 Submillimetre

The submillimetre atmospheric transmission spectrum above Mauna Kea, Hawaii, has been measured at a resolution of 0.005 cm^{-1} with a Fourier transform spectrometer (FTS) at the James Clerk Maxwell Telescope using the Sun as a source [1]. Column abundances of O_2, H_2O and O_3 determined from these spectra are found to be in excellent agreement with independent measurements and have been used as inputs to BTRAM. Figures 2 and 3 compare the BTRAM simulated atmospheric transmission spectrum with that observed in the 350 μm band [6]. The O_3 line measurements in particular provide a useful means of measuring the spectroscopic performance of the FTS. The measured lines are symmetric with widths of 0.007 cm^{-1}, which confirms the instrumental spectral resolution of 0.005 cm^{-1}. Furthermore, the wavenumber accuracy, as determined from a statistical analysis of 52 O_3 lines, is 0.0002 cm^{-1} rms, over an order of magnitude better than the resolution.
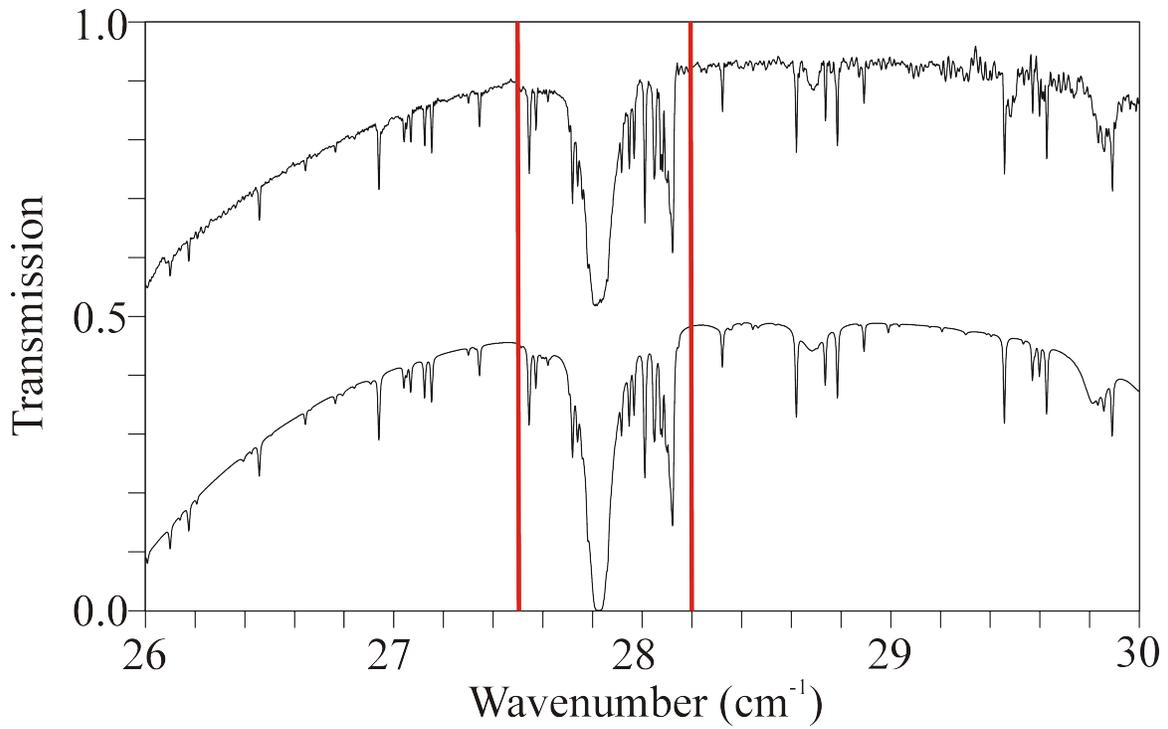
Figure 2. BTRAM atmospheric transmission spectrum (lower trace) computed for Mauna Kea, Hawaii, compared with measured atmospheric transmission spectrum (upper trace) offset by 0.5 for the 350 μm band. The data between the red bars is expanded in Figure 3, below.
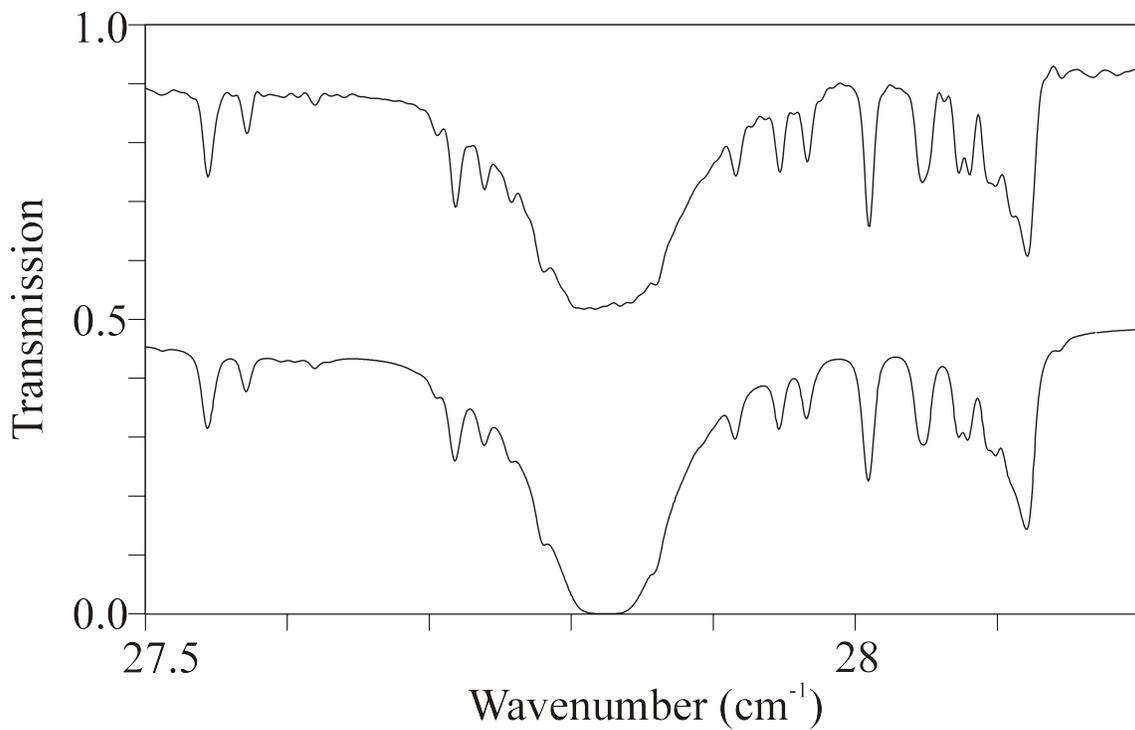
Figure 3. Expanded region of Figure 2 showing the detailed agreement in a complex part of the 350 μm band.
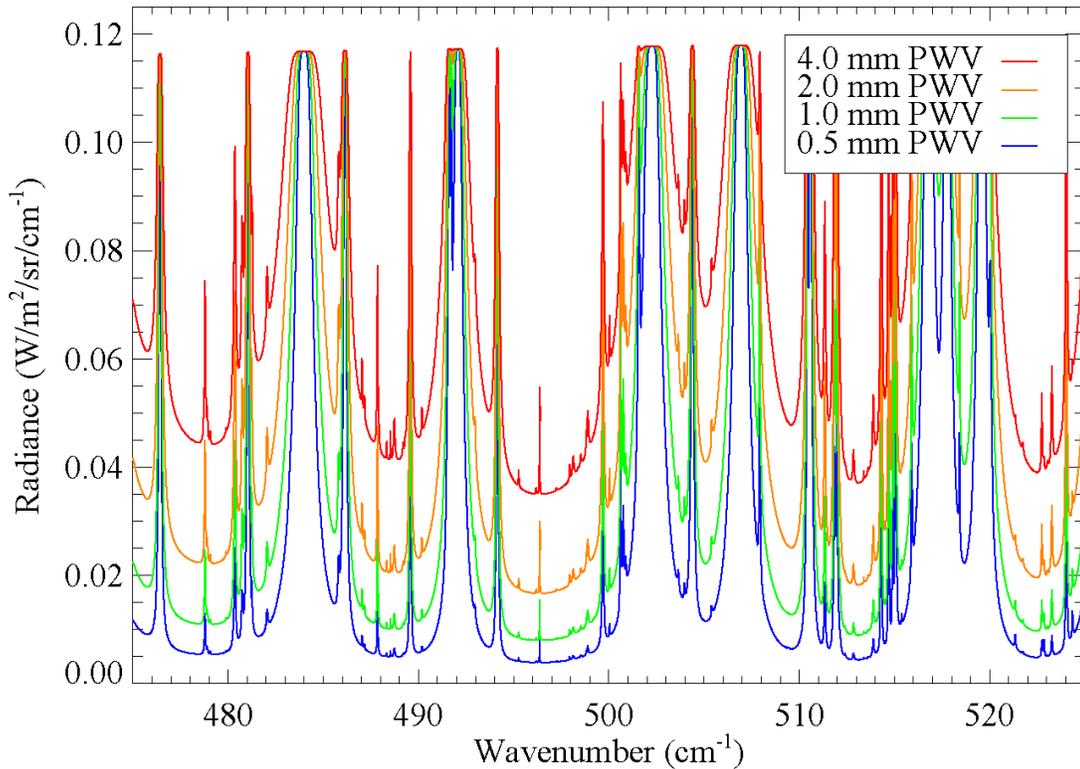
Figure 4. Atmospheric radiance above Mauna Kea, Hawaii as a function of PWV (0.5, 1, 2 and 4 mm) in the 20 μm spectral region used by the IRMA radiometer.

3.2 Mid-infrared

The Infrared Radiometer for Millimetre Astronomy (IRMA) is a device that has been developed by our group to produce accurate, real-time measurements of atmospheric PWV [7]. IRMA has several potential uses: as a monitor of phase distortion caused by atmospheric water vapour fluctuations along the line-of-sight of array antennae, as a site evaluation tool for the next generation of large telescopes, and for optimising the use of telescope time by providing real-time information on the atmospheric opacity. IRMA determines PWV amounts from measurements of atmospheric emission in a narrow spectral region around 20 μm, carefully selected to contain only rotational transitions of water vapour. Figure 4 shows the simulated BTRAM spectrum from Mauna Kea, Hawaii, for a range of PWV values from 0.5 mm, corresponding to excellent observing conditions, to 4 mm corresponding to poor conditions. By measuring the flux in this band with the sensitive radiometer the BTRAM model can be used to derive PWV amounts.

3.3 Near Infrared

BTRAM has been used to model the near infrared spectrum above the Chilean Andes to compare with spectra obtained from a number of high resolution echelle spectrometers. This work is in support of a series of site testing campaigns for the next generation of large telescopes. Figure 5 shows a small subset of normalised echelle order 50 data measured using MIKE, a high resolution echelle spectrometer mounted to the 6.5 m Clay telescope at Las Campanas Observatory in central Chile [8]. The target star for this calibration measurement was HR5174, a +5.15 apparent magnitude, 9800 K surface temperature, main sequence star used as a telluric standard star because it does not exhibit any photospheric spectral features. The MIKE measurement was taken at 2009-05-10T03:02:56, with an airmass of 1.009, and an exposure time of 33 seconds.
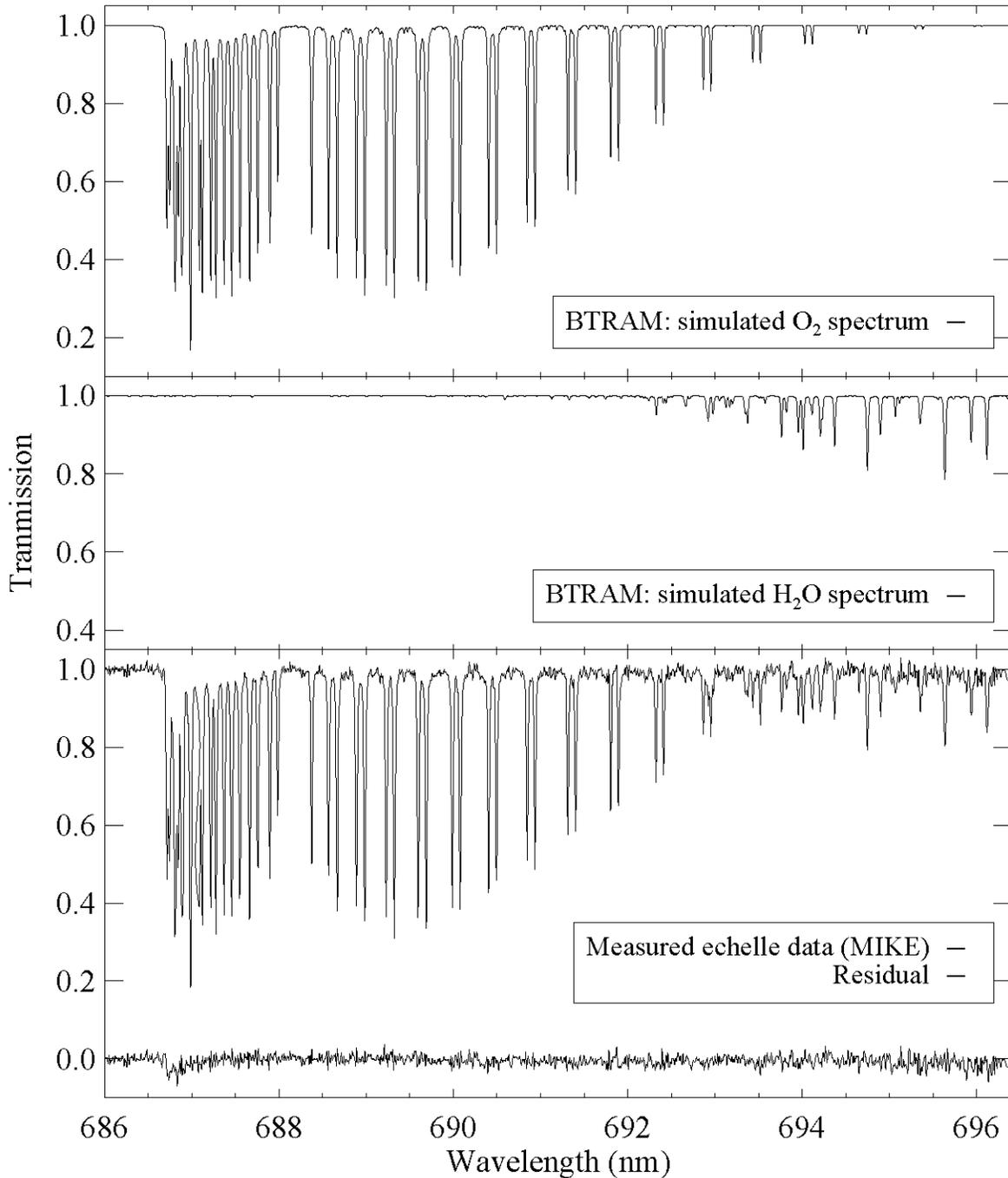
Figure 5. A simulation of the atmosphere above Las Campanas Observatory (LCO) was produced over the near infrared region using BTRAM. The top most trace is the simulated transmission for an atmosphere containing only Oxygen. The middle trace shows the same simulation for an atmosphere containing only water vapour. The water vapour abundance was set to 3.8 mm PWV, as determined for this time period by other means. The bottom plot shows normalised echelle data measured using the MIKE instrument, which is mounted to a 6.5 m telescope at LCO. The bottom plot also shows the residual when both the O_2 and H_2O traces are subtracted from the MIKE data. Apart from the region around 687 nm, where line blending begins to occur, the match between simulated spectra and measured spectra is quite remarkable.

The principal sources of opacity in this region are O_2 and H_2O, whose contributions are shown in the upper two panels. The lower panel shows the MIKE spectra together with the residual. The BTRAM simulated spectrum is seen to provide an excellent fit to the observed spectrum over a region containing a complex manifold of spectral features. Moreover, since the abundance and distribution of O_2 in the atmosphere is well known, it serves as an intrinsic calibration for the spectrum and thus the derivation of atmospheric water vapour content.

4 CONCLUSION

The paper describes the Blue Sky Transmission and Radiance Atmospheric Model (BTRAM), which was designed with the goal of creating a radiative transfer model that takes advantage of a modern programming language, is fully customisable by the user, and easy to extend and maintain. Although initially developed to model the atmosphere above Mauna Kea at submillimetre wavelengths, BTRAM has also proven to be extremely useful in modeling the atmosphere at mid- and near-infrared wavelengths. Three examples of the utility of BTRAM covering a wavelength range of three orders of magnitude, illustrating both atmospheric transmission and emittance are presented.

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