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1. INTRODUCTION

The launch of new satellite instruments such as the Atmospheric Infrared Sounder (AIRS) and the Infrared Atmospheric Sounding Interferometer (IASI) will allow the routine measurement of high spectral resolution thermal infrared radiances for the first time. With the high information content of these observations, increased accuracy in retrievals of important atmospheric properties such as temperature and humidity profiles becomes possible. However, a sophisticated understanding of the radiative transfer properties of the atmosphere is required for operational fast models, which are underpinned by a knowledge of the spectroscopic properties of atmospheric gas species.

The HITRAN database (Rothman et al., 1998) is widely used as a comprehensive source of fundamental parameters such as transition line strengths, positions and widths. The verification of databases against observational data is critical to establish their validity in radiative transfer applications, and so we have sought to quantify differences between HITRAN 96 and the most recent edition HITRAN 2000 (<http://www.hitran.com>) in the infrared region. The performance of each database can be judged by the success of line-by-line radiative transfer calculations in reproducing observed spectral radiances. For such comparisons to be meaningful it is essential that simultaneous measurements of radiances and atmospheric profiles of temperature and constituent gas concentrations are made. We have utilized data collected during the Measurement of Tropospheric Humidity (MOTH) campaign, using the extensive instrumentation installed on the Met Office C-130 aircraft. Infrared radiances were recorded with the Airborne Research Interferometer Evaluation System (ARIES), while aircraft atmospheric profiles were used as input

to the GENLN2 line-by-line radiative transfer code (Edwards, 1992).

Accurate simulations are also dependent on a sophisticated model of the water vapor continuum, which plays a significant role across the infrared spectrum. The CKD 2.4 continuum model as formulated by Clough et al. (1989) is widely used for this purpose. Comparisons between ARIES spectra and GENLN2 calculations allow the effectiveness of the continuum model to be judged.

2. AIRCRAFT MEASUREMENTS

The observations presented in this paper were made during the MOTH-Tropic campaign, which was based in the South Atlantic and occurred during April-May 1999. Two flights were made on predominantly clear-sky days flying over the ocean, A670 on 28 April and A676 on 6 May. During this period radiosondes were launched from Ascension Island (8° S, 14° W) to supplement the C-130 aircraft humidity profiles. The aircraft was equipped with a total water hygrometer (TWC) using absorption in the Lyman- α band, and a General Eastern dew point hygrometer which served to calibrate the TWC measurement. In addition, the Microwave Airborne Radiometer Scanning System (MARSS) recorded microwave brightness temperatures around 183 GHz, which were used to ensure the water vapor profile input to the GENLN2 model was representative of the atmospheric column. A full discussion of the methodology for determining humidity profiles for the MOTH campaign can be found in Taylor et al. (2002). Measurements of ozone and carbon monoxide mixing ratios were also made. The spectra were recorded at altitudes of 7-8 km (nadir views) or 35 m (zenith views). ARIES operated at a resolution of 0.482 cm⁻¹ over the spectral range 550-3000 cm⁻¹ (similar to IASI); details of the instrument specification and calibration are given in Wilson et al. (1999).

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3. RADIATIVE TRANSFER MODEL

The best representation of the atmospheric profile for each flight was translated onto a 98-level pressure grid for application in the GENLN2 radiative transfer code. In addition to the directly sampled atmospheric gases (H_2O , O_3 , CO), standard profiles of other radiatively active species were used. These were scaled where necessary by the most recent available (IPCC) data on atmospheric abundances. The line-by-line computations were performed at a spectral resolution of 0.01 cm^{-1} , and subsequently degraded to the ARIES resolution (accounting for the instrumental lineshape) to allow direct comparisons to be made.

GENLN2 calculations were carried out for both the HITRAN 96 and HITRAN 2000 databases, including spectral line parameters for the major gas species and infrared cross-sections for the heavier molecules. HITRAN 2000 was released in December 2000, with updates for individual molecules becoming available since then. The most important of these, in relation to this study, was the release of the update for water vapor line parameters in April 2001 which corrected some errors in the original database. The CKD 2.4 water vapor continuum was employed in all HITRAN model comparisons. The surface boundary condition for the model was established by retrieving simultaneously the sea-surface spectral emissivity and radiometric skin temperature (to within $\pm 0.1 \text{ K}$) with combined nadir and zenith ARIES views at low level above the ocean.

4. IMPACT OF HITRAN UPDATES

Since the atmospheric column and/or surface temperature viewed by ARIES may change somewhat over a 10 minute aircraft run, the spectra presented here consist of single 5 s views of approximately 500 m travel distance. Figure 1 (a) shows an ARIES upwelling brightness temperature spectrum recorded during the A670 flight, concentrating on the window region. The majority of the atmospheric absorption here comes from water vapor, both from weak individual spectral lines and the broad continuum absorption. The infrared ozone band is visible around 1050 cm^{-1} , and a number of minor gases, mainly halocarbon compounds, also need to be included in the simulations for good agreement with the observed spectra. Figures 1 (b) and (c) show the observed

(ARIES) minus calculated (GENLN2) brightness temperature residuals using the HITRAN 96 and HITRAN 2000 databases respectively. It is readily apparent that many of the residual errors present when including HITRAN 96 parameters in the GENLN2 calculation disappear when HITRAN 2000 is used instead. There appears to be insufficient ozone in the model profile wholly to account for the observed reduction in brightness temperature due to this gas; investigations into the accuracy of the MOTH ozone retrievals are continuing. The magnitude of residuals between 1100 and 1200 cm^{-1} has not been greatly improved by inclusion of HITRAN 2000 water vapor line parameters in the model. Tests show that these residuals cannot be removed by any reasonable variation in the water vapor profile, i.e. the increase in mixing ratio required is greater than the humidity measurement uncertainty (Taylor et al., 2002).

Values of average residual error (bias) and root-mean-squared (rms) deviation over the

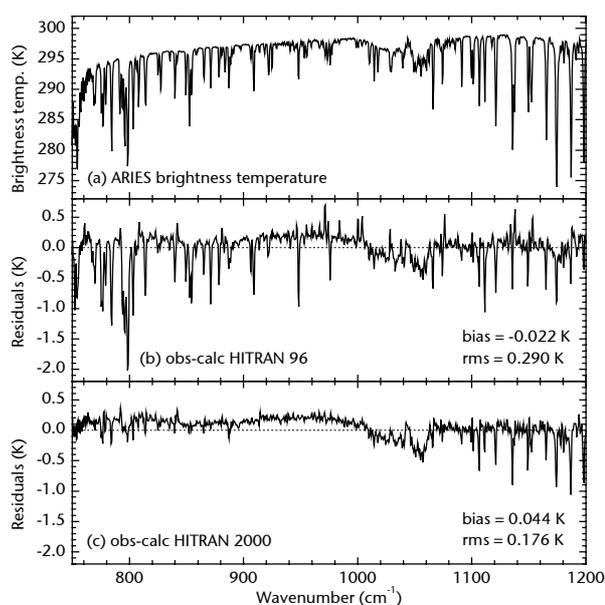


Figure 1. Comparison of observed ARIES spectrum and GENLN2 calculations over the range $750\text{--}1200 \text{ cm}^{-1}$ for MOTH flight A670: (a) ARIES radiance spectrum; (b) ARIES spectrum converted to brightness temperature; (c) observed minus calculated residuals with GENLN2 simulation incorporating HITRAN 96; (d) residuals with HITRAN 2000 parameters used in the simulation. Values of bias and rms in the lower panels denote the average residuals and root-mean-squared deviation of the residuals respectively.

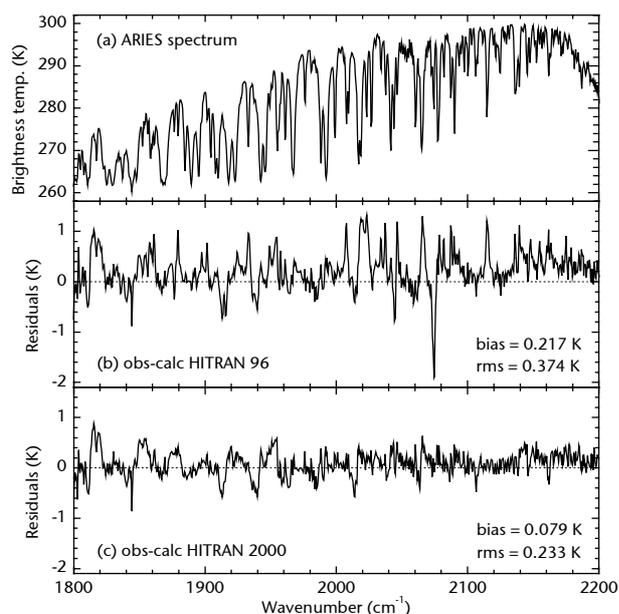


Figure 2. Comparison of observed ARIES spectrum and GENLN2 calculations over the range 1800-2200 cm^{-1} for MOth flight A670: (a) ARIES brightness temperature spectrum; (b) observed minus calculated residuals with GENLN2 simulation incorporating HITRAN 96; (c) residuals with HITRAN 2000 parameters used in the simulation. Values of bias and rms in the lower panels denote the average residuals and root-mean-squared deviation of the residuals respectively.

window region are included in Figure 1 for the HITRAN 96 and 2000 simulations. Since the radiance in this spectral region is greatly affected by the surface emission, variations in surface temperature will directly affect the bias values, and so this measure of the error should be treated with caution. A further consideration is the accuracy of the water vapor continuum, for which the CKD 2.4 formulation has been adopted here (see next section).

Figure 2 illustrates the effect of HITRAN updates on the 1800-2200 cm^{-1} region. The reduction in rms residual error by more than a third demonstrates the impact of revised data in HITRAN 2000. The intrinsic noise level of ARIES spectra is given by the noise equivalent brightness temperature ($\text{NE}\Delta T$) (Wilson et al., 1999). While some residuals in Figure 2 can be explained by instrument noise, others, for instance in the range 1100-1200 cm^{-1} in Figure 1, are larger than $\text{NE}\Delta T$ and therefore are likely to be caused by modeling errors. A more complete discussion of the impact of HITRAN

updates in the infrared, and further results, can be found in Newman and Taylor (2002).

5. WATER VAPOR CONTINUUM

Whereas the ARIES observations of upwelling radiation are a good proxy for IASI-like data, modeling downwelling radiances is a more rigorous test of the continuum absorption due to the strong signal against a cold background. We have analyzed ARIES zenith views recorded at low level to test the effectiveness of the CKD 2.4 continuum in the GENLN2 simulations. Figure 3 (top panel) shows an ARIES spectrum recorded during the A670 flight. The lower panel in Figure 3 (dotted line) illustrates that using the CKD 2.4 continuum model in the simulation results in significant (up to 3 K) residual errors. We have modified the continuum in the "microwindows" between the sharp lines to obtain agreement between observed and calculated spectra.

Figure 4 plots the self-broadening continuum coefficient for water vapor over the infrared window region (foreign broadening is negligible) for CKD 2.4 (solid line) and our modified continuum (dashed line). We have interpolated

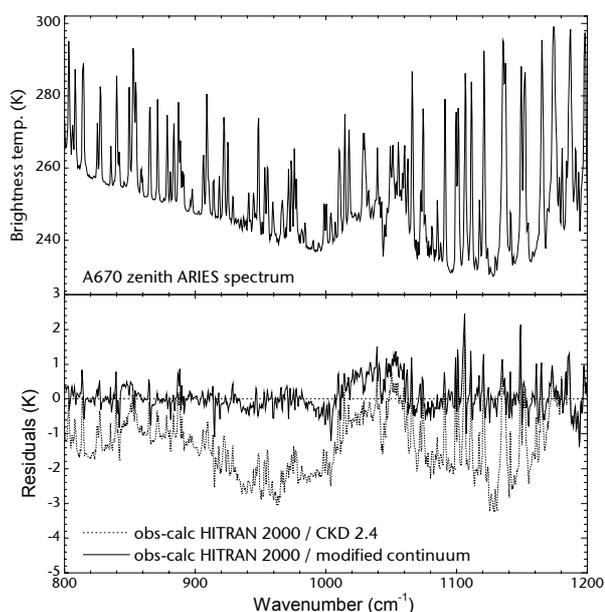


Figure 3. Comparison of observed ARIES zenith spectrum and GENLN2 calculations over the range 800-1200 cm^{-1} for MOth flight A670: (top panel) ARIES brightness temperature spectrum; (lower panel) observed minus calculated residuals with GENLN2 simulation incorporating CKD 2.4 water vapor continuum (dotted line) and modified continuum (solid line).

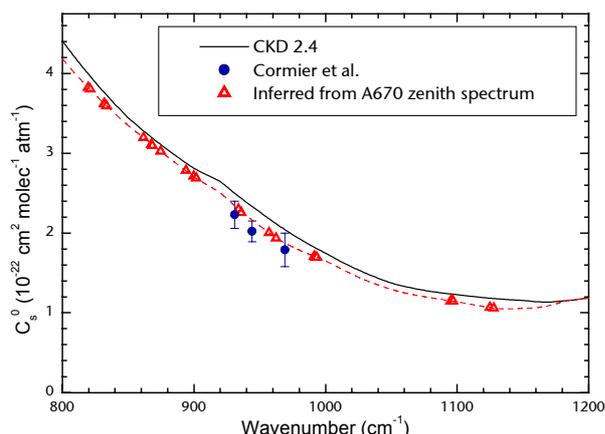


Figure 4. Comparison of the self-broadening continuum coefficient over the infrared window region from the CKD 2.4 model (solid line), laboratory data (circles with error bars) and retrieved from A670 ARIES/GENLN2 fits (triangles joined by dashed line).

the new continuum in regions of significant absorption, e.g. the ozone band around 1050 cm^{-1} . Also plotted in Figure 4 (symbols with error bars) are the results of a recent laboratory study (Cormier et al., 2002) using a laser absorption technique at three frequencies. Although the continuum coefficients Cormier et al. propose are lower than in this work, the uncertainty in the measurements makes these results entirely consistent with ours.

The lower panel in Figure 3 (solid line) shows the effect of the new continuum which, as expected, yields much improved agreement with the observations. A uniform reduction in the H_2O profile by 3-5% will also improve the residuals, but errors elsewhere (e.g. in the 5 μm region) are made worse by this alteration. Hence we believe the window region residuals are mostly due to the continuum model and not caused by an uncertain water vapor profile. In addition we have tested the new continuum against data recorded on a separate MOTH flight, A676, as an independent case study: here too the modified continuum is in much better agreement with ARIES spectra.

6. CONCLUSIONS

The new spectroscopy included in the HITRAN 2000 database is a significant improvement over previous versions of the database such as HITRAN 96, and is recommended for radiative transfer applications

in the infrared region, especially at high resolution. Operational weather center retrievals of temperature and humidity profiles, using radiances from new satellite instruments such as AIRS and IASI, will be more accurate as a result of the new data. There is evidence from ARIES observations that the CKD 2.4 model overestimates the water vapor continuum in the 800-1200 cm^{-1} window region, a result that is corroborated by laboratory measurements. Further work needs to be done on identifying any changes to the temperature dependence of the continuum in the infrared, which will require observations at higher latitudes.

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