Infra-red heating calculations with a water vapour pressure broadened continuum

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(Manuscript received 25 January 1973; in revised form 21 May 1973. Communicated by Dr. A. K. Betts)

SUMMARY

Previous heat budget studies relying on infra-red radiation calculations have not used a water vapour pressure dependent continuum absorption in the 830-1,250 cm\(^{-1}\) region of the infra-red spectrum. The purpose of this study was to investigate the differences in the infra-red divergence profiles caused by inclusion of the vapour pressure dependent continuum absorption.

The results indicate only a very small change in infra-red divergence from previous work for a typical midlatitude temperature, water vapour profile. However, for tropical temperature and moisture profiles, the new continuum data result in approximately 30 per cent more total tropospheric infra-red cooling than obtained using earlier continuum absorption data. In addition, it is shown that within a realistic range of tropical atmosphere moisture content, the continuum infra-red cooling may act to either stabilize or destabilize the lower layers of the troposphere.

1. INTRODUCTION

That observations of divergence of infra-red radiation (IR) have not agreed with calculations, even under reported clear conditions, has been noted since the first radiometeronde observations were reported by Suomi, Staley and Kuhn (1958). In general, observations exhibited greater divergence of IR in the lower troposphere than calculations predicted. It has been unclear whether the observations or the calculations, or both, have been in error.

Kuhn and Suomi (1963) ascribed this difference to particulate aerosols in a south-west US desert location. Cox (1969) suggested two plausible explanations for observed vs. calculated differences for tropical Pacific data. He concluded that the effect of a horizontal variation in surface temperature was misinterpreted as a vertical net flux divergence in the observations. This accounted for a major portion of the discrepancy. He suggested that water droplets in insufficient quantities to be classified as cloud account for the remainder of the low level discrepancy and that cirrus clouds were present between 300 and 100 mb. Gille and Ellingson (1970) also noted these discrepancies in tropical data.

Since 1964, a series of radiometeronde intercomparisons have been carried out with the objective of standardizing data acquired by radiometerondes of various countries. From these checks, Gille and Kuhn (1972) report the same discrepancy between observation and calculation noted above. Kuhn and Stearns (1971) compared radiometeronde data and IR calculations using an empirical continuum absorption parameter and showed that enhanced absorption in the continuum region could explain a substantial portion of the observation – calculation discrepancy.

Bignell (1970) reported new experimental results on the absorptive properties of the water vapour continuum in the 480 to 910 cm\(^{-1}\) region. The additional absorption noted increased with the partial pressure of water vapour and was found, contrary to previous work, to have a negative temperature dependence of two per cent per °C in the temperature range 21°C to 45°C. While Bignell gave no firm explanation, he, Burroughs, Jones and Gebbie (1968) suggested the possibility that the water dimer molecule (H\(_2\)O\(_2\))\(_2\) may be responsible for the absorption characteristics observed. Bignell gives a detailed summary of previous work in this area.

Platt (1972) showed comparisons of observations and calculations of the upward radiance in the 830-1,000 cm\(^{-1}\) spectral region as a function of altitude. These results
showed qualitative agreement between observations in the atmosphere and the laboratory-deduced Bignell water vapour pressure dependent absorption coefficients.

Ellingon (1972) computed infra-red heating rates using a Bignell type continuum absorption coefficient, however, the absorption coefficient was assumed to be independent of temperature.

2. Technique

The purpose of the research in this paper is to explore the effect of the Bignell, vapour pressure-broadened continuum absorption on IR radiation divergence calculations in the atmosphere. This is accomplished by comparing divergence calculations based on an isothermal, broadband, flux emissivity transfer program. The flux emissivities used in the transfer calculation are (a) reported by Staley and Jurica (1970) and (b) the new values computed using the Bignell data.

To obtain an indication of the effect of vapour pressure broadened continuum absorption in infra-red divergence, it is not necessary to use the most sophisticated radiative transfer method. A simplified broadband isothermal emissivity transfer scheme has been used with two sets of water vapour transmissivity data noted above; the resulting infra-red heating rates are compared for the total IR spectrum (100-2,500 cm\(^{-1}\)), the water vapour window (660-1,220 cm\(^{-1}\)) and the water vapour rotational band (100-660 cm\(^{-1}\)).

(a) Isothermal emissivity transfer calculation

The brief discussion which follows outlines the method used in this study to compute infra-red irradiance. The atmosphere has been assumed to consist of water vapour and carbon dioxide. Although ozone may be treated in an analogous way, for the purposes of this comparison it was neglected.

The radiative transfer equation in the absence of scattering may be written in the following way.

\[
F = \int_{P_1}^{P_2} B(T) \left[ \frac{\partial}{\partial p} (E(\text{cont}) + E(\text{rot}) + E(6.3) + E(\text{CO}_2) - E(\text{OVL})) \right] dp
\]

\[
+ \left( 1 - \int_{P_1}^{P_2} \left[ \frac{\partial}{\partial p} (E(\text{cont}) + E(\text{rot}) + E(6.3) + E(\text{CO}_2) - E(\text{OVL})) \right] dp \right) B(T_s) \tag{1}
\]

\(F\) is the upward or downward irradiance, \(B(T) = \sigma T^4\) (the Stefan-Boltzmann law), \(E(\_\_\_\_)\) is the broadband flux emissivity (defined in Eq. (3)), \(p\) is pressure, cont, rot, and 6.3 are the three portions of the water vapour absorption spectrum considered and CO\(_2\) represents the 15 \(\mu\)m CO\(_2\) absorption; OVL accounts for the overlap between the long wavelength side of the continuum and short wavelength side of the rotational water vapour absorption with the 15 \(\mu\)m carbon dioxide absorption band. \(T_s\) is the temperature of the background.

Eq. (1) was applied to temperature and water vapour profiles to provide upward and downward irradiance values as functions of height. A finite difference calculation of the IR heating rate was then made.

(b) Flux emissivity data

The continuum flux emissivity data reported by Staley and Jurica (1970) were obtained by a numerical integration of higher spectral resolution data found in Elsasser and Culbertson (1960). The resulting emissivity data were given as a function of two variables, pressure corrected precipitable water and temperature.

In our analysis, we must include a third independent variable, water vapour pressure, \(e\); with this additional variable, a precomputed tabular representation of the flux emissivity as used by Staley and Jurica (1970) becomes unworkable. Since we desired to retain the time-saving feature of a broadband emissivity, the following computational scheme was developed.
The broadband emissivity for an absorbing gas of amount \( u \), temperature \( T \), is

\[
E(u, T) = \int_0^\infty \frac{W(\nu, T)}{\sigma T^4} \left[ 1 - \frac{\tau(\nu, u, T, e)}{\nu} \right] d\nu
\]  

(2)

where \( W(\nu, T) \) is the Planck function, \( \nu \) the wave number and \( \tau \) the spectral transmissivity.

(i) **Continuum region:** Eq. (2) was rewritten in the following manner for the continuum absorption in order to allow an analytic solution to the integral.

Bignell expressed the total absorption coefficient as shown in Eq. (3).

\[
k(\nu) = (T, p, e) = k_1(\nu, T) p + k_2(\nu, T) e
\]

(3)

where \( k_1 \) is the absorption coefficient at unit total pressure for foreign broadening and \( k_2 \) is the absorption coefficient at unit partial vapour pressure for the vapour pressure dependent absorption, \( e \) is the water vapour pressure and \( p \) is the total pressure. For the 8 to 12 \( \mu \)m window interval, Bignell states \( k_2(\nu) \gg k_1(\nu) \); therefore, assuming an exponential relation between the spectral transmissivity, \( \tau_\nu \), and Eq. (3) multiplied by \( u \), we have Eq. (4)

\[
\tau_\nu(u, T, e) = \exp(-k(\nu, T) eu).
\]

(4)

From Bignell's tabulation of \( k_2(\nu, 20^\circ C) \) the window interval from 660 to 1,210 cm\(^{-1}\) was divided into five sub-intervals. For each sub-interval the absorption coefficient was assumed to be a linear function of wave number and the classical intercept (a), slope (b), coefficients were evaluated. In a like manner, the Planck function was expressed as a linear function of wave number, \( \nu \), for each sub-interval. In this instance, a set of coefficients dependent upon temperature was derived. Substituting the two linear functions (Eq. (5))

\[
W(\nu) = a + \beta \nu
\]

\[
h(\nu) = a + b \nu
\]

(5)

into the numerator of Eq. (2) yields

\[
E(u, T, e) = \int_0^{\nu f} \frac{\left[ 1 - \exp(-(a + b \nu)ue) \right] (\alpha + \beta \nu)}{\sigma T^4} d\nu
\]

(6)

Values of the parameters \( a, b, a \) and \( b \) for each sub-interval are given in Table 1.

Eq. (6) may then be integrated to yield

\[
\sigma T^4 E(u, T, e) = a(\nu_2 - \nu_1) + \frac{\beta}{2} (\nu_2^2 - \nu_1^2) + \frac{\alpha}{\text{bue}} \left[ \text{exp}(-\text{bue} \nu_2) - \text{exp}(-\text{bue} \nu_1) \right] - \frac{\beta}{\text{bue}} \left[ \text{exp}(-\text{bue} \nu_2) \left( \frac{1}{\text{bue}} - \nu_2 \right) - \text{exp}(-\text{bue} \nu_1) \left( \nu_1 - \frac{1}{\text{bue}} \right) \right].
\]

(7)

**TABLE 1.** LINEARIZATION PARAMETERS FOR SPECTRAL ABSORPTION COEFFICIENT AND PLANCK FUNCTION

<table>
<thead>
<tr>
<th>wave no. (cm(^{-1}))</th>
<th>Absorption coefficient parameters ( T = 20^\circ C )</th>
<th>Planck function ( T = 0^\circ C ) parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( a )</td>
<td>( b )</td>
</tr>
<tr>
<td>660-810</td>
<td>109.1</td>
<td>-0.117</td>
</tr>
<tr>
<td>810-900</td>
<td>53.1</td>
<td>-0.0482</td>
</tr>
<tr>
<td>900-1,050</td>
<td>9.7</td>
<td>0</td>
</tr>
<tr>
<td>1,050-1,140</td>
<td>-31.1</td>
<td>0.0389</td>
</tr>
<tr>
<td>1,140-1,210</td>
<td>-55.2</td>
<td>0.0690</td>
</tr>
</tbody>
</table>
Eq. (7) was evaluated for each of the five sub-intervals listed in Table 1 and the results summed to cover the 660-1,210 cm\(^{-1}\) region.

An effective temperature, \(T_{\text{eq}}\), and effective water vapour pressure, \(e_{\text{eq}}\), are defined in Eq. 8 to account for the effects of a non-homogeneous atmosphere on the broadband flux emissivity utilized in Eq. (7).

\[
T_{\text{eq}} = \frac{\int T \, du}{\int du}
\]

\[
e_{\text{eq}} = \frac{\int e \, du}{\int du}
\]

In Eq. (8), \(T\) is temperature, \(e\) is vapour pressure and \(u\) is precipitable water. In addition, a diffusivity factor of 1.66 was used to convert from a radiance emissivity to a flux emissivity.

The temperature dependence of \(k_{\nu}(T)\) was specified as proportional to the dimer (H\(_2\)O)\(_2\) concentration. The dimer mole fraction, \(C\), was determined from Eq. (9) which was derived from basic physical chemistry arguments given by Eisenberg and Kauzman (1969).

\[
C = \frac{1}{2} \left\{ \left[ 2 + \frac{P_r \exp(C_1 - C_2/T)}{e} \right] - \left[ \left( 2 + \frac{P_r \exp(C_1 - C_2/T)}{e} \right)^2 - 4 \right]^{1/2} \right\}
\]

where \(C_1 = 13.0096\), \(C_2 = 2878.225\) K and \(P_r\) is a reference pressure of one atmosphere. The consequences of this assumption are discussed in a later section.

A comparison of a numerical integration using a 10 cm\(^{-1}\) increment in Eq. (2) showed agreement with the analytical result from Eq. (8) to within one tenth of one percent while the analytic method was faster by a factor of fifteen.

(ii) Rotational water vapour: While updating the broadband emissivity data, the contribution from the rotational water vapour band was recalculated using spectral data more recent than those used by Staley and Jurica (1970). The regression equation depiction of the spectral transmissivity given by Smith (1969) was selected. These spectral data were then used in Eq. (2) which was numerically solved to yield the broadband rotational emissivity.

(iii) Carbon dioxide: The technique used to update the CO\(_2\) emissivities from Smith’s data was analogous to that outlined above for rotational water vapour. The problem of overlap was treated in a manner analogous to that given previously by Staley and Jurica, however, the updated transmissivity data were used. A pressure correction exponent of 0.40 was used for the optical depth of CO\(_2\).

3. Comparison of broadband flux emissivities

A comparison of the broadband flux emissivity for the continuum given by Staley and Jurica with those calculated in the present study for 20°C is shown in Fig. 1. Instead of
tending toward an upper limit of unity, the flux emissivity asymptotically approaches a value equal to the fraction of the total energy, $\sigma T^4$, in the specific spectral interval. Clearly, for the very moist cases (high vapor pressure) the emissivity obtained by applying the Bignell data is as much as a factor of two larger than that given by Staley and Jurica. Fig. 2 shows a similar comparison for $-40^\circ$C. Here again the vapor pressure dependence may cause significant differences.

![Figure 2](image)

**Figure 2.** Flux emissivity of the water vapor continuum given by Staley and Jurica and that calculated from Bignell data for $T = -40^\circ$C.

Figs. 3 and 4 show a similar comparison between Staley and Jurica and the current study for the water vapor rotational band and the carbon dioxide 15 $\mu$m band. For the rotational water band for an optical depth of 1 cm, the Staley and Jurica data appear to be approximately two per cent too low. For CO$_2$, at $20^\circ$C, between 0-1 cm and 100 cm Staley and Jurica’s values tend to be about 10 per cent lower than those calculated from Smith’s spectral data for CO$_2$.

![Figure 3](image)

**Figure 3.** Flux emissivity for 15 $\mu$m CO$_2$ band given by Staley and Jurica and that calculated from Smith (1969) for $T = 20^\circ$C.

4. **Comparison of Calculated Irradiances**

Figs. 6-9 enable one to compare the results of the evaluation of the transfer equation using Staley and Jurica’s flux emissivity values in Eq. (1) and using the new emissivity results presented in this paper. The solid lines represent the heating rate calculated using the new emissivity data and the dashed lines are the differences between the heating rates
represented by the solid line and that computed using Staley and Jurica's emissivity values. For perfect agreement, the dashed line would be vertical at zero. The dashed line to the right of the zero indicates that the new calculated represents less heating (or more cooling) than that calculated using Staley and Jurica's data.

Only the total IR heating, the continuum and water vapour rotational components are depicted in Figs. 6-9. In the total heating, however, the effects of CO₂, the 6-3 μm band and an overlap correction are taken into account. For this reason, the two components (cont and rot) do not sum directly to form the total.

(a) Midlatitude case

The temperature and water vapour data shown in Fig. 5 were taken from a model 45° N latitude July profile (Environmental Science Services Administration 1966) and were used in calculating the IR heating profiles shown in Fig. 6.

In the comparison shown in Fig. 6, the new emissivity values result in a 3 per cent larger divergence of net radiation in the surface to 150 mb layer. While this is a relatively minor change, the vertical distribution of the change in the vertical is more impressive. Cooling values of the lowest layers increased while those of the upper layers decreased slightly. Turning to the contribution of the continuum alone, one sees that it is indeed the continuum which is responsible for larger cooling rates near the surface. However, slight changes in the rotational water component reduce the midtropospheric maximum from its Staley and Jurica value.
Figure 6. Total IR spectrum, water vapour continuum, and rotational water vapour IR heating rates (solid lines) and differences between Staley and Jurica results and this paper (dashed lines), for midlatitude data.

Figure 7. Tropical temperature and water vapour profiles used in IR heating rate comparisons.

(b) Tropical case

Fig. 7 shows the temperature and moisture profiles used in the tropical comparisons. The set labelled GUAM represents an average over the spring season of 1965 for that location. The other profiles labelled DIS were observed at the ship Discoverer for 3 June 1969 during the BOMEX experiment.

Let us first look at Fig. 8, a comparison of the calculations using the GUAM data. The most dramatic feature of this comparison of calculations is that the total tropospheric (surface to 100 mb) cooling has increased by 31 per cent. This increase is largely due to the enhanced cooling by the continuum (over twice as much), although the rotational water vapour contribution to the cooling increased by 15 per cent. Further, we note a strong cooling maximum accentuated near the surface by the new continuum data. This agrees qualitatively with the effects expected by Bignell (1970) and with the observations reported by Cox (1969).
Figure 8. Total IR spectrum, water vapour continuum, and rotational water vapour IR heating rates (solid lines) and differences between Staley and Jurica results and this paper (dashed lines) for Guam data.

Figure 9. Total IR spectrum, water vapour continuum, and rotational water vapour IR heating rates (solid lines) and differences between Staley and Jurica results and this paper (dashed lines) for Discoverer data.
The second tropical comparison of IR heating rates is shown in Fig. 9. The *Discoverer* sounding shows significantly more water vapour than the GUAM data. The IR cooling maximum is not the lowest layer but displaced upward between 875 and 925 mb. This is caused by the continuum reaching near opacity in the downward irradiance calculation. The increased continuum absorption has had the same effect as a low level cloud with decreased cooling beneath and enhanced cooling near its top. The ability of the moisture profile to significantly change the low troposphere IR heating distribution through the opacity of the continuum may be of major significance in an understanding of tropical dynamics. A simple comparison of Figs. 8 and 9 shows how the change in moisture profiles changes the influence of IR heating in the 875 to surface layer from a stabilizing to destabilizing tendency. The second pronounced IR heating minimum near 575 mb in Fig. 9 is primarily due to the rotational water vapour band although the continuum is still contributing approximately $-0.5^\circ$C per day at this level.

In order to illustrate more clearly the relationship of the vertical IR heating rate profiles to the precipitable water a series of calculations was made using a power law water vapour distribution expressed by Eq. (10)

$$q(p) = q(p_0)\left(\frac{p}{p_0}\right)^\lambda$$

(10)

where $q(p)$ is the mixing ratio, $p$ is pressure, $p_0$ is surface pressure and $\lambda$ is a positive dimensionless number. For a given $q(p_0)$ the total integrated optical depth is uniquely related to $\lambda$ such that larger values of $\lambda$ imply smaller precipitable water.

Fig. 10 shows the continuum contribution to the IR heating rate for five values of $\lambda$ in Eq. (10). The *Discoverer* temperature profile shown in Fig. 9 was used for all five computations. Clearly, as the total precipitable water changes the vertical distribution of the IR continuum heating rate changes dramatically. For large $\lambda$ there is a pronounced low level cooling maximum, while for small $\lambda$ the cooling maximum at the surface is suppressed and the cooling at higher levels is enhanced. The range of precipitable water represented in Fig. 10 exceeds the range found in nature at tropical latitudes; nevertheless, the changes

![Figure 10. Dependence of the water-vapour continuum IR heating rate on vertical distribution of water vapour. Lambda is the exponent in the moisture power law expression (Eq. (10)) and u is precipitable water.](image-url)
in the induced stability over a subrange, curves 2, 3, and 4, are significant and more representative of real extremes. Interestingly, the total tropospheric continuum heating rate decreased by less than 10 per cent from the smallest to the largest value of $\lambda$.

By using Eq. (9) to express the temperature dependence of the Bignell continuum absorption coefficient, we have adopted the dimer explanation for the enhanced absorption. In order to ascertain the effect of this assumption, the heating rate calculation for the Discoverer data was repeated assuming a temperature independent continuum absorption coefficient. The results of this comparison are shown in Fig. 11. The solid line in Fig. 11 is the same as the continuum line in Fig. 9; the dashed line is the difference between the calculations with and without the temperature dependent absorption coefficient. The effect of neglecting the negative temperature dependence is to enhance the cooling of the 925 mb to surface layer and to suppress the cooling by the continuum at higher altitudes.

![Figure 11. Effect of temperature dependent absorption coefficient on water vapour continuum IR heating rate.](image)

5. Conclusions

The Bignell vapour pressure broadened continuum coefficients may significantly alter the IR heating estimates deduced from calculations. While only slight differences of IR heating calculations were noted for typical midlatitude temperature and moisture profiles, total tropospheric cooling estimates in the tropical cases were increased by 30 per cent. The cooling by the continuum itself was twice as great as previous estimates in these instances.

In addition to altering the total tropospheric energy loss by IR, the continuum absorption may account for both stabilizing and destabilizing influences in the lower troposphere. The stabilizing-destabilizing effect depends on the opacity of the continuum and thus primarily on the total amount of water vapour. Heretofore, the change between a stabilizing and destabilizing effect has been thought to be dependent upon clouds or a discontinuity in the moisture profile. It is now possible to obtain a like result with only a different total amount of water vapour while keeping the same relative vertical distribution of the gas.

The temperature dependence of the continuum absorption coefficient significantly affects the IR divergence calculation. While a dimer concentration temperature dependent
function was used in this study, it is important to verify the correct temperature dependence of the Bignell absorption coefficients to at least \(-20^\circ\text{C}\). The negative temperature dependence assumed in this study tended to reduce the stabilizing role of IR in the lowest layers.\(^*\)

**Acknowledgment**

This research was supported by the Atmospheric Sciences Section of the National Science Foundation, Grant GA-36302.

**References**


\(^*\) Since the submission of this paper, a paper by J. T. Houghton and A. C. L. Lee appearing in Nature Physical Science, Vol. 258, 21 August 1972 has been brought to the author's attention. Houghton and Lee's conclusions essentially agree with the results shown above.