Development and recent evaluation of the MT_CKD model of continuum absorption

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Water vapour continuum absorption is an important contributor to the Earth’s radiative cooling and energy balance. Here, we describe the development and status of the MT_CKD (Mlawer–Tobin–Clough–Kneizys–Davies) water vapour continuum absorption model. The perspective adopted in developing the MT_CKD model has been to constrain the model so that it is consistent with quality analyses of spectral atmospheric and laboratory measurements of the foreign and self continuum. For field measurements, only cases for which the characterization of the atmospheric state has been highly scrutinized have been used. Continuum coefficients in spectral regions that have not been subject to compelling analyses are determined by a mathematical formulation of the spectral shape associated with each water vapour monomer line. This formulation, which is based on continuum values in spectral regions in which the coefficients are well constrained by measurements, is applied consistently to all water vapour monomer lines from the microwave to the visible. The results are summed-up (separately for the foreign and self) to obtain continuum coefficients from 0 to 20000 cm$^{-1}$. For each water vapour line, the MT_CKD line shape formulation consists of two components: exponentially decaying far wings of the line plus a contribution from a water vapour molecule undergoing a weak interaction with a second molecule. In the MT_CKD model, the first component is the primary agent for the continuum between water vapour bands, while the second component is responsible for the majority of the continuum within water vapour bands. The MT_CKD model should be regarded as a semi-empirical model with strong constraints provided by the known physics. Keeping the MT_CKD continuum consistent with current observational studies necessitates periodic updates to the water vapour continuum coefficients. In addition to providing details on the MT_CKD line shape formulation, we describe the most recent update to the model, MT_CKD_2.5, which is based on an analysis of satellite- and ground-based observations from 2385 to 2600 cm$^{-1}$ (approx. 4 μm).

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Continuum absorption and emission by atmospheric water vapour has a critical impact on the weather and climate of the Earth [1,2]. Near the surface, the radiative effects of the water vapour continuum contribute as much as 40 per cent of the total longwave radiative cooling rate, considerably affecting the thermodynamic structure of the atmosphere. Higher in the troposphere, the percentage of the cooling rate owing to the water vapour continuum is smaller but still significant. The impact of water vapour continuum absorption on the energy balance of the Earth is similarly profound, decreasing the outgoing longwave irradiance by as much as 10 W m$^{-2}$. Clearly, it is important for studies of atmospheric processes that our understanding of the water vapour continuum be well established.

For many years, no definitive argument existed as to what form of or process related to water vapour was responsible for the observed continuum absorption. An important development in the understanding of this effect was the introduction of the Clough–Kneizys–Davies (CKD) continuum model [3,4], which demonstrated that the observed properties of this absorption could be derived from the assumption that the continuum was owing to interactions between a single absorbing water vapour molecule and another molecule, which could be either water vapour (self continuum) or a different molecule (foreign continuum). The philosophy in the development of the CKD continuum was to use the most well-established measured values for continuum absorption coefficients (e.g. [5]) to fit a variation of the impact line shape (symmetrized as in Van Vleck & Huber [6]): the modified line shape was constrained to be of the form of a product between the impact line shape and a reasonably simple, spectrally dependent ‘χ-function’. This approach is semi-empirical in the sense that the known physics as reflected by the Van Vleck and Huber (VVH) line shape formalism was incorporated, but the line shape was modified via the χ-function to be consistent with observations. The derived semi-empirical CKD line shape was then consistently applied to all water vapour lines from the microwave to the shortwave, thereby extrapolating knowledge of the continuum from spectral regions in which it was relatively well known to those in which it was not. (The associated continuum absorption coefficients result from summing-up the contributions from all water vapour lines.) The line shape that resulted from this procedure was consistent with the interpretation that the observed continuum absorption was owing to the intermediate and far wings of allowed transitions of the water vapour monomer.

After the CKD model was created, continuum absorption in the spectral regions on which the line shape formulation was based was analysed by a number of reliable laboratory- and field-based measurements, some of which agreed with the original laboratory values and some of which did not. In addition, similar measurements with implications for the water vapour continuum were made in other spectral regions, which provided a crucial assessment of the applicability of the line shape used in the CKD model to the entire spectrum. These studies led to modifications to the CKD continuum coefficients in certain spectral regions, which were implemented in a series of revised versions of the CKD model. However, despite these modifications, the CKD line shape was not re-derived to remain consistent with the coefficients. Therefore, in spectral regions in which no reliable measurements of continuum absorption existed, these later versions of the CKD...
model had exactly the same continuum values as the original version, even though the associated line shape was known to be flawed. The development of these modified versions was consistent with the functional definition of the water vapour continuum that had been adopted by the CKD developers—that of slowly varying absorption owing to water vapour which, when added to line contributions, was needed to agree with the observations.

This inconsistency was rectified with the development of the MT_CKD (Mlawer–Tobin–Clough–Kneizys–Davies) continuum formulation [7]. While the primary motivation for the development of this new formulation was the restoration of consistency between the line shape formulation and the existing set of reliable measured continuum values, an additional motivation was to alter the functional form used for the fit and, by implication, the interpretation of the physical basis for the water vapour continuum. Continuum absorption by water vapour has the properties that it is much greater within water vapour bands and less between bands than the continuum implied by the Lorentz line shape applied to water monomer lines, which is derived from the clearly non-physical assumption that the collision time of the molecular interaction involved is instantaneous, i.e. the impact approximation. As a result, the $\chi$-function used in the CKD formulation had values greater than unity (super-Lorentzian) close to line centre and less than unity (sub-Lorentzian) far from line centre. The far-wing line shape behaviour, which determined the continuum absorption coefficients in between water vapour bands, was readily understood physically: refining the impact approximation to account for a finite duration of collision decreases the line shape far from the centre of the line. (The line shape must decrease at least exponentially as the distance from line centre approaches infinity [4,8].) In the CKD formulation, a $\chi$-function with behaviour in the far line wings given by a simple variation of an exponentially decreasing function allowed the observed continuum behaviour between bands to be accurately fitted. The super-Lorentzian behaviour of the line shape closer to line centre, responsible for the continuum absorption within water vapour bands, is not so straightforwardly associated with a physical mechanism related to the absorbing water vapour molecule. The approach adopted in CKD to model this absorption was conceptually consistent with there being an unknown mechanism that caused additional absorption associated with the intermediate wings of allowed monomer transitions. In Clough et al. [3], no physical basis was explicitly suggested for this additional absorption; the observed in-band continuum values were reproduced in the CKD formulation by fitting parameters in the $\chi$-function that controlled the behaviour of the empirically derived line shape within approximately $100\text{cm}^{-1}$ of line centre. This super-Lorentzian behaviour was combined with the sub-Lorentzian behaviour far from line centre into a single $\chi$-function that multiplied the Lorentz line shape.

In the years after the development of the CKD model, little progress had been made in identifying a mechanism that would allow water vapour monomer transitions to have sufficient super-Lorentzian absorption to explain the observed in-band continuum. Therefore, the MT_CKD continuum used a revised formulation; it employed a second term to be added to the term responsible for the sub-Lorentzian far-wing continuum contribution, in contrast to the multiplicative $\chi$-function formulation of the CKD model. This approach is conceptually consistent with the existence of a water vapour absorption source in

Phil. Trans. R. Soc. A (2012)
addition to that associated with collisionally broadened water vapour monomer absorption lines (including their sub-Lorenztian far wings). From observation, the in-band continuum absorption is aligned with the location of the water vapour monomer bands; therefore, any interaction between the absorbing water vapour molecule and another molecule (water vapour or ‘foreign’) that is responsible for this additional absorption must be sufficiently weak so as to permit access to the same rovibrational modes of monomer transitions and sufficiently brief to cause these transitions to be greatly broadened. In this interpretation of the MT_CKD continuum, monomer transitions occur not only in the form of sharp-featured collisionally broadened lines with wings that decrease exponentially with distance from line centre, but also in a broad continuum resulting from weak interactions between a water vapour molecule and a second molecule. This overlapping of allowed and broadened transitions also occurs in collision-induced absorption bands observed in various spectral regions (e.g. [9,10]). For example, in the case of molecular oxygen, which does not have a permanent dipole moment, these transitions result from ‘forbidden’ interactions that become accessible upon the generation of a short-lived dipole moment as a result of the collision. Many of these collision-induced bands overlap spectrally with lines from allowed transitions (e.g. magnetic dipole transitions in the 1.27 μm band of molecular oxygen).

The ability of the MT_CKD formulation to fit the measured continuum values should not be interpreted, however, as decisive proof that the in-band continuum absorption is owing to weak interactions involving a water vapour molecule. It is also likely that a method similar to the CKD χ-function approach, albeit using more complicated functions, could have been used to fit the measured data. The actual source of in-band water vapour continuum absorption associated with the monomer will be conclusively determined only with the generation of an \textit{ab initio} calculation, using the quantum mechanical properties of the water vapour monomer that reproduces the known continuum values. However, the success of the MT_CKD formulation in reproducing observed continuum absorption provides firm support to the conclusion that there is water vapour continuum absorption that is owing to the water vapour monomer.

A main objective of this paper is to present a recent modification to the MT_CKD continuum model in the 4 μm region based on spectral radiance measurements from both satellite- and ground-based instruments. The analysis that led to this modification is detailed in §4. Section 2 presents background information on the CKD and MT_CKD continuum formulations, including some historical information related to the CKD formulation and revisions to the CKD model prior to the development of MT_CKD. Section 3 presents detailed information about the MT_CKD continuum formulation, as well as descriptions of previous modifications made to the MT_CKD model. Section 5 provides a summary finally.

2. Background

\textit{(a) MT_CKD and line-by-line radiative transfer model}

In a radiative transfer calculation, the division between what is considered absorption owing to spectral lines and that owing to continuum is somewhat
arbitrary, with the only absolute requirement being consistency in the definition of each so that the appropriate total absorption is preserved. In the line-by-line radiative transfer model (LBLRTM) [7], all absorption beyond 25 cm$^{-1}$ from line centre is defined as continuum absorption. This definition provides a calculational benefit: the spectral dependence of all absorption owing to a spectral line is weak at this distance from line centre, obviating the need for the evaluation of a complicated spectral function when this part of each line is considered during an LBLRTM calculation. An additional factor encouraging the truncation of the more complicated ‘line’ part of the calculation is that the dependence of the absorption coefficient (in cm$^2$ molecule$^{-1}$) on the density of the colliding molecules becomes a simple linear function away from the central line region, simplifying the parametrization of the absorption owing to this part of the line. Therefore, in LBLRTM, the sum of the contributions from all lines beyond 25 cm$^{-1}$ from their respective line centres is considered to be continuum absorption. As it is essential for the continuum contribution from a line to be continuous 25 cm$^{-1}$ from its centre, the continuum contribution inside of 25 cm$^{-1}$ must be non-zero.

A definition of the water vapour continuum coefficient in this central region of the line that preserves continuity and the desired slow spectral variation of the continuum is the sum of (i) the difference between the line contribution and the Lorentz line contribution (varies with wavenumber inside of 25 cm$^{-1}$) and (ii) the value of the Lorentz line shape 25 cm$^{-1}$ from line centre (i.e. the ‘Lorentz pedestal’; fixed with wavenumber inside of 25 cm$^{-1}$). These two components of continuum absorption for each line inside of 25 cm$^{-1}$ are combined with the contribution outside of 25 cm$^{-1}$ described above to form the continuum. The sum of these contributions over all water vapour lines is a continuous, slowly varying function, which is pre-computed and tabulated at 10 cm$^{-1}$ intervals in the MT_CKD (previously CKD) model. In an LBLRTM calculation, the stored values are interpolated in wavenumber and scaled from a reference collider density value to obtain the appropriate absorption coefficient.

The MT_CKD continuum model also includes parametrizations of continuum absorption owing to carbon dioxide, ozone, nitrogen and oxygen, including a number of collision-induced continuum absorption bands in the thermal and solar spectral regions. For CO$_2$, the continuum provides a mechanism to include the appropriate contribution of the far wings, a role analogous to the water vapour continuum parametrization. There is an important difference, however, between the treatment of the line contribution within 25 cm$^{-1}$ for CO$_2$ and H$_2$O lines. As the line shapes of CO$_2$ lines are commonly subject to the effects of line coupling [11], the difference between the actual and Lorentz line shape is not a simply parametrized, slowly varying spectral function. Therefore, the MT_CKD CO$_2$ continuum parametrization does not include the first of the two terms described above that are included in the H$_2$O continuum within 25 cm$^{-1}$ of line centre. Instead, LBLRTM, which includes a first-order treatment of CO$_2$ line coupling constructed using the Lamouroux et al. [12] databases and software for the P, Q and R branches, treats this contribution to the absorption as part of the ‘line’. As for H$_2$O, all absorption further than 25 cm$^{-1}$ from line centre is considered part of the continuum—the impact of line coupling is appropriately accounted for in the stored continuum coefficients. Any further adjustment to the line shape in the wings (i.e. $\chi$-function not equal to unity) is dealt with empirically, as detailed in §3 below. There is also a contribution to the continuum within 25 cm$^{-1}$ of line

Phil. Trans. R. Soc. A (2012)
Development, evaluation of MT_CKD model

centre that is needed for continuity. As the impact of line coupling for a single line is asymmetric with respect to its line centre, this is a more complicated function than the Lorentz pedestal used for $\text{H}_2\text{O}$. (The line contribution within $25 \text{ cm}^{-1}$ for each $\text{CO}_2$ line is reduced by this same function to preserve to appropriate total absorption. The values of this function $\pm 25 \text{ cm}^{-1}$ from line centre are equal to the Lorentz line shape (i.e. $\chi = 1$) adjusted for line coupling at these points.) This baseline continuum function within $25 \text{ cm}^{-1}$ is combined with the contributions from the wings of all lines; these contributions are computed for all $\text{CO}_2$ lines at the reference temperature of 296 K, which are then summed-up and stored every $2 \text{ cm}^{-1}$ in MT_CKD.

The line shape formalism in LBLRTM is owing to Van Vleck & Huber [6], with the absorption coefficient ($\text{cm}^2 \text{ molecule}^{-1}$) given by

$$k(n) = R(n)\sigma(n) \quad (2.1)$$

with

$$R(n) = \nu \tanh\left(\frac{\beta\nu}{2}\right) \quad (2.2)$$

and

$$\sigma(n) = \langle f(n) + f(-n) \rangle, \quad (2.3)$$

where $R(n)$ is the radiation field term and $\sigma(n)$ is the symmetrized power spectral density function. This VVH formalism has been chosen as it is applicable to all spectral domains, it assures radiation balance between absorption and emission for a general line shape function $f(n)$ and it satisfies important sum rules. In order to represent a physical process, $\sigma(n)$ must decay for large values of $\nu$ at least as fast as an exponential function [4]. This condition is not obeyed by the Lorentz line shape function that defines the ‘line’ contribution of water vapour lines within $25 \text{ cm}^{-1}$ of line centre in LBLRTM, but this does not pose an issue as the ‘line’ contribution is not defined further than $25 \text{ cm}^{-1}$ from line centre. Instead, as a result of the definition of the continuum adopted above, the need for rapid functional decay far from line centre affects only the behaviour of the continuum.

(b) The Clough–Kneizys–Davies continuum

To provide context for the MT_CKD line shape formulation presented below, essential details of the CKD continuum formulation are provided here. More extensive information on the CKD formulation can be obtained from the study of Clough et al. [3,4].

The CKD continuum model was derived based on a series of laboratory measurements [5,13] in the microwave/sub-millimetre spectral region and the infrared regions of 330–1060 and 1400–2300 cm$^{-1}$. These experiments measured absorption owing to water vapour for a variety of temperatures in the windows between water vapour lines, from which the contribution from the lines (as defined above) was removed. The resulting absorption coefficients were then divided by the appropriate radiation terms (see equation (2.2)), producing the ‘continuum coefficient’. These results verified the well-known fact that there are two distinct contributions to the continuum absorption, one with continuum coefficients proportional to the density of molecules other than water vapour (foreign continuum) and another proportional to the density.

Phil. Trans. R. Soc. A (2012)
of water vapour (self continuum). These results were consistent with the interpretation that the continuum absorption is due to collisional effects and is dependent on the time between collisions. These measurements indicated that there was no discernible dependence on temperature for the foreign continuum, whereas the self-continuum measurements showed an increase in absorption coefficient with decreasing temperature.

The CKD water vapour continuum was developed on the basis of a semi-empirical fit to these experimentally determined values for continuum coefficients. By ‘semi-empirical’, it is meant that known physical mechanisms, such as a non-instantaneous duration of collision, are incorporated into the adopted formalism, but the guiding objective of this formalism is to attain agreement between measurements and derived continuum values. This perspective was incorporated through the determination of two functions $\chi(\nu)$ (one each for the foreign and self continua) in terms of which the foreign- and self-broadened absorption coefficients are defined as

$$k(\nu) = R(\nu) \sum_i \tilde{S}_i(T) \frac{1}{\pi} \left[ \frac{\alpha_i}{(\nu - \nu_i)^2 + \alpha_i^2} \chi(\nu - \nu_i) + \frac{\alpha_i}{(\nu + \nu_i)^2 + \alpha_i^2} \chi(\nu + \nu_i) \right],$$

(2.4)

where the sum is performed over all water vapour lines and $\tilde{S}_i$ is the intensity of the transition at wavenumber $\nu_i$ and halfwidth $\alpha_i$. Equation (2.4) is consistent with the VVH formalism defined in equations (2.1)–(2.3). A value of unity for the function $\chi(\nu)$ corresponds to the impact approximation, with a line shape in the infrared equal to the Lorentz function,

$$L(\nu - \nu_i) = \frac{1}{\pi} \frac{\alpha_i}{(\nu - \nu_i)^2 + \alpha_i^2}. \quad (2.5)$$

(In this paper, the terms ‘sub-Lorentzian’, ‘super-Lorentzian’, and so on are referenced to equation (2.4) with $\chi(\nu) = 1$.) It is interesting to consider as an example the functional form

$$\chi(\nu) = e^{-(\nu / \nu_D)^p} \quad \text{where} \quad p \geq 1. \quad (2.6)$$

Adoption of such a $\chi$-function would negate the impact approximation, allow the symmetrized autocorrelation function to be analytical at the time of collision, and, with appropriate values for $\nu_D$ and $p$, could provide agreement with both the observed line shape near line centre and the observed sub-Lorentzian absorption between bands. However, such a functional form would not provide a mechanism to produce the observed super-Lorentzian continuum values within water vapour bands and, therefore, can only serve as a starting point in the determination of the semi-empirical function $\chi$.

After removing the ‘line’ contribution from the continuum coefficients, the CKD formulation can be written as

$$\tilde{C}(\nu) = \langle \phi(\nu) + \phi(-\nu) \rangle_c = \sum_i \tilde{S}_i [L_c(\nu - \nu_i) \chi(\nu - \nu_i) + L_c(\nu + \nu_i) \chi(\nu + \nu_i)],$$

(2.7)
where $L_c(v - v_i)$ is the Lorentz line shape with the intensity peak at line centre removed,

$$L_c(v \pm v_i) = \begin{cases} \frac{1}{\pi} \frac{\alpha_i}{25^2 + \alpha_i^2} & |v \pm v_i| \leq 25 \text{ cm}^{-1}, \\ \frac{1}{\pi} \frac{\alpha_i}{(v \pm v_i)^2 + \alpha_i^2} & |v \pm v_i| \geq 25 \text{ cm}^{-1}, \end{cases}$$

(2.8)

and the function $\chi'$ is defined in terms of the $\chi$-function as follows:

$$\chi' (v \pm v_i) = \begin{cases} 1 + [\chi (v \pm v_i) - 1] \frac{25^2}{(v \pm v_i)^2 + \alpha_i^2} & |v \pm v_i| \leq 25 \text{ cm}^{-1}, \\ \chi (v \pm v_i) & |v \pm v_i| \geq 25 \text{ cm}^{-1}. \end{cases}$$

(2.9)

Note that since the halfwidth $\alpha_i = \alpha_i^0 (\rho/\rho_0)$ is proportional to the collider density $\rho$, where $\alpha_i^0$ is the self-broadened halfwidth at atmospheric density $\rho_0$, the continuum coefficients are also proportional to $\rho$, consistent with observed behaviour. The procedure followed in the development of CKD was the determination of functional forms for $\chi'$ for both the foreign and self continua that permitted agreement between the Burch-measured values and the continuum coefficients calculated from equation (2.7). The two functions that were derived were

$$\chi'_f (v \pm v_i) = 6.65 e^{-(v \pm v_i/75)^2}$$

(2.10)

and

$$\chi'_s (v \pm v_i) = 8.63 e^{-(v \pm v_i/400)^2} + \left[ 0.83 \left( \frac{v \pm v_i}{250} \right)^2 + 0.033 \left( \frac{v \pm v_i}{250} \right)^4 \right] e^{-|v \pm v_i/250|},$$

(2.11)

where the wavenumber quantities are expressed in units of inverse-centimetre and $\chi'_s$ is specified at 296 K. The $\chi$-functions implied by these functions are shown in fig. 4 of Clough et al. [3] and indicate the three necessary qualitative features: values near unity close to line centre as a result of the validity of the impact approximation for interactions that occur at large distances between the absorbing and colliding molecules; values greater than unity between approximately 10 and 100 cm$^{-1}$ from line centre, consistent with the super-Lorentzian continuum behaviour within water vapour bands; and exponential decay far from line centre, resulting in the analyticity of the corresponding symmetrized autocorrelation function. To compute the CKD continuum coefficients, these line shape functions were applied to all water vapour lines from the microwave to the shortwave using the most accurate existing line parameter data. This effectively served to extrapolate information about the nature and intensity of continuum absorption from the spectral regions in which the Burch measurements were made to spectral domains less well probed, such as the shortwave. The observed temperature dependence of the self continuum was accounted for by extrapolating the continuum coefficients at 296 K to 260 K using the self-continuum measurements performed at all temperatures.

Phil. Trans. R. Soc. A (2012)
(ranging between 296 and 338 K) in the Burch experiments. As stated above, the multiplicative $\chi$-function in this formalism was consistent with the interpretation that the intermediate and far wings of lines associated with the allowed monomer transitions were the cause of the observed continuum features, with the actual monomer line shape consistent with the CKD line shape given by equations (2.7)–(2.11). In this interpretation, there was an unidentified physical mechanism responsible for the in-band super-Lorentzian absorption.

In the years since the generation of the CKD continuum, there were a number of field- and laboratory-based measurement efforts that provided more accurate determination of continuum absorption coefficients in certain spectral domains. Revised coefficients would no longer be consistent with the CKD formulation, but instead be associated with a different set of values for the free parameters in equation (2.10) and/or (2.11) or, potentially, a revised formulation. Rather than modifying the underlying CKD formulation each time when new accurate continuum measurements became available, new versions of the CKD continuum were generated with modified coefficients in isolated spectral regions (see below). Although this resulted in improved measurement–model validations, the CKD continuum thereby forfeited its internal consistency. For example, certain measurements implied that the foreign continuum in the centre of the water vapour $\nu_2$ band (1400–1800 cm$^{-1}$) was generally lower than given by the original CKD fit, a result that had implications related to the value of the foreign $\chi$-function in the region in which it is super-Lorentzian. However, only the foreign continuum coefficients in the $\nu_2$ band of the CKD model were modified as a result of these measurements, and not the analogous (i.e. in-band) spectral regions in any other water vapour bands. In addition, it is clear from equation (2.7) that the values of continuum coefficients are dependent on the intensities $\tilde{S}_i$ of water vapour transitions, quantities that are frequently the subject of spectroscopic laboratory investigations. However, neither the CKD continuum coefficients were recomputed as a result of revised line intensities, nor were the free parameters in the CKD formalism refitted. Consequently, there were spectral regions, such as the shortwave, in which the CKD continuum coefficients had never been modified despite improvements to our understanding of the relevant spectroscopy.

A brief summary of important versions of the CKD water vapour continuum follows, with the date of implementation and motivation for each revision:

- CKD _0 (1989): this refers to the original version of the CKD water vapour continuum model, consistent with equations (2.10) and (2.11). Initially, it was thought based on certain observations that the CKD _0 foreign continuum values in the window region 800–1200 cm$^{-1}$, a spectral region in which absorption owing to the foreign continuum is relatively insignificant, were too small. Therefore, for a brief period of time, a ‘fudge’ factor was inserted in all window regions from the infrared to the visible to increase the continuum coefficients. It is this altered version of the continuum model that was used by Clough et al. [2] and is referred to as ‘CKD’ in that work. However, these modifications were eliminated after a short time and the original coefficients restored (and used by Clough & Iacono [14]). The short-lived modified revision is not considered as an official version of the CKD continuum.
Development, evaluation of MT_CKD model

- CKD_2.1 (1993): the most significant modifications were increased self-continuum coefficients in the window region from 800 to 1100 cm\(^{-1}\), based on spectral radiance data taken by the NOAA Wave Propagation Laboratory group in Kavieng, New Guinea, in January 1993 [15]. A 'bump' centred at 930 cm\(^{-1}\) was added to the self coefficients, a feature that scaled with water vapour as did the self continuum, but was not thought to be associated with the water vapour monomer owing to its presence in a spectral domain far from the presence of strong water vapour lines. In addition, the foreign continuum coefficients were decreased in the \(\nu_2\) band of water vapour (1200–2200 cm\(^{-1}\)) to attain better agreement with the measurements of Burch [13]. CKD_2.1 was used in the development of the original version of the fast radiation code RRTM [16].

- CKD_2.2 (1996): the self-continuum coefficients were increased by approximately 30 per cent in the microwave region to attain better agreement with atmospheric measurements.

- CKD_2.4.1 (1999): the most significant changes were made to the foreign continuum between 300 and 700 cm\(^{-1}\) as a result of surface measurements in the Arctic [17]. In the cold, dry conditions of this region, the spectral region at the edge of the water vapour rotation band (400–600 cm\(^{-1}\)) is no longer opaque at the surface, as is normally seen at lower latitudes. This allows the properties of the water vapour absorption in this region to be probed, and, as a result of these measurements, led to the determination that the CKD foreign water vapour continuum coefficients needed revision.

3. The development of the MT_CKD formulation

It was clear from the multiple modifications made to the CKD water vapour continuum coefficients that the CKD line shape formulation was flawed. Therefore, an effort was undertaken to modify the formulation to re-establish consistency between the line shape formulation and the most up-to-date measurements of the water vapour continuum. As a result, the computed continuum coefficients in spectral regions without compelling continuum measurements would also be consistent with the latest measurements. As discussed above, the multiplicative \(\chi\)-function that characterized the CKD approach was replaced by a revised formulation that was not suggestive of super-Lorentzian behaviour in the near-to-intermediate wings of allowed transitions of the water vapour monomer.

(a) Continuum absorption coefficients used in the fitting procedure

In the least-squares fitting procedure that was employed to determine values for the free parameters in the MT_CKD formulation, strongly weighted constraints were placed with respect to continuum absorption coefficients that were well grounded in accurate field measurements to ensure that the new continuum in those regions agreed with those values within the measurements' respective uncertainties. In addition, in certain spectral regions, the CKD continuum absorption coefficients were used as lesser-weighted constraints to ensure that continuity with the previous continuum model could be attained to as great an extent as possible.
For the foreign continuum, the continuum coefficients from the following spectral regions were used in the least-squares fitting procedure (all values in inverse centimetres):

- 0, 10: CKD_2.4.1 values used, based on Burch’s [13] measurements and ground-based measurements from the Southern Great Plains (SGP) site of the Department of Energy (DoE) Atmospheric Radiation Measurement (ARM) programme [18].
- 480–750: CKD_2.4.1 values used.
- 1300–2000: modified values of the CKD_2.4.1 coefficients derived from measurements from the high-spectral-resolution infrared sounder (HIS) [21].

For the self continuum, the continuum coefficients from the following spectral regions were used in the least-squares fitting procedure (all values in inverse-centimetres):

- 0: CKD_2.4.1 value used, based on ground-based measurements from the DoE ARM SGP site.
- 1310–1540, 1660–2040: CKD_2.4.1 values used.
- 1550–1650: used values from Tobin et al. [23].

(b) The MT_CKD formulation

The following empirically derived equations satisfactorily reproduced the absorption coefficients (see §3a) used as constraints in the fitting process, and were used to generate the MT_CKD_1.0 continuum coefficients.

(i) MT_CKD foreign continuum

The continuum is the sum of two contributions: the ‘allowed’ term and the ‘weak interaction’ term. The allowed term is given by equations (2.7)–(2.9) with a χ-function given by

\[
\chi_a(\nu \pm \nu_i) = \left(1 + \frac{|\nu \pm \nu_i|}{\gamma_a}\right) \exp \left(-\frac{|\nu \pm \nu_i|}{\gamma_a}\right) \quad \gamma_a = 61.5 \text{ cm}^{-1} .
\]

The weak interaction term is given by the following equation:

\[
\sum_i \frac{\tilde{S}_i \alpha_{WI}/\pi}{\alpha_{WI}^2 + (\nu - \nu_i)^2} \left\{ \xi_{i, WI} \exp \left[-\left(\frac{\nu - \nu_i}{\gamma_{WI}}\right)^2\right] \right\} \quad \alpha_{WI} = 70.09 \text{ cm}^{-1} \quad \gamma_{WI} = 54.05 \text{ cm}^{-1},
\]
Development, evaluation of MT_CKD model

where the sum is over all lines $i$ with strength $S_i$ and position $\nu_i$. The relative strength of interaction term $\zeta_{i, WI}$ is given by

$$
\zeta_{i, WI} = \begin{cases} 
A_\uparrow \exp \left[ -\frac{(E_i''/\eta_\uparrow)^2}{\Delta J_i > 0 \text{ or } \Delta J_i = 0, \Delta K_{a,i} > 0 \text{ or } \Delta J_i = 0, \Delta K_{c,i} = 0, \Delta K_{a,i} > 0} \right] 
\Delta K_{a,i} = 0, \Delta K_{c,i} > 0, 
\end{cases}
$$

$$
A_\uparrow = 0.0658, \quad \eta_\uparrow = 255.9 \text{ cm}^{-1},
A_\downarrow = 0.0596, \quad \eta_\downarrow = 411.5 \text{ cm}^{-1}, \quad (3.3)
$$

where, for the transition $i$, $E_i''$ is the lower energy state, and $J_i$, $K_{a,i}$ and $K_{c,i}$ are the rotational quantum numbers. (‘R-branch’ transitions correspond to the subscript ‘$\uparrow$’ and ‘P-branch’ transitions to ‘$\downarrow$’.) The exponential term in equation (3.3) is present to make the weak interaction term relatively less spectrally broad than the water vapour monomer absorption bands, consistent with observations. The large difference between $\eta_\uparrow$ and $\eta_\downarrow$ does not reflect the need for a qualitatively different parametrization of this ‘narrowing’ effect for the ‘$\uparrow$’ and ‘$\downarrow$’ transitions, but rather the generally different magnitude of the $E''$ terms for the ‘$\uparrow$’ and ‘$\downarrow$’ transitions.

The contributions of the allowed and weak interaction terms to the MT_CKD foreign continuum are shown in figure 1.

(ii) MT_CKD self continuum

As for the foreign, the continuum is the sum of the ‘allowed’ term and the ‘weak interaction’ term. The allowed term is given by equations (2.7)–(2.9) with a $\chi$-function given by

$$
\chi_a(\nu \pm \nu_i) = \exp \left[ -\left( \frac{|\nu \pm \nu_i|}{\gamma_a} \right)^{p_a} \right] \quad p_a = 1.462, \quad \gamma_a = 310.5 \text{ cm}^{-1}. \quad (3.4)
$$

The weak interaction term is given by the following equation:

$$
\sum_i \frac{\tilde{S}_i \alpha_{WI}/\pi}{\alpha_{WI}^2 + (\nu - \nu_i)^2} \left\{ \zeta_{WI} \exp \left[ -\frac{(\nu - \nu_i)^2}{\gamma_{WI}} \right] \right\}
\alpha_{WI} = 87.72 \text{ cm}^{-1}, \quad \gamma_{WI} = 306.6 \text{ cm}^{-1}, \quad (3.5)
$$

where the sum is over all lines $i$ with strength $S_i$ and position $\nu_i$. The relative strength of interaction term $\zeta_{i, WI}$ is given by the same functional form as equation (3.3) with $A_\uparrow = 1.660, \eta_\uparrow = 62.77 \text{ cm}^{-1}, A_\downarrow = 1.561, \text{ and } \eta_\downarrow = 105.1 \text{ cm}^{-1}$.

(c) Modifications to the MT_CKD continuum model

As was the case for the CKD continuum formulation, in the years since the development of the MT_CKD formulation and the release of MT_CKD_1.0, a number of well-founded measurement-based studies have indicated that the MT_CKD continuum absorption coefficients needed adjustment in certain spectral regions. As a result, revisions to the continuum model have been released
with modified coefficients in these regions; however, the MT_CKD line shape formulation has not been adjusted to reflect these changes. Notable MT_CKD model versions include:

— MT_CKD_1.1 (2004): the MT_CKD_1.0 foreign coefficients agreed well with the Tobin et al. [17] continuum values near 430 cm$^{-1}$ that were used in the least-squares fitting procedure described above, but these values were not particularly consistent with the continuum values from the same study at slightly lower (400–415 cm$^{-1}$) and higher (445–450 cm$^{-1}$) wavenumber values. This led to the MT_CKD_1.0 continuum values being somewhat greater than the corresponding CKD_2.4.1 values in this region. Reconsideration of this issue after the release of MT_CKD_1.0 led to the release of MT_CKD_1.1 with foreign continuum coefficients from 250 to 550 cm$^{-1}$ modified to be more consistent with those in CKD_2.4.1.

— MT_CKD_2.0 (2007): this revision to the CO$_2$ continuum is relevant to the analysis presented in §4. Coinciding with the release of LBLRTM_v11.1, the first version of this model with first-order line coupling implemented for the P, Q and R branches of CO$_2$ bands, a complete recalculation of the CO$_2$ continuum was performed so that it would be consistent with the newly implemented line shape. In the region of the CO$_2$ $v_3$ band (approx. 2350 cm$^{-1}$), the computed CO$_2$ continuum was lowered by approximately 25 per cent to obtain consistency with atmospheric infrared sounder (AIRS) measurements. These values remained in MT_CKD until the analysis presented here, and can be found in the last column of table 1.
Table 1. MT_CKD_2.5 and MT_CKD_2.4 CO2 continuum scaling factors. Values are relative to CO2 continuum coefficients computed with first-order line coupling and $\chi = 1$—see description of MT_CKD_2.0 in §3.3 for more details.

<table>
<thead>
<tr>
<th>wavenumber (cm$^{-1}$)</th>
<th>MT_CKD_2.5</th>
<th>MT_CKD_2.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>2380</td>
<td>0.690</td>
<td>0.754</td>
</tr>
<tr>
<td>2390</td>
<td>0.691</td>
<td>0.757</td>
</tr>
<tr>
<td>2395</td>
<td>0.718</td>
<td>0.758</td>
</tr>
<tr>
<td>2400</td>
<td>0.807</td>
<td>0.760</td>
</tr>
<tr>
<td>2405</td>
<td>0.927</td>
<td>0.761</td>
</tr>
<tr>
<td>2410</td>
<td>1.033</td>
<td>0.763</td>
</tr>
<tr>
<td>2420</td>
<td>1.135</td>
<td>0.767</td>
</tr>
<tr>
<td>2430</td>
<td>1.220</td>
<td>0.772</td>
</tr>
<tr>
<td>2440</td>
<td>1.296</td>
<td>0.776</td>
</tr>
<tr>
<td>2450</td>
<td>1.366</td>
<td>0.781</td>
</tr>
<tr>
<td>2460</td>
<td>1.432</td>
<td>0.787</td>
</tr>
<tr>
<td>2470</td>
<td>1.495</td>
<td>0.793</td>
</tr>
<tr>
<td>2480</td>
<td>1.555</td>
<td>0.799</td>
</tr>
<tr>
<td>2500</td>
<td>1.555</td>
<td>0.812</td>
</tr>
<tr>
<td>2550</td>
<td>1.542</td>
<td>0.847</td>
</tr>
<tr>
<td>2600</td>
<td>1.460</td>
<td>0.882</td>
</tr>
</tbody>
</table>

— MT_CKD_2.01 (2007): based on a preliminary analysis of AERI-ER measurements from the DoE ARM Northern Slope of Alaska (NSA) site, the foreign continuum coefficients from 250 to 550 cm$^{-1}$ were increased.

— MT_CKD_2.4 (2008): detailed analysis [24] of AERI-ER measurements at the DoE ARM NSA site, including those from the Radiative Heating in Underexplored Bands Campaign [25], as well as analysis of microwave measurements [26], resulted in modifications to the foreign and self-continuum coefficients in the 0–600 cm$^{-1}$ region.

The following section provides details about the measurement-based analysis which is the basis for MT_CKD_2.5, the most recent version of the continuum model. Another continuum-related measurement dataset that may have an impact on future versions of MT_CKD consists of recent laboratory investigations (e.g. [27]) performed as part of the Continuum Absorption at Visible and Infrared wavelengths and its Atmospheric Relevance (CAVIAR) programme. CAVIAR measurements have supported the existence of continuum absorption aligned with monomer absorption bands, but also have provided compelling evidence that there is continuum absorption associated with pure water vapour which is in agreement with ab initio calculations of the absorption spectrum of true water–water bound states (i.e. water dimer) [28]. Validated water dimer absorption will need to be included in LBLRTM calculations and, hence, the MT_CKD continuum, but as it is not associated with monomer transitions, these features cannot be generated by the MT_CKD line shape formulation. Dimer absorption may present an additional challenge for MT_CKD in that...
Table 2. Measurement of datasets used in this study to determine MT_CKD_2.5 continuum coefficients. PWV, precipitable water vapour.

<table>
<thead>
<tr>
<th>instrument</th>
<th>platform</th>
<th>dates</th>
<th>PWV range (cm)</th>
<th>temperature and H$_2$O profile information</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIRS</td>
<td>satellite, over ARM TWP site</td>
<td>Sep 2002–Oct 2003</td>
<td>4.0–5.6</td>
<td>for each case, 2 collocated RS90 radiosondes with staggered launches, PWV scaled to agree with microwave measurement</td>
<td>Aumann et al. [29]</td>
</tr>
<tr>
<td>IASI</td>
<td>satellite, global over ocean</td>
<td>Apr 2008</td>
<td>0.3–5.5</td>
<td>ECMWF analysis</td>
<td>Richter &amp; Wagner [30]</td>
</tr>
<tr>
<td>AERI</td>
<td>ground-based, ARM SGP site</td>
<td>Jan 1999–Dec 2001</td>
<td>0.5–5.0</td>
<td>collocated RS-80 radiosondes, PWV scaled to agree with microwave measurement</td>
<td>Knuteson et al. [19,20]</td>
</tr>
</tbody>
</table>

self-continuum coefficients near 1600 cm$^{-1}$ that constrained the least-squares fit used to develop the MT_CKD_1.0 self continuum have been suggested (I. V. Ptashnik 2007, personal communication) to be actually owing to the dimer, which would necessitate a re-derivation of the MT_CKD line shape formulation for the self continuum.

4. Continuum absorption in the ‘bandhead’ of the carbon dioxide 4.3 $\mu$m band

We now present a recent analysis based on comparisons between LBLRTM calculations and measurements from three different instruments in the 2385–2600 cm$^{-1}$ (3.85–4.20 $\mu$m) spectral region that resulted in the revised continuum model MT_CKD_2.5. The measurement datasets used in this study are summarized in Table 2.

An interesting feature of the $v_3$ band of CO$_2$ is its ‘bandhead’ at approximately 2385 cm$^{-1}$, a consequence of the frequency gap between consecutive rotational lines in this band’s R-branch transitioning from positive to negative values. This results in a relatively abrupt termination of R-branch absorption lines at this wavenumber value, and an associated dramatic decrease in the atmospheric opacity with increasing wavenumber values in the vicinity of the bandhead (Figure 2). For example, for a satellite measurement in a typical terrestrial atmosphere, the transition between radiance measurements being sensitive to stratospheric conditions to those sensitive to boundary layer conditions (passing through all intervening vertical layers) occurs over a spectral interval of 40–50 cm$^{-1}$ (Figure 3). Especially given the significant dependence of the Planck function on temperature for wavenumbers >2000 cm$^{-1}$, spectrally resolved satellite measurements from this limited spectral region contain a great deal of...
information on atmospheric temperature profiles, and therefore hold enormous potential for temperature remote sensing if accurate knowledge of the absorption properties of all gases that are active in this region can be obtained.

As seen in figure 2, the key absorbers with continuum absorption in the spectral region past the CO$_2$ $\nu_3$ bandhead (i.e. 2385–2500 cm$^{-1}$) are N$_2$, CO$_2$ and H$_2$O. In LBLRTM, these absorbers are included in this region as a combination of continuum and line absorption. The version of the model used for the baseline results in this study is an extension (see below for specifics) of LBLRTM_v11.6, referred to herein as ‘LBLRTM_v11.6+’.

Details about the optical depth calculation in LBLRTM_v11.6+ related to these three key absorbers are as follows:

— N$_2$: the nitrogen collision-induced fundamental absorption band centred at approximately 2330 cm$^{-1}$ is included in MT_CKD_2.4 based on the highly accurate formulation of Lafferty et al. [31]. This implementation includes temperature dependence and includes the varying efficiencies of nitrogen and oxygen molecules as collision partners with the absorbing nitrogen molecule. The efficiency of water vapour as a collision partner is not accounted for, contributing a small amount of additional uncertainty in the determination of the CO$_2$ continuum coefficients presented below. Should the efficiency of water vapour be as high as that measured by Baranov [32], a moderate reduction in the amount of absorption attributed to the water vapour continuum in this analysis may be warranted.

— CO$_2$: to form LBLRTM_v11.6+, LBLRTM_v11.6 was modified to include the line positions and intensities in the spectral range 597–2500 cm$^{-1}$ from the Carbon Dioxide Spectral Database (CDS), maintained by Tashkun, as implemented in the hitran_mipas_pf3.2 line file [33,34]. The first-order line-coupling coefficients were then recalculated using the formalism of Niro et al. [11]. No additional non-Voigt modifications were made to the
Figure 3. For the 36 cases in the AIRS dataset (see text): (a) average AIRS brightness temperature measurements (solid line) and corresponding calculations using LBLRTM_v11.6+/MT_CKD_2.4 (dashed line); (b) average residuals between AIRS and LBLRTM_v11.6+/MT_CKD_2.4; (c) average residuals after the CO$_2$ continuum in LBLRTM_v11.6+ was modified; (d) average residuals after temperature dependence of the CO$_2$ continuum was added to the model version used in (c); (e) average residuals after a modification to the water vapour continuum in LBLRTM_v11.6+ was added to the changes used in (d)—the resulting model is LBLRTM_v11.7 and the continuum version is MT_CKD_2.5. (Online version in colour.)
Development, evaluation of MT_CKD model

(lines i.e. $\chi = 1$). The CDSD line parameters and coupling coefficients were validated within the $\nu_2$ and $\nu_3$ bands using measurements from the AIRS and the infrared atmospheric sounding interferometer (IASI).

— $\text{H}_2\text{O}$: under typical conditions, absorption owing to $\text{H}_2\text{O}$ in this region is dominated by the self continuum. For both the self and foreign continuum, the coefficients in MT_CKD_2.4 follow from the mathematical continuum formulation described above (i.e. they are the same as in MT_CKD_1.0).

(a) Measurements used in the analysis

Comparisons between spectrally resolved radiometric measurements and corresponding line-by-line radiation calculations provide a powerful technique for evaluating and improving the spectroscopic parameters used by radiative transfer models. These spectral radiative closure studies necessitate a simultaneous critical evaluation of the quality of the measurements, the spectroscopic information used in the calculation and the atmospheric properties used by the model to represent the atmospheric state within the field of view of the instrument. Even with thorough attention given to these three key components of a closure study, the determination of ‘truth’ in these studies can be elusive. For example, residuals in one spectral region might suggest an issue with an input temperature profile, but those in another may not. Two spectral regions influenced by the same species can provide differing levels of measurement–model agreement, leaving it unclear which region’s absorption parameters may need modification. Different instruments may provide contradictory messages.

These examples underscore two important necessities of a closure study—that key uncertainties receive appropriate consideration and what constitutes ‘agreement’ between the measurements and calculations is defined. One uncertainty that all radiative closure studies have to deal with is the degree to which the atmospheric profile input to the radiative transfer model is representative of the conditions seen by the radiometric instrument. Radiosondes can provide an excellent first guess with respect to temperature and water vapour profiles, as is the case for two of the three measurement datasets used in this study, but they have known limitations. The high uncertainty associated with water vapour profiles from radiosondes in cold and dry conditions (e.g. [35]), such as the upper troposphere, will not have an effect on the analysis presented here as the relevant water vapour absorption is due to the self continuum and therefore occurs near the surface. For the same reason, uncertainty in the representativeness of the water vapour profile owing to radiosonde drift during flight is not an issue for the ground-based study shown here, and has been dealt with appropriately for the satellite-based study that uses radiosondes (see below). Other issues related to profile representativeness do affect the analysis presented here, such as the impact of radiosonde drift on temperature profiles relevant to $\text{N}_2$ and $\text{CO}_2$ radiative processes and, for the satellite studies, the ability of a single temperature and water vapour profile to represent the distribution of conditions within the instrument’s field of view. These issues prevent a clear understanding of what constitutes ‘truth’ in a radiative closure study such as the one presented here. As a result, it is necessary that the definition of agreement between measurement and model be based on the concept of consistency across as wide a set of conceptual dimensions as possible given the experimental design: consistency

Phil. Trans. R. Soc. A (2012)
between results from different instruments, viewing geometries, atmospheric properties, as well across spectral bands from the same species and bands from different species.

This study uses three different instruments that provide spectrally resolved measurements past the bandhead of the CO$_2$ $v_3$ band; two satellite-based and one ground-based instrument (table 2). This variety in perspectives on the radiating environment, plus the diversity of water vapour loadings associated with two of the three datasets, provides confidence that our analysis will be sufficiently broad.

One validation dataset, provided by L. Strow and S. Hannon (UMBC), consists of clear sky, night-time, ocean AIRS measurements made during the ‘phase 1’ AIRS validation over the DoE ARM Tropical Western Pacific (TWP) site between September 2002 and April 2003. This dataset was used extensively in the tuning of the AIRS operational fast forward model [36]. The input profiles, provided on the AIRS standard 100 layers, were based on the Tobin et al. [37] ‘best estimate’ profiles, constructed from radiosonde launches specifically timed to coincide with AIRS overpasses. Two radiosonde launches were used for each best estimate profile, with launches timed to account for the time taken for the sondes to ascend over their altitude range in order that the combination of the upper and lower parts of the profiles would adequately represent the instantaneous profile observation captured by the AIRS measurements. The best estimate water vapour profiles were scaled to agree with the column water vapour measured by a collocated ground-based microwave radiometer. The ozone profiles were from European Centre for Medium-range Weather Forecasting (ECMWF) analyses. The CO$_2$ profiles were taken from the US standard atmosphere, but scaled to have a volume mixing ratio of approximately 372ppm. The carbon monoxide and methane profiles from the US standard atmosphere were scaled to give a good fit in the relevant spectral regions. All other trace gas profiles were from the US standard atmosphere. The set of 36 AIRS matches used in this analysis corresponds to only eight of these best estimate profiles. While this AIRS/ARM dataset provides a limited number of profiles and a limited range of column water vapour values (4.0–5.6cm), it offers a relatively accurate specification of the atmospheric state (although it has a bias in the average sea surface temperature of around $-0.2$ K).

A global dataset of 129 clear sky, night-time, ocean, near-nadir IASI measurements has been supplied by M. Matricardi (ECMWF) along with the corresponding ECMWF analysis information (surface temperature, temperature, water vapour, ozone). This is a subset of the dataset discussed by Matricardi [38]. All cases are from the time period 1–10 April 2008, and correspond to a wide range of column water vapour values. The constant CO$_2$ mixing ratio (below 0.1Mb) for each profile ranges from 382 to 394 ppm. The ECMWF analysis used as input to LBLRTM should certainly not be regarded as ‘truth’ for the atmospheric and surface state. There are some obvious moist biases in the water vapour in this dataset, particularly in the tropics, as well as an average high bias of around 0.2 K in the sea surface temperatures supplied. However, averaging the large number of profiles in this dataset reduces instrument noise issues and diminishes the effect of random differences between the true state and the ECMWF model.

The ground-based dataset used in this study is from the AERI [19,20]. For more than a decade, AERI instruments have been located at the DoE ARM SGP site in Oklahoma and the NSA site in Barrow, Alaska. Their accuracy and
Development, evaluation of MT_CKD model

reliability have led to their use in numerous studies (e.g. [22] and references therein). Three years worth of AERI SGP data—from the beginning of 1999 to the end of 2001—have been used for this work. Atmospheric temperature and humidity profiles are from 240 clear sky, collocated RS-80 radiosondes, with the column water vapour scaled to agree with an on-site microwave radiometer. The need for this scaling of column water vapour arises from demonstrated inaccuracies in RS-80 water vapour measurements (e.g. [39]) and the consequent need to reduce the random error in column water vapour [40] for radiative closure analysis. The AERI measurements used in this study are continuous in time and the radiosondes are launched from the same location as the AERI is situated, thereby minimizing errors in the representativeness of the atmospheric state used as input to the model. The AERI SGP dataset offers a wide range of atmospheric conditions, with column water vapour values ranging from around 0.5 to 5 cm. For these ground-based model–measurement comparisons, there are no issues with uncertainty in the surface parameters, a factor that differentiates this dataset from the satellite-based measurements that are also used in this study.

(b) Comparison between measurements and unmodified model

For all three datasets used in this study, comparisons between measurements and LBLRTM_v11.6+ were performed. For the AIRS dataset, figure 3a presents the average measured and calculated brightness temperatures, while figure 3b shows the average measurement–calculation residuals. Similarly, figure 4a shows the average IASI brightness temperatures and corresponding model calculations for the cases analysed in this study. The average differences between the measurements and calculations are shown in figure 4b. Finally, figure 5a shows the average AERI radiance measurements and corresponding calculations and figure 5b shows the measurement–calculation residuals.

As the residual results shown in figures 3–5 are for cases spanning a large range of water vapour loadings and atmospheric temperature profiles, they are limited in their ability to identify specific deficiencies in the calculation of optical depths for individual species in the model. However, the comparisons with the measurements from all three instruments paint a consistent picture that the optical depth computed by LBLRTM is not sufficient to provide closure with radiometric observations.

Measurement–model comparisons for individual cases can provide a better qualitative indication of possible model deficiencies. Figure 6a(i), b(i) shows the residuals associated with two AERI (figure 6a(i)) and two IASI (figure 6b(i)) measurements. For each instrument, one measurement corresponds to a low (black curve) water vapour loading and one to a high (grey curve) loading, where the residuals for each case shown are generally representative of the residuals for other cases analysed with similar column amounts of water vapour. For the dry case for each instrument, there are discernible measurement–calculation discrepancies between 2400 and 2450 cm\(^{-1}\). (It should be emphasized that, for the IASI cases, no adjustment has been made to account for errors in surface temperature, so for the black curve shown in figure 6b(i), the effective ‘zero line’, which can be determined from the residuals in the most transparent spectral region (2500–2600 cm\(^{-1}\)), is approximately +0.5 to +0.75 K. Figure 6a(ii–v), b(ii–v) indicates, for each instrument, the sensitivity of the modelled radiances to four modifications.
to model parametrizations:

— A 10 per cent adjustment to the CO$_2$ continuum in MT_CKD_2.4.
— The scaling to the MT_CKD continuum that was determined by Strow et al. [36] based on comparisons with AIRS cases (same dataset used here) and ground-based measurements.
Figure 5. Same as figure 3, except for the 240 cases in the AERI dataset (see text). Comparisons are for radiances and in ‘radiance units’, 1 r.u. = 1 mW (m² sr cm⁻¹)⁻¹. (Online version in colour.)

— An adjustment to the MT_CKD self continuum consistent with the measurements of Burch & Alt [5].
— A 25 per cent adjustment to the N₂ continuum in MT_CKD_2.4. (Note: this change is in excess of the estimated uncertainty for this absorber.)
Figure 6. (a) The AERI residuals with MT_CKD_v2.4 and the sensitivity of modelled downwelling (AERI) radiances to the preliminary AER CO₂ continuum adjustment, Strow et al.’s [36] H₂O continuum adjustment, the self H₂O continuum suggested by the Burch laboratory measurements and a 25% change in the N₂ continuum, for a wet and a dry case. (b) The IASI residuals with MT_CKD_v2.4 and the sensitivity of modelled upwelling brightness temperatures to the same parameters for the same variables, for a wet and a dry case. The sensitivity is defined as the calculation for the perturbed condition minus the calculation for the reference condition.

The results in figure 6a(ii), b(ii) suggest that the adjustment shown to the CO₂ continuum would substantially reduce the spectral residual in the dry case, but there would still be remaining residuals in the moist case. The
AERI sensitivity results for the CO$_2$ and N$_2$ perturbations indicate that even an optical depth deficiency unrelated to H$_2$O will result in a significant correlation of radiance residuals with respect to water vapour loading. This is because of the strong (compared with the atmospheric window) dependence of emitted radiance in this spectral region on temperature, coupled with the substantial correlation between temperature and water vapour abundance. This behaviour complicates the interpretation of the ground-based residuals. In contrast, neither the CO$_2$ nor the N$_2$ perturbation is distinguishable for the two IASI cases analysed in figure 6. An analysis of the complete ground- and satellite-based datasets, each corresponding to a wide range of water vapour loadings, will allow deficiencies in modelling ‘dry’ and ‘wet’ absorption to be distinguished.

(c) Residual analysis and modifications to MT_CKD

Water vapour continuum absorption in the spectral region past the CO$_2$ $\nu_3$ bandhead is dominated by the self continuum, which, because of its quadratic dependence on H$_2$O concentration, is extremely weak for dry atmospheres. Therefore, in this analysis, IASI and AERI cases with low H$_2$O column amounts can be used to analyse the accuracy of the ‘dry’ absorber with significant uncertainty, the CO$_2$ continuum. Figure 7a shows the measured IASI brightness temperatures in the spectral region of interest for those cases in our dataset having less than 2 cm of precipitable water vapour (PWV), as well as corresponding LBLRTM_v11.6+ calculations. Figure 7b shows the measurement–calculation residuals for these cases. The shaded bar in this figure shows the range of brightness temperature residual values for which the measurement and model are considered to be in agreement. The width of this bar is based on IASI measurement uncertainty, while the bar’s placement is determined by the residuals in the very transparent 900 cm$^{-1}$ region (not shown) for the same set of cases. For this subset of cases, the average measured and calculated brightness temperatures in the 900 cm$^{-1}$ region agree, implying that on average there is no overall error from any inaccuracy in the sea surface temperature and lower atmosphere water vapour abundances used in these calculations; for other PWV-based subsets of IASI cases used in this study, these residuals are non-zero, so the IASI plots in this paper explicitly show this shaded ‘zone of agreement’.

Figure 8a,b shows, respectively, the AERI radiance measurements and associated LBLRTM_v11.6+ calculations for cases corresponding to 0–2 cm of PWV and the radiance residuals for these cases. Both the IASI and AERI residuals indicate that the MT_CKD_2.4 CO$_2$ continuum in the spectral region past the $\nu_3$ bandhead is not able to provide suitable radiative closure.

Based on these ‘dry’ results, an empirical adjustment to the CO$_2$ continuum was determined and implemented in MT_CKD_2.5. The derived scale factors for the region near and past the bandhead are shown in table 1. (These values are relative to the continuum coefficients computed with line coupling and $\chi = 1$. The corresponding MT_CKD_2.4 scale factors are also shown for reference.) Where this analysis offered no new evidence, such as within the $\nu_3$ band, the continuum coefficients in MT_CKD_2.5 remained similar to those in MT_CKD_2.4. The residuals resulting from the model change are shown for the dry IASI and AERI cases in figures 7c and 8c, respectively.
The applicability of the adjusted CO$_2$ continuum coefficients for conditions other than those for which they were derived was evaluated using IASI and AERI cases with higher PWV values. Figures 9 and 10 show the results for these two instruments for cases with PWV = 2–4 cm, with figures 9a–c and 10a–c showing results analogous to those shown in figures 7 and 8. Similarly, figures 11

*Phil. Trans. R. Soc. A* (2012)
and 12 present the IASI and AERI results for cases in each dataset with PWV in the range of 4–6 cm. The IASI residuals for these higher PWV cases show a distinct feature from 2390 to 2400 cm\(^{-1}\), which, because of its proximity to the bandhead, is suggestive of an additional deficiency in the specification of CO\(_2\) absorption, possibly in the CO\(_2\) continuum. However, as these residuals are within 25 cm\(^{-1}\) of strong CO\(_2\) lines on the low wavenumber side of the bandhead, it is also possible that these measurement–calculation differences may be owing to an issue involving the portion of the absorption line considered by LBLRTM to be the ‘local line’ contribution.
Figure 9. Same as figure 3, except for the 60 cases in the IASI dataset with precipitable water vapour values between 2 and 4 cm (see text). See text for explanation of the shaded ‘zone of agreement’. (Online version in colour.)

The first-order line coupling coefficients for CO$_2$ depend on temperature and, in LBLRTM, coefficients are stored at four temperatures—340, 296, 250 and 200 K—with linear interpolation performed for temperatures in between. The unscaled continuum coefficients in MT_CKD have been computed based on a calculation.

Phil. Trans. R. Soc. A (2012)
Development, evaluation of MT_CKD model

of CO$_2$ line absorption using the line coupling coefficients at a single temperature (296 K). However, if the temperature dependence of the line coupling coefficients significantly impacts the line shape more than 25 cm$^{-1}$ from line centre, then there may be need for the continuum coefficients also to be parametrized accounting for temperature dependence. The MT_CKD_2.5 empirical adjustment described above not only accounts for a non-unity $\chi$-function but also effectively adjusts for any temperature dependence of the continuum coefficients for temperatures not near 296 K. (That is, the MT_CKD_2.5 scale factors in table 1 have been derived based on the profiles in the 0–2 cm PWV IASI and AERI datasets.

Figure 10. Same as figure 5, except for the 48 cases in the AERI dataset with precipitable water vapour values between 2 and 4 cm (see text). (Online version in colour.)
and are appropriate for the general range of temperatures that characterize the main emitting layers for cases in these datasets, but there is no guarantee that these scale factors will apply to CO$_2$ absorption at different temperatures.) To evaluate the level of temperature dependence in the CO$_2$ continuum, continuum

*Phil. Trans. R. Soc. A* (2012)
coefficients were calculated at 340, 250 and 200 K, and compared with those computed at 296 K and stored in MT_CKD (figure 13). As can be seen, there is notable dependence on temperature in the spectral region past the bandhead up to approximately 2435 cm\(^{-1}\). From the values plotted in this figure, a parametrization was developed for MT_CKD_2.5 to account for this temperature dependence while leaving the IASI and AERI results for the 0–2 cm PWV range unchanged. The results for the various PWV bins for the IASI and AERI datasets can be seen in figures 7d, 8d, 9d, 10d, 11d and 12d.
The hump-like feature seen previously is no longer present, establishing that its cause was the lack of temperature dependence in the CO$_2$ continuum parameterization in MT$_{-}$CKD$_{-}$2.4.

The remaining measurement–calculation residuals shown in these figures for the IASI and AERI datasets are spectrally smooth and increase with PWV. Given that absorption sources other than water vapour have been analysed and adjusted, these residuals are probably owing to a deficiency in the MT$_{-}$CKD parametrization of the water vapour continuum. In this spectral region between water vapour bands, the optical depth of the foreign continuum is not significant; so we consider what is known about the accuracy of the self continuum in window regions in the infrared and near-infrared. As discussed in §2, extensive analysis of surface-based radiance measurements in the infrared atmospheric window (800–1000 cm$^{-1}$) has determined the self-continuum absorption to impressive accuracy (approx. 5%) in this region. In both the MT$_{-}$CKD and CKD self-continuum models, the coefficients in analogous window regions (such as 2400–2600 cm$^{-1}$) are predominantly the result of the component of mathematical line shape formulation (e.g. equation (3.4)) needed to fit the known values in the infrared window. As discussed above, the MT$_{-}$CKD self continuum in the infrared window primarily arises from the far wings of water vapour lines in the pure rotation band, which are approximately 800 cm$^{-1}$ from that window. The assumption that equation (3.4) defines the far-wing behaviour of water vapour lines may be sufficient for computing the self-continuum coefficients at 2400 cm$^{-1}$ that arise from the far wings of lines in the $\nu_2$ fundamental band (at approx. 1600 cm$^{-1}$; i.e. 900 cm$^{-1}$ away), but there is no reason to expect that the contributions of the very far wings of lines in the pure rotation band (>2000 cm$^{-1}$ away) will be
Development, evaluation of MT_CKD model

correctly accounted for. The datasets analysed here provide an excellent field-measurement-based opportunity to evaluate the applicability of the line shape given by equation (3.4) far from line centre.

Laboratory-based studies in near-infrared window regions have also indicated that the MT_CKD and CKD self-continuum coefficients may be too low. Self-continuum measurements at 296 K presented by Burch & Alt [5] for the 2400–2640 cm\(^{-1}\) spectral region are two to four times greater than those produced by the MT_CKD formulation. (Calculations (not shown) using the Burch & Alt [5] coefficients do not provide suitable radiative closure for the datasets analysed here.) Bicknell et al. [41] presented laboratory measurements of the water vapour continuum at spectral locations situated within windows between water vapour bands at approximately 4600 cm\(^{-1}\) (2.17 \(\text{\mu m}\)) and approximately 6140 cm\(^{-1}\) (1.63 \(\text{\mu m}\)). Assuming that the self continuum is the predominant source of continuum absorption and accounting for the uncertainty in the measurement at 4600 cm\(^{-1}\), the measured self-continuum values in this study are 6–12 times higher than those in MT_CKD. At 6140 cm\(^{-1}\), the measurements are two to four times greater. Another laboratory measurement relevant to the issue of continuum absorption in window regions is owing to Fulghum & Tilleman [42]. This measurement was performed at 9466 cm\(^{-1}\), a location at the edge of a near-infrared window, for an atmosphere with a water vapour volume mixing ratio of 0.022. For these conditions, the foreign continuum provides approximately 10 per cent of the total continuum optical depth in MT_CKD. This laboratory measurement is consistent with an increase of a factor of 2–3 in the MT_CKD self-continuum coefficients in this region. The results from these three near-infrared laboratory studies were not used to develop the MT_CKD self-continuum line shape formulation described in §3. Had this formulation been constrained to agree with the well-established infrared window continuum values plus these near-infrared measurements, the functional form for the allowed term (i.e. equation (3.4)) would have had to be modified.

To evaluate whether the 2385–2600 cm\(^{-1}\) IASI and AERI results shown above are consistent with the laboratory measurements of Bicknell et al. [41] and Fulghum & Tilleman [42], the least-squares fitting procedure described in §3 was repeated including these additional constraints. This necessitated that the exponential piece of the allowed term (equation (3.4)) be modified to include a second term to permit a slower decay at ‘long range’ (i.e. very far wings of lines),

\[
\chi_a(v - v_i) = \frac{1}{1 + S_{lr}} \left\{ \exp \left[ - \left( \frac{|v - v_i|}{\gamma_a} \right)^{p_a} \right] + S_{lr} \exp \left[ - \left( \frac{|v - v_i|}{\gamma_{lr}} \right)^{p_{lr}} \right] \right\}. \quad (4.1)
\]

For the three long-range parameters, \(S_{lr}\), \(p_{lr}\) and \(\gamma_{lr}\), the least-square fit yielded 0.128, 1.384 and 5365 cm\(^{-1}\), respectively. The parameters still present from the original version of this term, \(p_a\) and \(\gamma_a\), underwent small shifts (to 1.641 and 338.6 cm\(^{-1}\), respectively) to maintain agreement with the unmodified constraints in the infrared window. With these values, the fit was able to provide agreement within the stated uncertainties with the laboratory measurements at 4600, 6410 and 9466 cm\(^{-1}\), while providing equivalent results to the MT_CKD formulation with respect to all existing constraints. In the region past the CO\(_2\) \(\nu_3\) bandhead (2385–2500 cm\(^{-1}\)), the continuum coefficients derived from the new fit were greater than those in MT_CKD by factors ranging from 4.8 to 7.4 (table 3).
Table 3. MT_CKD_2.5 H₂O self-continuum scaling factors relative to MT_CKD_1.0 coefficients.

<table>
<thead>
<tr>
<th>wavenumber (cm⁻¹)</th>
<th>scale factor</th>
<th>wavenumber (cm⁻¹)</th>
<th>scale factor</th>
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<td>2500</td>
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<td>1.18</td>
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</table>

These values are not as large as those found in recent laboratory-based analyses of water vapour continuum absorption in this region [43,44], and are also smaller than the scale factors advocated by Strow et al. [36] from field measurements. All studies consistently point to the need for greater absorption than in MT_CKD_1.0.

These new continuum values were then used in LBLRTM calculations and compared with measurements in the IASI and AERI datasets. The associated average measurement–calculation residuals are shown in figures 7e, 8e, 9e, 10e, 11e and 12e. For all categories analysed, the calculations are in agreement with the measurements within the respective uncertainties. Figures 9e and 11e, taken together, indicate that either a modest decrease or increase in the derived MT_CKD_2.5 water vapour continuum coefficients would negatively impact the level of agreement in one of the two datasets analysed in these figures. To provide an independent check on this self-continuum modification, calculations were performed for the AIRS dataset described above. The comparisons between measurement and calculation are shown in figure 3e. As all AIRS cases correspond to PWV values greater than 4cm, only a single category of cases is shown. (The residuals for each analysis step described herein are shown in figure 3a–d for completeness.) Figure 3e indicates that the adjustments made to the CO₂ and H₂O continua in MT_CKD result in very good agreement between the calculations and the AIRS measurements. This, coupled with the positive results with respect to the IASI and AERI cases, further validates these modifications, which have been adopted in MT_CKD_2.5.

5. Summary

The MT_CKD water vapour continuum has been developed to provide an accurate specification of an important source of molecular absorption in the atmosphere. This paper presented the perspective underlying the
development and evolution of the MT_CKD continuum model: fidelity to accurate observational assessments of continuum absorption, coupled with the use of a mathematical line shape formulation to extrapolate knowledge of the continuum from data-rich to data-poor spectral regions. Given that the primary intended application is for atmospheric radiation calculations, special emphasis is placed on ensuring that the MT_CKD continuum is consistent with well-regarded field-based measurement datasets. The MT_CKD model inherited its development philosophy from its predecessor, the CKD model, although its line shape formulation was revised to be consistent with the hypothesis that a source other than collisionally broadened monomer transitions is responsible for the majority of the in-band continuum absorption. This paper also presented the details of a radiative closure study in the region past the bandhead of the CO2 $\nu_3$ band that led to a recent revision to the continuum, MT_CKD_2.5. In this closure study, consistent results were obtained from measurement sources from different platforms and across a wide range of atmospheric conditions, providing additional confidence in the conclusions of the study.

Analysis of future measurement datasets will not only provide additional basis for adjusting the MT_CKD continuum coefficients in certain spectral regions, but will also provide stringent tests of the model’s foundational principles. The revisions to the continuum coefficients that have been implemented since the development of the MT_CKD line shape formulation and the release of MT_CKD_1.0 are already sufficient to justify an adjustment to the values of the fitted parameters in the formulation and, perhaps, even the functional forms it employs. Clearly, this approach cannot reproduce observed continuum absorption features that do not arise from transitions associated with the water vapour monomer, such as those that have been ascribed to bound dimers (e.g. [45]). However, the scope of the needed modifications to MT_CKD_1.0 has not undermined the MT_CKD perspective that there exists a line shape that, when consistently applied to all water vapour monomer lines, yields an accurate representation of this important source of continuum absorption. As additional observational evidence of the continuum is obtained, this perspective will be tested.

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Phil. Trans. R. Soc. A (2012)


