Airborne and satellite remote sensing of the mid-infrared water vapour continuum

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Remote sensing of the atmosphere from space plays an increasingly important role in weather forecasting. Exploiting observations from the latest generation of weather satellites relies on an accurate knowledge of fundamental spectroscopy, including the water vapour continuum absorption. Field campaigns involving the Facility for Airborne Atmospheric Measurements research aircraft have collected a comprehensive dataset, comprising remotely sensed infrared radiance observations collocated with accurate measurements of the temperature and humidity structure of the atmosphere. These field measurements have been used to validate the strength of the infrared water vapour continuum in comparison with the latest laboratory measurements. The recent substantial changes to self-continuum coefficients in the widely used MT_CKD (Mlawer–Tobin–Clough–Kneizys–Davies) model between 2400 and 3200 cm\(^{-1}\) are shown to be appropriate and in agreement with field measurements. Results for the foreign continuum in the 1300–2000 cm\(^{-1}\) band suggest a weak temperature dependence that is not currently included in atmospheric models. A one-dimensional variational retrieval experiment is performed that shows a small positive benefit from using new laboratory-derived continuum coefficients for humidity retrievals.

**Keywords:** remote sensing; water vapour continuum; airborne measurements; satellite observations

1. Introduction

Water vapour absorbs over a very large range of wavelengths, from the microwave to the ultraviolet parts of the electromagnetic (EM) spectrum. It plays a major role in the Earth’s radiation balance [1], contributing both in the thermal infrared

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One contribution of 17 to a Theo Murphy Meeting Issue ‘Water in the gas phase’.
(supplying as much as 60% of the total clear sky longwave radiative forcing) and being responsible for approximately 55 per cent of atmospheric solar absorption. The basic spectrum of water vapour is well known and studied, based on numerous laboratory measurements in the scientific literature and compiled in line lists such as HITRAN [2]. However, in addition to the spectrum of atmospheric water lines, there is also an underlying, less structured absorption known as the water vapour continuum. This continuum is relatively poorly characterized, and a full understanding of its fundamental mechanism is still lacking [3].

The Clough–Kneizys–Davies (CKD) semi-empirical model of the continuum [4], more recently Mlawer–Tobin_CKD (MT_CKD) [5], has been used successfully for many years in atmospheric radiative transfer codes, and is capable of reproducing many of the observed water vapour features in the mid-infrared spectral region. Radiative closure studies such as those by Turner et al. [6] and Delamere et al. [7] have constrained the MT_CKD continuum model to improve the parametrization in some spectral intervals, leading to a demonstrable improvement in the ability to simulate the terrestrial infrared spectrum.

This is not to say that MT_CKD is capable of reproducing all observable spectral behaviour, however. For example, the temperature dependence of the continuum has been found not to be well captured when compared with recent laboratory data [8,9]. MT_CKD also appears to underestimate the strength of the continuum in some high-transmittance atmospheric windows by as much as an order of magnitude [10]. A unifying theory of the continuum is still lacking, with competing formulations based on the far wings of water lines [11] and on the existence of bimolecular complexes known as dimers [3]. A revived interest in dimers has seen some recent papers [12] suggesting an important role for dimers in contributing to atmospheric absorption optical depths.

An improved knowledge of water vapour spectroscopy, including the water vapour continuum, is of importance for optimal assimilation of satellite radiances from hyperspectral instruments such as the infrared atmospheric sounding interferometer (IASI) in numerical weather prediction (NWP). Increasingly, water vapour channels from sounders such as IASI are being used in NWP for one-dimensional variational retrievals of atmospheric water vapour, and errors in the underlying radiative transfer model will degrade the ability to retrieve humidity accurately. Water vapour channels with high-peaking Jacobians, or weighting functions, are of interest in acting as ‘anchoring’ channels for upper troposphere–lower stratosphere humidity, where the current generation of NWP models shows relatively large humidity biases [13].

The Continuum Absorption at Visible and Infrared Wavelengths and its Atmospheric Relevance (CAVIAR) NERC/EPSRC-funded consortium brings together expertise in atmospheric remote sensing, laboratory measurements and quantum mechanical modelling. The Universities of Reading, Leicester and Cambridge, University College London and Imperial College London, together with the Rutherford Appleton Laboratory (RAL), National Physical Laboratory (NPL) and the Met Office, have coordinated research into the causes and magnitude of the water vapour continuum across the EM spectrum. This study reports on investigations into the mid-infrared continuum based on aircraft and

1NERC is the Natural Environment Research Council, EPSRC is the Engineering and Physical Sciences Research Council, both UK funding agencies.
Table 1. CAVIAR airborne interferometers. Specifications for the two interferometers deployed on the FAAM BAe 146-301 research aircraft during the CAVIAR field campaigns.

<table>
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<tr>
<th>interferometer</th>
<th>operating institution</th>
<th>spectral range</th>
<th>spectral resolution (cm(^{-1}))</th>
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<td>Met Office</td>
<td>550–3000 cm(^{-1}) in two bands</td>
<td>1.0</td>
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<tr>
<td>tropospheric airborne Fourier transform spectrometer (TAFTS)</td>
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<td>80–800 cm(^{-1}) in two bands</td>
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satellite radiance measurements from the dedicated field campaigns described in §2. The data analysis methodology is outlined in §3, with derived continuum coefficients presented in §4 for the mid-infrared band (near 1600 cm\(^{-1}\)) and near-infrared window (near 2500 cm\(^{-1}\)). We test the impact of differing formulations of the water vapour continuum on one-dimensional variational retrievals in §5 and summarize in §6.

2. Field measurements

(a) Laboratory characterization with a traceable calibration target

The specifications for the two interferometers flown on the Facility for Airborne Atmospheric Measurements (FAAM) Bae 146-301 research aircraft are supplied in table 1. Research results from the tropospheric airborne Fourier transform spectrometer (TAFTS) instrument are presented by Green et al. [14]. An important work programme of the CAVIAR consortium was the pre-campaign laboratory characterization of both instruments using a low-temperature blackbody target designed at NPL. Importantly, the accuracy of the NPL target was assured through a traceable measurement chain to an absolute calibration standard.

Laboratory calibrations for ARIES were performed with NPL target temperatures in the range \(-75^\circ\text{C}\) to \(+30^\circ\text{C}\) (198–303 K). Figure 1 shows the level of agreement of ARIES measurements with the NPL-traceable target, which by design exhibits a high emissivity across the mid-infrared region of 0.9975. The ARIES signal-to-noise is highest in the spectral range shown here (600–1400 cm\(^{-1}\)). Some systematic biases compared with the NPL target are seen; we need to ensure that these biases are small compared with the spectral signature of the continuum that we aim to measure.

Observed biases relative to modelled NPL target radiances are shown in figure 2 for the full ARIES spectral range. For a target temperature of 288 K, the biases largely fall within \(\pm 0.3\text{K}\) across the spectrum, as shown by the equivalent radiance uncertainty at this temperature. The maximum bias increases for lower target temperatures, and exceeds 2 K for some wavenumbers at 213 K. These wavenumbers correspond to the overlap region of the two ARIES detectors near
mean NPL target temperature = 288.18 K

mean NPL target temperature = 242.95 K

mean NPL target temperature = 213.32 K

Figure 1. Airborne research interferometer evaluation system (ARIES) radiance measurements, spanning the 600–1400 cm\(^{-1}\) spectral range, compared with National Physical Laboratory (NPL) blackbody apparent temperature based on a modelled target emissivity of 0.9975. Three NPL target temperatures are shown, with a vertical scale spanning 2 K in each case. Data are taken from a composite set of repeated measurements from the laboratory experiments in 2009. (Online version in colour.)

1700–1750 cm\(^{-1}\). We account for this scene brightness-dependent uncertainty in the data analysis that follows. Importantly, for the atmospheric measurements discussed in this paper, the scene brightness temperature generally exceeds 230 K, for which we expect calibration errors not to exceed 1 K based on the NPL calibration results except at the extreme edges of the ARIES spectral response.

\textit{(b) CAVIAR campaigns}

Two field campaigns have been completed as follows:

2. Jungfraujoch, Switzerland, July–August 2009. High-altitude observations, designed to probe cold, dry atmospheric conditions above the bulk of the lower tropospheric water vapour absorption. Ground-based measurements were made from the High Altitude Research Station (7\(^{\circ}\)59\('\) E, 46\(^{\circ}\)33\('\) N, 3450 m a.s.l.).
Remote sensing of the \( \text{H}_2\text{O} \) continuum

Figure 2. Airborne research interferometer evaluation system (ARIES)-measured radiances, spanning the full instrument spectral range, compared with NPL blackbody target at three temperatures. The dataset is the same as displayed in figure 1. (a) ARIES measurements overlaid with calculated radiances based on a modelled target emissivity of 0.9975. (b) The observed–calculated bias for each target temperature. The radiance uncertainty based on a representative temperature bias is shown as the dashed line for each case, see figure for values. (Online version in colour.)

The instrumentation deployed allowed the simultaneous measurement of key atmospheric state variables (particularly temperature and humidity) with radiometric observations. The key measurements were

— Atmospheric profiling using FAAM aircraft \textit{in situ} probes, including Rosemount temperature sensors, a chilled mirror hygrometer and optical fluorescence water vapour sensor.
— Frequent dropsonde releases (with parachute-borne sensors measuring temperature and humidity) to map spatial and temporal variability.
— Associated radiosonde launches from nearby locations.
— Mid-infrared (ARIES) and far-infrared (TAFTS) radiances, both upwelling and downwelling, recorded from the FAAM aircraft.
— Ground-based solar tracking measurements of optical depth using NPL’s high spectral resolution interferometer, spanning the infrared to visible spectral regions [15].
— Coincident IASI mid-infrared radiances from MetOp satellite overpasses.
During the Camborne campaign, three FAAM flights were achieved in the desired conditions (cloud-free at all altitudes for an extended period of time). One flight in particular, on 18 September 2008, coincided with particularly good clear sky conditions, with a stable humidity structure as evidenced by four radiosonde balloons launched during that day. Figure 3 compares FAAM *in situ* relative humidity with a radiosonde profile where the aircraft tracked the balloon in a spiral ascent. The FAAM aircraft also released dropsondes at the top of the profile. Elevated levels of humidity can be seen between 200 and 450 hPa, with a relatively dry layer below that and then a moist boundary layer near the surface. The discrepancies between the various measurements are limited to within ±10% relative humidity for much of the profile, with slightly higher departures at higher levels. Overall, the level of agreement in figure 3 gives confidence in the absolute accuracy of the humidity data.

Nine FAAM sorties were flown during the second campaign in Switzerland. These flights provided a larger set of clear sky measurements from which to investigate the strength of the infrared water vapour continuum.

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Figure 3. Comparison of relative humidity (RH) profiles recorded with Facility for Airborne Atmospheric Measurements (FAAM) chilled mirror hygrometer, FAAM dropsondes and a radiosonde balloon launched from the Met Office station in Camborne on 18 September 2008. The aircraft tracked the balloon as it ascended. (a) RH with respect to water, with the dotted line indicating where ice saturation will occur. (b) Differences of the other measurements relative to the radiosonde. (Online version in colour.)
3. Methodology

Studies at the Met Office have focused on retrieving continuum cross sections using ARIES and IASI radiances together with simulations, for which we use the line-by-line radiative transfer model (LBLRTM; [5]) v. 11.7. LBLRTM takes as input vertical profiles of temperature, mixing ratios of water vapour, ozone and carbon monoxide, and surface parameters (skin temperature and emissivity) which we base on FAAM BAe 146 in situ, dropsonde and remote sensing measurements. Other trace gases of importance for infrared radiative transfer have mixing ratios defined by climatology. The model radiances are convolved with the instrument response function of ARIES or IASI to facilitate a direct comparison. The strength of self- and foreign-broadened continua has been varied in the LBLRTM code to derive new estimates for the continuum coefficients.

The retrieval of continuum strengths is acutely sensitive to the assumed atmospheric profile of humidity, which necessitates accurate measurements of water vapour in the field. Substantial efforts were made during the campaigns to assemble as comprehensive a dataset of humidity profiles as possible, with separate measures of water vapour concentrations from aircraft probes in addition to dropsondes and radiosondes. Nevertheless, even relatively small uncertainties in the absolute water vapour mixing ratio, of the order of 5–10%, are problematic in the data analysis.

In order to minimize the effects of profile uncertainties, a one-dimensional variational approach has been taken in the ARIES and IASI data analysis, whereby the selective use of channels sensitive to CO₂ and H₂O has been employed to retrieve an improved profile of temperature and humidity for each case. It is important to avoid using channels sensitive to the water vapour continuum in the retrievals when it is the continuum itself that is the subject of the investigations (with generally unknown uncertainty in strength). Therefore, only channels with very weak continuum contributions have been used for this initial stage. We apply a maximum threshold of 10 per cent contribution by the (MT_CKD) continuum to the optical depth owing to water vapour in any channel used for atmospheric retrieval.

As commonly used in one-dimensional variational retrievals, we can define a cost function $J$ which we seek to minimize,

$$J(x) = (x - x_a)^T S_a^{-1} (x - x_a) + [y - F(x)]^T S_e^{-1} [y - F(x)],$$

where $x$ is the state vector including vertical profiles of temperature and humidity, $x_a$ is the a priori (first guess, or background) state vector, $y$ represents the observed radiances, $F$ is the forward model (LBLRTM), and $S_a$ and $S_e$ are the error covariance matrices of the a priori state and the observed radiances, respectively.

The one-dimensional variational retrieval, as detailed in Rodgers [16], performs the iteration

$$x_{i+1} = x_a + (K_i^T S_e^{-1} K_i + S_a^{-1})^{-1} K_i^T S_e^{-1} [y - F(x_i) + K_i (x_i - x_a)],$$

where $x_{i+1}$ is the retrieved state vector following iteration $i$ and $K$ is the Jacobian representing the derivative of forward-modelled radiances with respect to the state vector. The effectiveness of the retrieval depends, crucially, on accurately
specifying the error characteristics in the matrices $S_a$ and $S_b$. In particular, the use of a globally fixed background error covariance matrix $S_a$, such as from the Met Office or ECMWF operational schemes, may fail to represent accurately the profile uncertainty for a given time and location, and it should be possible to improve upon it in the unusual circumstances of a targeted set of dropsonde observations in the area.

Figure 4 shows an example of how a flight-specific error covariance matrix has been constructed. An ensemble of aircraft and dropsonde humidity profiles is shown in figure 4a, giving a set of departures from the mean profile in figure 4b. The variance of the departures as a function of pressure is shown in figure 4c. The profiles show remarkable consistency in the range 450–600 hPa, resulting in a very low variance (and high confidence) at these levels. Conversely, the lower part of the profiles, which is generally where the dropsondes were falling in and around mountainous terrain, exhibits high variance and low confidence in these values being representative of the flight as a whole. If treated as an
uncertainty, then the variance represents the diagonal of a covariance matrix (the off-diagonal terms can be similarly calculated). By including temperatures in the state vector \( \mathbf{x} \), a covariance matrix may be calculated that includes cross covariances (correlated errors) between humidity and temperature structures. (It is relevant to note here that this technique will probably overestimate the uncertainty in a particular profile because the ensemble will include real spatial and temporal variability. Nevertheless, it should capture at least partially the error associated with an observation \( \mathbf{y} \) that is slightly offset in time and space from the first guess profile \( \mathbf{x}_a \).)

In the original CKD definition of the continuum [4], the continuum coefficients are defined in terms of number density,

\[
k_{\text{abs}}(\nu, T) = R(\nu, T) \left[ \left( \frac{\rho_s}{\rho_o} \right) \tilde{C}_s(\nu, T) + \left( \frac{\rho_f}{\rho_o} \right) \tilde{C}_f(\nu, T) \right] + k_{\text{local}}, \tag{3.3}
\]

Here \( k_{\text{abs}} \) is the total absorption coefficient owing to water vapour (units cm\(^2\) per molecule) defined as a function of wavenumber (reciprocal wavelength) \( \nu \) in cm\(^{-1}\) and temperature \( T \) (K). \( \tilde{C}_s \) and \( \tilde{C}_f \) are the coefficients for the self and foreign water vapour continua, respectively (cm\(^3\) per molecule), \( \rho_o \) is the reference number density at 1 atm and 296K (molecule cm\(^{-3}\)), \( \rho_s \) is the density of water vapour and \( \rho_f = \rho_o - \rho_s \) is the foreign gas density (air excluding water vapour). The radiation field term is

\[
R(\nu, T) = \nu \tanh \left( \frac{hc_\nu}{2k_B T} \right), \tag{3.4}
\]

where \( h \) is Planck’s constant, \( c \) is the speed of light and \( k_B \) is Boltzmann’s constant. The term \( \tanh(hc_\nu/2k_B T) \) can be considered unity with negligible temperature dependence over the spectral range studied here. The local line shape, \( k_{\text{local}} \), is defined as a Lorentz line shape for each water vapour line within \( \pm 25 \text{ cm}^{-1} \) of the line centre minus the Lorentz line shape value at \( \pm 25 \text{ cm}^{-1} \). Everything else contributing to the water vapour absorption, including the \( \pm 25 \text{ cm}^{-1} \) ‘pedestal’ term, is classed as the continuum and included in the coefficients.

Several definitions of the continuum exist in the literature. Following Paynter et al. [9], it is possible to normalize the continuum coefficients to 1 atm pressure of the ‘self’ or ‘foreign’ gas and include the radiation term so that

\[
k_{\text{abs}}(\nu, T) = [p_s C_s^o(\nu, T) + p_f C_f^o(\nu, T)] \frac{T_o}{T} + k_{\text{local}}, \tag{3.5}
\]

where \( p_s \) and \( p_f \) are the water vapour and foreign gas pressure, respectively, and \( T_o = 296 \text{ K} \) is the reference temperature. The term \( T_o/T \) arises from the ideal gas relation \( p = \rho k_B T \); it is important to include it, otherwise continuum coefficients at temperatures other than \( T_o \) need to be adjusted for direct comparison with MT_CKD coefficients [8].

In this study, we compare continuum coefficients derived for different ambient temperatures. We follow Rowe et al. [17] by expressing the water vapour absorption as

\[
k_{\text{abs}}(\nu, T) = \frac{\rho_s}{\rho_o} C_s(\nu, T) + \frac{\rho_f}{\rho_o} C_f(\nu, T) + k_{\text{local}}, \tag{3.6}
\]
where the coefficients $C_{s,f}$ have units cm$^2$ per molecule and, again, the radiation field term is included in the coefficients. For atmospheric conditions, the second (foreign gas) term dominates for in-band absorption, whereas the first (self continuum) term is dominant in the out-of-band window regions [4]. LBLRTM allows the continuum strength to be perturbed by a chosen amount. In the 1400–2000 cm$^{-1}$ spectral region the foreign continuum optical depth dominates; hence, the perturbation need only be applied to the foreign continuum at these frequencies. The optimum continuum strength is found that reduces observed–calculated residuals to zero for the continuum-sensitive channels.

The channel selection for ARIES and IASI profile-constraining retrievals avoids channels sensitive to trace gases (such as methane and ozone) as well as those with a large contribution from the water vapour continuum. Given the optimum retrieved profile, it is then possible to use forward model calculations with LBLRTM to analyse the non-fitted continuum channels (specifically, the observed–calculated residuals). We need to take account of sources of error in the residuals when deriving continuum coefficients, resulting both from uncertainties in the radiances measurements and from the LBLRTM simulations. We consider here (as frequency-dependent terms)

1. ARIES and IASI random noise owing to detector sensitivity (‘instrument noise’).
2. ARIES calibration uncertainty. This has been determined as a function of scene temperature using the CAVIAR NPL cold blackbody dataset (figure 2).
3. Uncertainty in surface temperature and emissivity (downward views only). This uncertainty is much less for scenes over ocean than over complex terrain such as the Swiss Alps.
4. Uncertainty in the spectroscopy of HITRAN line parameters. A radiances error has been estimated using the error code specifications in HITRAN, and performing a series of LBLRTM Monte Carlo runs with appropriate perturbations.
5. Uncertainty in the LBLRTM constrained profile. The one-dimensional variational technique supplies an estimate of the error in the retrieved profile that can be transformed into an effective radiances uncertainty.

To obtain a total uncertainty, we assume these error sources are independent and combine in quadrature (i.e. calculate the root sum of the squares of the individual errors).

4. Results

Here, we seek to constrain the strength of the foreign continuum in the $v_2$ water vapour band between 1300 and 2000 cm$^{-1}$ and the self continuum in the relative window region between 2400 and 3200 cm$^{-1}$ based on ARIES and IASI remote sensing measurements compared with radiative transfer simulations. We also compare our results with laboratory measurements performed at the RAL as part of the CAVIAR project. The experimental methodology and data analysis techniques involved in extracting continuum coefficients from the
laboratory spectra are discussed in detail by Ptashnik et al. [10] (self continuum) and [18] (foreign continuum). In brief, the water vapour spectra were recorded using a Bruker IFS-125 high-resolution Fourier transform spectrometer at RAL’s Molecular Spectroscopy Facility (http://www.msf.rl.ac.uk/). Sensitivity to the weak continuum absorption was achieved through the use of long- and short-path cells which use mirrors at both ends to reflect radiation across the length of the cell many times. Measurements were carried out over a range of temperatures and for both pure water vapour and water–air mixtures. The contribution owing to the self continuum has been subtracted from the water–air continuum coefficients to leave purely the foreign gas continuum. The continuum coefficients were derived in a way compatible with the MT_CKD definition.

(a) Foreign continuum strength between 1300 and 2000 cm$^{-1}$

A typical spectrum of observed–calculated residuals is shown in figure 5b for the mid-infrared region 1200–2400 cm$^{-1}$. This region is dominated by the strong $v_2$ water vapour band centred at 1600 cm$^{-1}$, with the underlying foreign gas broadened water vapour continuum (mainly owing to N$_2$). Data are taken from the Camborne campaign in 2008 with ARIES viewing downwards at high altitude over ocean just north of the radiosonde station. An LBLRTM simulation has been run for this case based on a retrieved profile of temperature and humidity using ARIES channels insensitive to the continuum (see §3). The residuals at some frequencies exceed 2 K, largely owing to high instrument noise at these frequencies or uncertainties in the radiative transfer modelling.

For selected continuum-sensitive channels, shown as the black dots in figure 5b, the brightness temperature residuals using LBLRTM (which here includes the MT_CKD 2.5 model of the continuum) are typically within ±2 K. Because the atmospheric profile has been well constrained from the one-dimensional variational retrieval, we seek to attribute these remaining residual differences to errors in the modelled continuum strengths.

A further comparison is shown in figure 5c where the MT_CKD foreign water vapour continuum coefficients have been replaced by CAVIAR (RAL) laboratory-derived coefficients. There is some improvement in the magnitude of the residual differences, particularly in the wings of the $v_2$ band. However, in the centre of the band near 1600 cm$^{-1}$, the residuals are consistently negative with the CAVIAR (RAL) continuum. As we discuss below, we ascribe this negative residual (which implies insufficient continuum optical depth in the simulation) to a potential strengthening of the foreign continuum at atmospheric temperatures colder than those used for the laboratory measurements (296 K).

An important advantage for ARIES is the capability to look upwards as well as downwards. This obviates the need to model accurately emission and reflection from the Earth’s surface, and gives sensitivity to different channels as the water vapour optical depth above the aircraft varies. One such case from the Jungfraujoch campaign is shown in figure 6a, with particular sensitivity at the centre of the strong water vapour band. In this case, ARIES measures a colder brightness temperature in continuum-sensitive channels than suggested by LBLRTM with a foreign continuum strength of MT_CKD × 1.00. Figure 6b, showing a combined foreign continuum strength from many Jungfraujoch cases, suggests that an MT_CKD scaling factor less than 1.0
Figure 5. (a) Downward-looking brightness temperature spectrum from ARIES over ocean near Camborne on 18 September 2008, recorded at an altitude of 10 km on the FAAM BAe 146 aircraft. The spectrum is the mean of 117 fields of view. (b) Spectral residuals showing the difference between the mean ARIES observation and a line-by-line radiative transfer model (LBLRTM) simulation using as input the one-dimensional variational retrieved profile of temperature and humidity. The black dots are a subset of the spectral channels that have been selected for their sensitivity to the water vapour (foreign) continuum. The simulation was performed with the default version of LBLRTM incorporating the MT_CKD continuum. (c) Spectral residuals as in panel (b) where the CAVIAR (RAL) laboratory-derived continuum has been applied in place of MT_CKD. (Online version in colour.)

is required to bring simulation and observation into agreement. CAVIAR (RAL) laboratory results [18] are also shown, indicating that MT_CKD_2.5 may overestimate the strength of the foreign continuum by 20–40% in this spectral region.

The uncertainty in the derived continuum strength, shown as the error bars in figure 6, contains a contribution from spectroscopic line parameter uncertainty for both ARIES and CAVIAR (RAL) fits. This part of the uncertainty is not, therefore, independent between the two sets of measurements.

Figure 7 summarizes recent results for the mid-infrared strong water vapour band from four sources and compares them with MT_CKD_2.5. The CAVIAR work (RAL laboratory analysis and retrieval-based continuum derivation from ARIES and IASI) is shown along with data from Rowe & Walden [20]. They
used ground-based interferometer measurements in Antarctica to obtain foreign continuum coefficients for atmospheric temperatures below $-25^\circ\text{C}$. Rowe and Walden’s results imply that, relative to MT_CKD, the foreign continuum is up to 50 per cent lower below 1490 cm$^{-1}$, and up to 20 per cent higher above 1850 cm$^{-1}$.

There is some support for the Antarctica results from the ARIES and IASI data, particularly in the 1400–1500 cm$^{-1}$ range. The CAVIAR (RAL) data also show a stronger continuum than MT_CKD above 1900 cm$^{-1}$, although they do not reproduce the weaker continuum below 1500 cm$^{-1}$. All four datasets show that the continuum cross section has a neutral or positive spectral gradient over the range 1585–1605 cm$^{-1}$ at the centre of the band, in contrast to a 10 per cent
Figure 7. (a) Four determinations of foreign continuum coefficients in the range 1300–2000 cm$^{-1}$, compared in each case with the MT_CKD_2.5 formulation. (a) CAVIAR (RAL) coefficients based on laboratory data at 296 K; (b) ARIES derivation from Jungfraujoch CAVIAR flights; (c) IASI derivation from three CAVIAR case studies; (d) ground-based measurements by Rowe & Walden [20] in Antarctica corresponding to atmospheric temperatures around $-30^\circ$C. (Online version in colour.)

It is important to define the effective temperature at which the field measurements are most sensitive. Rowe & Walden [20] proposed that a temperature dependence may play a role in the foreign continuum which would help to explain their cold temperature results. For the ARIES and IASI remote sensing measurements, we define the continuum Jacobian as

$$\frac{\partial R_i}{\partial (C_{f})_{i,j}} = R_i((C_{f})_{i,j} = (C_{f,MT_CKD})_i) - R_i((C_{f})_{i,j} = 0),$$  \hspace{1cm} (4.1)

where the radiance at the observation altitude, $R_i$, at frequency $i$, is calculated for a set of atmospheric vertical levels $j$ using LBLRTM and the default MT_CKD_2.5 foreign continuum coefficients $(C_{f,MT_CKD})_i$, and separately for the same set of vertical levels with the continuum contribution to the optical depth at level $j$ set to zero. The difference, as defined by the equation, is the Jacobian for each $i, j$. 

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Figure 8. Example continuum Jacobian for downwelling radiance, as computed using equation (4.1) at a reference wavenumber of 1598.5 cm$^{-1}$, for the Jungfraujoch flight on 4 August 2009. The observation pressure level is 565 hPa. (a) Water vapour vertical profile as measured by the aircraft instrumentation and re-gridded as input for LBLRTM; (b) Jacobian with respect to foreign continuum, displayed as a function of atmospheric pressure, with units W m$^{-2}$ sr$^{-1}$ (cm$^{-1}$)$^{-1}$/[100% MT_CKD continuum coefficient]; (c) Jacobian with respect to foreign continuum, displayed as a function of atmospheric temperature. The horizontal dashed line shows the Jacobian-weighted mean temperature for which the continuum strength is retrieved, 261 K in this case. (Online version in colour.)

The continuum Jacobian for an example Jungfraujoch case is shown in figure 8. The mean temperature at which the continuum strength is retrieved is computed as the Jacobian-weighted temperature. The range of mean temperatures for the Jungfraujoch cases analysed in this study was between 255 and 265 K.

Rowe et al. [17] define their effective temperature weighting function in a similar same way as in equation (4.1), and in updated work [20] report weighted mean temperatures of approximately $-30^\circ$C for their results. We summarize the effective temperatures applicable to the results shown in figure 7 in table 2.

For the ARIES results and those of Rowe & Walden [20] displayed in figure 7, both derived from spectrometer zenith data, the (normalized) continuum Jacobians and therefore the effective temperatures for different spectral channels are relatively spectrally invariant. For nadir measurements such as the IASI observations, however, there is considerable spectral variation in the effective...
Figure 9. Spectral variation of effective temperatures, defined as described in the text, for IASI continuum coefficients displayed in figure 7. Data are shown for IASI cases near Camborne, UK, on 18 September 2008 (diamonds) and for cases near the Jungfraujoch, Switzerland, on 27 July 2009 and 1 August 2009 (triangles and squares, respectively). (Online version in colour.)

Table 2. Effective temperatures for continuum coefficients. Range of temperatures applicable to the data sources shown in figure 7. For the laboratory data, the cell temperature was measured directly; for the remotely sensed data, the mean temperature at which the atmospheric signal was observed has been determined as described in the text.

<table>
<thead>
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<th>data source</th>
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<tr>
<td>ARIES data recorded over Jungfraujoch</td>
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<tr>
<td>IASI case studies</td>
<td>247–281</td>
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<td>Rowe &amp; Walden [20]</td>
<td>around 243</td>
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temperatures for different channels. Figure 9 shows this spectral dependence. It is clear that channels towards the edge of the $v_2$ band are sensitive to much warmer temperatures than those nearer band centre owing to continuum Jacobians peaking closer to the surface (due to the greater transparency of the atmosphere at frequencies away from band centre).

Interestingly, this means that the IASI and Rowe & Walden [20] results are sensitive to similarly low temperatures (255 K or less) at the centre of the $v_2$ band where broadly there is mutual agreement. The 296 K laboratory continuum
coefficients are markedly smaller at 1600 cm\(^{-1}\), whereas the ARIES results at 255–265 K fall somewhere in between. We consider this to be the best evidence that a weak temperature dependence to the foreign continuum is genuine. Paynter et al. [9] (see their fig. 16) detected a small trend in foreign continuum coefficients between 1580 and 1610 cm\(^{-1}\) over the temperature range 296–351 K, which is additional evidence of a slight strengthening of the foreign continuum with decreasing temperature in this spectral interval.

We note that continua other than those owing to H\(_2\)O are present in the infrared atmospheric spectrum. Most pertinently, the broad collision-induced absorption by O\(_2\) in the fundamental band centred near 1550 cm\(^{-1}\) is a significant absorber. However, the O\(_2\) continuum data used in MT_CKD [21] were based on measurements over the 193–293 K temperature range, i.e. applicable to the expected range in the real atmosphere. We have tested the impact for a test case (that shown in figure 5) and have found that the O\(_2\) continuum has an impact of (at maximum) 1.4 K. Therefore, the O\(_2\) continuum absorption would need to be in error by a significant fraction to account for the residual differences we observe.

(b) The 2400–3200 cm\(^{-1}\) continuum

The MT_CKD continuum model has undergone regular revisions to take account of new data. One spectral region subject to large changes recently in v. 2.5 is in the range 3–5 \(\mu\)m (2000–3200 cm\(^{-1}\)) based on analysis of satellite- and ground-based infrared measurements [22]. Other work has previously suggested that past versions of MT_CKD underestimated the magnitude of the self continuum in this region [9]. Most recent experimental data [10,23] clearly demonstrate that the self continuum in this window is more than an order of magnitude stronger than it was in the MT_CKD_2.4 model. Here, we seek to test a new set of continuum strengths based on RAL data [10] with recent versions of MT_CKD. Figure 10a compares self-continuum cross sections for MT_CKD_2.4 and MT_CKD_2.5 with the CAVIAR (RAL) data. The revision to the MT_CKD coefficients is as high as a factor of 10 near 2700 cm\(^{-1}\). CAVIAR (RAL) coefficients are higher still.

Validation of the self continuum in this region in the real atmosphere, when relying on passive infrared radiometry, involves an unusual combination of conditions; the weakness of the continuum requires a very high water vapour concentration for adequate detection, and contamination by solar radiation limits observations to night time. Fortunately, archive ARIES data recorded in the tropics were available for this purpose. As described by Taylor et al. [24], non-continuum water vapour lines in the ARIES spectrum have been used to constrain the water vapour profile in this validation dataset. Low-altitude upward-looking measurements are shown in figure 10b. Residual differences between LBLRTM simulations, which have been run with MT_CKD_2.4, MT_CKD_2.5 and CAVIAR (RAL) continuum coefficients, and ARIES brightness temperatures are shown in figure 10c–e. While large discrepancies between observation and model are seen when using MT_CKD_2.4 (some residuals of 5–10 K), these are much reduced with MT_CKD_2.5. Using the CAVIAR (RAL) coefficients achieves excellent agreement with the ARIES data at 2450 cm\(^{-1}\), with slightly negative residuals at wavenumbers above this.
Figure 10. (a) Water vapour self (H$_2$O–H$_2$O) continuum cross section, at a reference temperature of 296 K, for the MT_CKD_2.4 formulation (dashed line) and MT_CKD_2.5 (solid line) together with values derived from RAL laboratory data (data points with error bars, [10]). (b) ARIES upward-looking brightness temperatures from low altitude recorded during the MOTH-Tropic campaign near Ascension Island on 6 May 1999. (c–e) Residual differences (observed–calculated) between ARIES and LBLRTM brightness temperatures where the modelled continuum strength is adopted from MT_CKD_2.4, MT_CKD_2.5 and CAVIAR (RAL), respectively. (Online version in colour.)
We estimate that the ARIES spectrum for this warm, tropical atmosphere is sensitive to temperatures in the range 290–300 K (the self continuum has a quadratic dependence on the water vapour mixing ratio, and the continuum emission is therefore concentrated in the very lowest layers of the atmosphere for ARIES zenith views). It is therefore reasonable to use the ARIES spectrum to compare directly self-continuum coefficients defined at the standard reference temperature of 296 K. Baranov et al. [8] note that the temperature dependence in MT_CKD does not compare well with some laboratory studies, particularly at temperatures much higher than 296 K; however, we expect that deviations from the MT_CKD temperature dependence will not markedly affect our data analysis here. We have neglected the effects of aerosols in our clear sky simulations, which in theory could contribute to the optical depth in this spectral region. However, the pristine atmospheric conditions around Ascension Island mean that tropospheric concentrations of aerosol were low.

Continuum absorption owing to N\textsubscript{2} and CO\textsubscript{2} is important in this spectral region. Mlawer et al. [22] test the sensitivity of atmospheric spectra in ‘dry’ and ‘wet’ conditions in order to separate out the effect of the water vapour continuum from other gases. The modified continuum coefficients from their work have been adopted in the MT_CKD 2.5 release. Our results (figure 10) are broadly supportive of the changes from MT_CKD 2.4; we cannot judge on these results alone whether the CAVIAR (RAL) or MT_CKD 2.5 coefficients are most suitable for radiative transfer simulations. We note that the uncertainty bounds in the CAVIAR (RAL) laboratory data overlap with MT_CKD 2.5 between 2400 and 2800 cm\textsuperscript{-1} and it is only near 3200 cm\textsuperscript{-1} (a proposed water vapour dimer feature; [25]) that the two models differ significantly. The ARIES calibration uncertainty of 1–2 K at this extreme end of the instrument spectral range may also account for some of the residuals remaining in figure 10.

It may not appear that even an order of magnitude change in the strength of the self continuum near 2700 cm\textsuperscript{-1} is of major importance for satellite remote sensing, because the continuum is already so weak. However, for this reason, the atmospheric infrared sounder (AIRS) channel at 2616 cm\textsuperscript{-1} has frequently been cited as a ‘super window channel’ and used to infer sea surface temperatures (SSTs) directly on account of assumed high transmittance [26]. SSTs derived in this way may need revision based on a new understanding of continuum strength in this spectral region. Spectral bands near 3.7 \mu m (2700 cm\textsuperscript{-1}) on spaceborne instruments such as the moderate resolution imaging spectroradiometer are also used for the retrievals of cloud droplet sizes [27], which may be sensitive to underlying radiative transfer assumptions about the water vapour absorption [28].

There is evidence from laboratory measurements that MT_CKD may underestimate the continuum strength in other near-infrared spectral windows, as discussed elsewhere [18].

5. Results applied to one-dimensional variational retrievals

Satellite observations sensitive to the \nu\textsubscript{2} band of water vapour between 1300 and 2000 cm\textsuperscript{-1} are used at NWP centres for the estimation of water vapour profiles. In recent years, instruments with spectral resolutions of the order of 1 cm\textsuperscript{-1},
such the AIRS and the IASI, have demonstrated positive impact on the forecast of meteorological variables [29,30]. The computational cost of assimilating large numbers of observations means that typically only a small subset of channels is actually used. The 300-channel subset of Collard [31] is optimized for maximum information content, although not all these channels are used operationally [29]. Increased use of spectral information from IASI-like observations may be possible in future through the use of principal components for spectral compression and noise filtering [32].

In order to test the possible benefit of an improved formulation of the water vapour continuum, we perform a one-dimensional variational retrieval experiment using a set of observations from the CAVIAR case study near Camborne, UK, on 18 September 2008. We base this on the [31] channel selection augmented with additional continuum channels to test their impact. The combined channel selection is 345 channels including 183 used operationally at the Met Office (figure 11). The case study consists of clear sky IASI observations over ocean together with FAAM dropsonde releases for the same time and location. Camborne radiosonde balloon ascents bracketed the IASI overpass time. As discussed earlier in §3, we use an ensemble of sonde observations to construct a background error covariance matrix for temperature and humidity. For the purposes of this retrieval experiment, we select one dropsonde from a high-altitude run of the FAAM BAe 146 aircraft to represent the first guess of the temperature and humidity profile. This dropsonde (released at 1042 UTC on 18 September 2008) was not well collocated with the clear sky IASI observations. We choose a different dropsonde (released at 1026 UTC) to represent our best estimate of the ‘truth’ because this measurement was made to coincide in time and space with the IASI observations. For the observation error covariance matrix (\(S\) in equation (3.1)), we use the IASI instrument noise supplemented by a 0.2K error term to represent approximately radiative transfer errors; the errors are assumed spectrally uncorrelated.

Figure 11 shows results for a retrieval using four clear sky IASI fields of view. In figure 11b, we show the spectral residuals for one example spectrum where the forward model, incorporating the MT_CKD_2.5 continuum, has been initialized with the background (first guess) profile. The residuals in the 1300–2000 cm\(^{-1}\) band are largely negative, which implies that there is insufficient water vapour optical depth in the model profile. By contrast, the temperature sounding channels in the CO\(_2\) band centred at 667 cm\(^{-1}\) do not exhibit a marked bias, indicating that the model temperature profile is consistent with the IASI observation. Observed–model residuals before and after the one-dimensional variational retrieval are shown in figure 11c. The retrieval succeeds in reducing the spectral residuals for the both average and r.m.s. differences.

The retrieval results in terms of the humidity state vector are shown in figure 11d,e. Relative to the 1026 UTC dropsonde ‘truth’, the background profile is too dry between 400 and 500 hPa. The retrieval does a good job of successfully producing a positive humidity increment at these levels, although the magnitude of the increment is slightly overdone. There also appears to be a spurious increment in low-level humidity near the surface at 900–1000 hPa that is not captured in the ‘true’ profile. There is also a substantial increase in humidity between 300 hPa and the top of the atmosphere in the retrieval. For these vertical levels, the Camborne radiosonde ascents have been interpolated in time.

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Figure 11. Retrieval results with the forward model (LBLRTM) incorporating the MT_CKD_2.5 water vapour continuum. 
(a) Observation vector (average IASI brightness temperature for the selected footprints with retrieval channels highlighted). 
(b) An example first guess residual (observation minus model using background profile, retrieval channels highlighted). 
(c) Residuals for retrieval channels before and after retrieval; mean and r.m.s. residuals are shown in the figure. 
(d) Humidity state vector displaying the model background, retrieved profile for four IASI footprints and a profile labelled ‘truth’ derived from the best collocated dropsonde measurement. 
(e) Retrieved humidity increment for the four observations compared with the ‘true’ expected difference. 
(f) Jacobians for the retrieval channels with respect to the water vapour mixing ratio where the continuum-sensitive channels for IASI (the same channels as shown in figure 7) are highlighted. (Online version in colour.)
to constitute the background. It is recognized that the corrections applied to radiosonde data to account for the effects of solar heating are imperfect [33], so we cannot validate the retrieval performance here in the upper atmosphere. The water vapour Jacobians (figure 11f) show that the retrieval channels have a

Figure 12. Retrieval results with the forward model (LBLRTM) incorporating the CAVIAR (RAL) water vapour continuum. See figure 11 caption for details. (Online version in colour.)
sensitivity peaking generally between 200 hPa and the surface. The temperature retrieval (not shown) produces a small increment which, for most vertical levels, is less than ±1 K.

Figure 12 shows retrieval results where the forward model, LBLRTM, now includes the CAVIAR (RAL) continuum coefficients in place of MT_CKD. The retrieval humidity increment is not too dissimilar to that shown in figure 11. However, there is a qualitative improvement in the size of the increment near 400–500 hPa where the retrieval is a good match to the dropsonde ‘truth’. There is also a reduced increment near the surface. Arguably, the ‘CAVIAR’ retrieval matches the validation profile less well near 550 hPa than the ‘MT_CKD’ retrieval.

Quantitatively, the post-retrieval brightness temperature residual and r.m.s. are improved when using the CAVIAR (RAL) continuum, from −0.39 to −0.27 K and from 0.58 to 0.49 K, respectively. Although not a large difference, it does imply that the retrieval is better able to converge with the CAVIAR coefficients. The one spectral interval where the residuals remain large is the centre of the ν2 band near 1600 cm⁻¹. There are also discrepancies in this interval between the various studies shown in figure 7. If due to a genuine temperature dependence, then this may account for the residual difference in figure 12c where we have applied laboratory continuum coefficients derived at 296 K.

6. Summary

The aim of this study was to test the applicability of the MT_CKD continuum under real atmospheric conditions and validate new laboratory-derived CAVIAR (RAL) continuum coefficients. Both aircraft and satellite infrared radiances, collocated with intensive observations of the atmospheric state, have been analysed with the aid of line-by-line simulations. The self continuum in the 2400–3200 cm⁻¹ region has undergone substantial revision in the latest MT_CKD_2.5 release, and we confirm that this version is in much better agreement with ARIES airborne radiances in a tropical atmosphere than MT_CKD_2.4. The CAVIAR (RAL) self continuum [10] is slightly higher than MT_CKD_2.5 across this part of the infrared spectrum; both these sets of coefficients are compatible with the ARIES measurements to within experimental error.

A one-dimensional variational technique has been applied to regions of the spectrum insensitive to the continuum in order to reduce uncertainties in the atmospheric profiles, and thereby improve the accuracy of derived coefficients. In the 1300–2000 cm⁻¹ region, ARIES and IASI retrieved foreign continuum coefficients are broadly in agreement with the MT_CKD_2.5 foreign continuum, although discrepancies persist. In the 1400–1500 cm⁻¹ range, the inferred foreign continuum is weaker than MT_CKD; between 1900 and 2000 cm⁻¹, the ARIES and IASI coefficients are somewhat higher. This result is corroborated by the recent results of Rowe & Walden [20]. However, the CAVIAR (RAL) laboratory measurements of the foreign continuum [18] do not show such significant departures from MT_CKD in these ν2 band wings. We interpret these differences as evidence of a weak temperature dependency in the strength of the foreign continuum, because the remote sensing measurements (ARIES, IASI; [20]) were all sensitive to relatively low atmospheric temperatures compared with the 296 K laboratory data.
All sources of continuum strengths we consider benefit from good to signal-toupper-noise at the centre of the band near 1600 cm$^{-1}$. Here, the laboratory and ARIES results suggest a continuum strength of 60–85% and 70–90% of the MT_CKD value, respectively. By contrast, the IASI results and those of Rowe & Walden [20], which are sensitive to lower atmospheric temperatures of 255 K or less, are in much better accord with MT_CKD. We consider this is the strongest evidence available that the foreign continuum exhibits an increasing strength with decreasing temperature at the centre of the $\nu_2$ band.

The $\nu_2$ band is used at NWP centres for the retrieval of humidity from satellite instruments such as IASI. Although the number of channels used operationally is currently limited, there are potential benefits from using more spectral information, including more continuum-sensitive channels. An accurate knowledge of the water vapour radiative transfer is a prerequisite, however, without which the humidity retrievals may be degraded. We have tested the MT_CKD_2.5 and CAVIAR (RAL) continua in a retrieval experiment, applied to IASI observations during an intensive observation period. The observed–retrieved brightness temperature residuals for an example channel selection are reduced with the CAVIAR (RAL) coefficients, and the retrieved humidity profile is qualitatively closer to the validation sonde ‘truth’. However, significant residuals remain near 1600 cm$^{-1}$, which we suspect is due to application of 296 K laboratory coefficients to channels where the continuum sensitivity peaks closer to 250 K. We anticipate that future models of the foreign continuum used in infrared remote sensing may need to include temperature-dependent terms, as is currently formulated in MT_CKD for the much stronger temperature dependence of the self continuum.

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