Solar heating by ozone in the tropical stratosphere

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(Received 28 January 1981; revised 23 June 1981)

SUMMARY

The solar heating caused by ozone absorption in the tropical stratosphere has been calculated by direct integration over wavelength. Ozone concentration profile, cloud cover and albedo are shown to be the main parameters affecting the heating rate. Variations in the heating rate due to the temperature dependence of ozone absorption, are found to be small.

1. INTRODUCTION

As part of a study of the radiative balance of the tropical stratosphere, the solar heating due to ozone has been calculated. Earlier studies of the contribution from ozone absorption, e.g., those of Murgatroyd and Goody (1958) and Rodgers (1967), have all used a single absorption curve. More recently Lindzen and Will (1973) have suggested simple analytic formulae for the absorption due to each ozone absorption band. This approach has been used by Schoeberl and Strobel (1978) to predict ozone absorption for their global numerical model. Because of the importance of this ozone heating in the middle and upper stratosphere, it has been calculated directly, enabling various factors to be examined individually.

2. CALCULATION OF THE HEATING RATES

Throughout the work height is specified in terms of relative pressure, \( \phi = p/p_0 \), where \( p_0 \) = standard pressure at the ground. It is most convenient to use the subsidiary variable \( z = -\ln \phi \). A plane stratified atmosphere is assumed with a parallel beam of solar radiation, entering at the top (pressure \( \phi_t \)). Only absorption of radiation is considered, scattering is ignored. The lower boundary is taken to be a perfect diffuse reflector specified by an effective albedo \( a^* = (\text{albedo}) \) (fractional cloud cover). To correct for the earth's curvature, a correction \( M(\phi) \) is used. For geometric height \( h \), (corresponding to pressure \( \phi \)) and solar zenith angle \( \psi \)

\[
M(h) = \frac{1 + h/R}{(\cos^2 \psi + 2h/R)^{1/2}} \quad \text{(Houghton 1963)}
\]

\( \psi = \arccos(\sin \delta \sin \lambda + \cos \delta \cos \lambda \cos \omega t) \),

\( \delta = \) solar declination for the day,

\( \lambda = \) latitude,

\( R = \) earth's radius,

\( \omega = \) rate of rotation of the earth,

\( t = \) time from local noon.

The heating rate has been calculated at specified pressure levels rather than as the mean flux divergence across a layer. This avoids instability, when calculating the contribution of individual bands. These have contributions which can vary by ten at the same level, making a difference method unstable.

The basic formula for the heating rate caused by absorption of the direct solar beam at wavelength \( \lambda \) is:

\[
\dot{\theta}_\lambda(\phi) = -\frac{c(\phi)}{c_p} \frac{\partial F_\lambda(u)}{\partial u}. \quad \text{(2)}
\]

Then the instantaneous heating rate at level \( \phi \) for wavelength \( \lambda \) is:

\[
\dot{\theta}_\lambda(\phi) = \frac{k_\lambda(\phi) c(\phi)}{c_p} F_\lambda(\phi_0) \exp\{-s_\lambda(\phi, \phi)\} \quad \text{(direct heating)}
\]

\[
+ \frac{k_\lambda(\phi) c(\phi)}{c_p} 2\pi I_\lambda(\phi_0) E_2(\tau_\lambda(\phi, \phi)) \quad \text{(diffuse heating from reflection)} \quad \text{(3)}
\]

\( u = \) mass of the absorber per unit cross sectional area of the beam, measured along

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the beam from the top of the atmosphere to level concerned

\[ F_0(\phi) = \text{solar flux at wavelength } \lambda \text{ at the top of the atmosphere} \]

\[ k_\lambda(\phi) = \text{absorption coefficient at wavelength } \lambda, \text{ pressure } \phi \]

\[ c(\phi) = \text{mass mixing ratio of the absorber at pressure } \phi \]

\[ \tau_s(\phi', \phi) = \int_{\phi'}^{\phi} M(\phi') k_\lambda(\phi') \frac{c(\phi')}{g(\phi')} P_0 d\phi' \]

(4)

= slant optical depth from the top of the atmosphere

\[ \tau_s(\phi_0, \phi) = \int_{\phi}^{\phi_0} k_\lambda(\phi') \frac{c(\phi')}{g(\phi')} P_0 d\phi' \]

(5)

= vertical optical depth from the base of the atmosphere

\[ E_2(\tau_s) = \text{second exponential integral } = \frac{1}{\omega^2} \exp(-\omega \tau_s, d\omega) \]

\[ g(\phi) = \text{acceleration due to gravity at level } \phi \]

\[ c_p = \text{specific heat of a gas at constant pressure} \]

\[ I_\lambda(\phi_0) = \text{the intensity of the perfect diffuse surface at the bottom of the atmosphere, viz.} \]

\[ I_\lambda(\phi_0) = \pi^{-1} a^* F_0(\phi_0) \exp(-\tau_s(\phi_0, \phi_0)) \cos \beta, \]

(6)

where \( \cos \beta = M^{-1}(\phi_0) \).

In the wavelength regions where oxygen and ozone absorption overlap, \( \tau_s \) is replaced by \( \tau_s(\text{O}_3) + \tau_\lambda(\text{O}_2) \) and similarly for the vertical depth.

These formulae and the methods of calculation are described in more detail in Edwards (1970).

To interpolate the mass mixing ratio between each pair of data levels the expression, \( c(\phi) = f(\phi') \) has been used (Rodgers and Walshaw 1966). This enables explicit expressions to be found for \( \tau_s \) and \( \tau_\lambda \). The integration over wavelength for each band is done by Simpson's Rule with \( \Delta \lambda = 5 \text{ nm} \). This step size is a compromise between accuracy and the size of the input data tables. Finally this instantaneous heating rate is integrated over the daylength by using an 8-point Gaussian quadrature from noon to sunset and doubling. This avoids the near singularity in \( M \) at sunset.

3. Selection of the Solar and Absorption Data

The values of the solar flux tabulated by Allen (1958) and quoted by Goody (1964) have been chosen as representative, except for the spectral region 180–240 nm, where Brewer and Wilson's (1965) data have been preferred. A cubic spline interpolation has been used to prepare a table at 5 nm intervals for integration. A spline method has been chosen, because it has smoothing properties and reduces polynomial oscillation (Alberg, et al. 1967).

The following selection of the data for ozone absorption has been made. For the region 130–200 nm Watanabe's data have been taken from the review by Schultz, et al. (1963). In the near ultra violet and visible regions the selection is that suggested by Inn and Tanaka (1957). This uses their own absorption coefficients for the Hartley band and Vigroux's (1953) for the Huggins and Chappuis bands. Because Vigroux's coefficients are given at each maximum and minimum, their spacing in wavelength is irregular. Since the absorption coefficient of ozone is a fairly smooth function, this has been explicitly assumed and the coefficients have been interpolated at 5 nm intervals for integration, by again using a cubic spline.

For the Hartley, Huggins and part of the Chappuis band (475–650 nm), Vigroux tabulates the temperature variation of his absorption coefficients in the form \( r_\lambda(\theta) = k_\lambda(\theta)/k_\lambda(18), = \theta - 30, -44, -59, -92 \text{ °C} \). \( r_\lambda(\theta) \) has been averaged for the wavelength range of \( \lambda \) from -2.5 to +2.5 nm about each wavelength tabulated. Then a least
squares straight line has been fitted to the meaned ratios to give an absorption coefficient
of the form

\[ k_A(\theta) = k_A(18)(a_A + \beta A\theta) \]

Although Inn and Tanaka's absorption coefficients have been used for the Hartley
band, this linear correction has been applied to them. In regions where Vigroux does not
give a temperature effect, there is assumed to be none. As Vigroux has reported no change
in the absorption coefficients of the Huggins band for a pressure range of 200:1, pressure
independence has been assumed for all the absorption bands.

Similarly a selection of data has been made for oxygen absorption. For the continuum
region from 130–175 nm, Watanabe's coefficients have been taken from Schultz, et al. (1963).
To integrate over each band within the Schumann Runge system (180–200 nm) requires a
much narrower interval than 5 nm, so the following approximation has been made. From
Farmer et al. (1968), a stepped graph of the equivalent widths has been plotted. Then a
smooth curve has been drawn through the steps, so that the area under the curve approxi-
mately equals the area under the steps. The approximate absorption coefficients are then
read off from the constructed curve. For the continuum region from 200–240 nm the
absorption coefficients measured by Ditchburn and Young (1962) have been used. These
coefficients have a linear dependence on pressure but none on temperature.

4. Selection of the atmospheric data

The only tropical station in the N. American ozonesonde network is Allbrook Field
in the Canal Zone (9.0°N, 79.6°W). A sample of 20 soundings for 1963–4, taken from
Hering (1964–5) shows no obvious seasonal trend, so a mean ascent (A) has been constructed
from 7 data levels, Fig. 1. No direct rocket soundings of ozone for the tropical upper

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**Figure 1.** The Canal Zone mean ozonesonde ascent (A) joined to the constructed ozone profile (1) for the
upper stratosphere.
atmosphere are available. Rather than taking an entirely theoretical profile, a mean profile (1) has been constructed from the data shown in Fig. 2. The profile (1) has been joined to the mean ascent (A) by a single step, using the interpolation formula \( c = f_\phi \) (Fig. 1). For oxygen a constant mass mixing ratio of 0.2315 has been used below 80 km with that of the Cospar atmosphere (CIRA 1965) above this level.

Since the mean temperature profile corresponding to the ozone profile (A) is very close to the US substandard atmosphere's profile for 15°N, listed in the US Standard Atmosphere Supplements (1966), the substandard temperature profile has been used. The topmost data level for absorption is set at 110 km \((z = 15.0)\) to allow for the removal of energy from the solar beam by absorption in the mesosphere.

A simple climatological approach has been used for the cloud data. Conover (1965) reports an albedo of about 0.9 for thick cumulonimbus. This has been uniformly applied to the survey of planetary brightness by Booth and Tayler (1968) to yield a cloud cover at 10°N of 0.22. Hence, an effective albedo, \( a^* = 0.2 \) is obtained, as a global estimate for the latitude. A value of \( a^* = 0.4 \) has been used to represent desert areas in the tropics.

For the average tropical cumulonimbus, the height of the cloud top has been fixed at 6.48 km \((z = 0.784)\), (Donne 1962, Rodgers 1967). Kantor and Graham (1968) observed very high tropical cumulonimbus off the US Gulf coast. For these a height of 17.4 km \((z = 2.465)\) has been used together with an \( a^* = 0.9 \). The various combinations of height and effective albedo are listed in Table 1.
TABLE 1. THE CLOUD CONDITIONS OF THE ASCENTS USED FOR THE HEATING PROFILES

<table>
<thead>
<tr>
<th>CLOUD CONDITIONS</th>
<th>ASCENT CODE NUMBER</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I</td>
</tr>
<tr>
<td>Cover and Albedo</td>
<td>c</td>
</tr>
<tr>
<td>No reflection</td>
<td>0</td>
</tr>
<tr>
<td>Tropical average</td>
<td>0.22</td>
</tr>
<tr>
<td>Desert</td>
<td>1</td>
</tr>
<tr>
<td>Cumulonimbus</td>
<td>1</td>
</tr>
<tr>
<td>Height</td>
<td>km</td>
</tr>
<tr>
<td>Ground</td>
<td>0.15</td>
</tr>
<tr>
<td>Average CuNb</td>
<td>6.48</td>
</tr>
<tr>
<td>High CuNb</td>
<td>17.4</td>
</tr>
</tbody>
</table>

5. INTERPRETATION OF THE SOLAR HEATING RATES

Solar energy absorbed by ozone may either increase the translational kinetic energy of the molecules (i.e., heating) or it may cause photodissociation to oxygen. These excited oxygen molecules may either take part in further chemical reactions or deactivate by reradiation. The calculations by Hunt (1965) show that the diurnal variation of ozone is fairly small below the 65 km level. Therefore temporary energy storage caused by the increase in concentration of an excited species can be ignored below 65 km. An estimate of the energy radiated by oxygen molecules in the 1-27 band has been made for ascent II, using the data of Evans (1967). Although this radiation is equivalent to 10% of the solar heating at 71.5 km, it decreases rapidly at lower levels. Thus the calculated heating rates are considered to give the potential temperature rise for levels up to 71.5 km (z = 10.0). Above this level, 'heating rates' measure the primary removal of energy from the solar beam.

The heating profiles have been calculated for a vertical spacing Δz = 0.5 km, which is a compromise between a well-defined profile and computation time.

Using the simplest possible ascent, I, two trials have been done to check the accuracy of the integrations. Using a 16-point Gauss formula for the integration over the day, gives the same results as the 8-point one to 5 significant figures, so errors from this integration can be ignored. The first order estimate of the error in using Simpson's Rule for the integration over wavelength is given by e(%) = 100(S₄₈ - S₂₉)/15(S₄₈), Noble (1964). For this trial, some absorption bands have been slightly shortened, so all have 4ν ordinates. At levels below 71.5 km (z = 10.0), |ε| < 1.5%. This integration over the day and all subsequent ones are done at the summer solstice for the Allbrook Field station.

To examine the accuracy of the integration over path length, the heating rates obtained for ascent II with alternate levels omitted have been compared with those obtained using all levels. The largest differences, magnitude 4–6%, occur where the ozone concentration is varying rapidly with height. As it is doubtful whether ozone fine structure has much effect on heating, twice the error of the wavelength integral has been estimated for the complete calculation. Thus, 3% is taken as the maximum error up to the level z = 10.0.

6. RESULTS FOR THE SOLAR HEATING RATES

The effects of different cloud conditions are shown in Fig. 3. Comparing the results for ascents (II, III) with IV and (V, VI), it is seen that the effective albedo is much more important than the cloud height in determining the amount of heating by reflection.

Figure 4 shows the contribution to the total heating rate by each band. The Hartley band has been divided into two sections to examine the effect of the overlapping oxygen continuum. The heating maximum is largely provided by the HA part of the Hartley band between 240–300 nm, while at lower levels the Huggins and especially the Chappuis bands predominate. Although the HB part of the Hartley band from 200–240 nm, which overlaps the oxygen continuum, provides 10% of the total heating at the maximum, it is not important at other levels. The overlapping oxygen continuum is not significant at any level.
Figure 3. The effect of various cloud conditions.

\[ R = \frac{\text{total heating}}{\text{heating by absorption of downward flux alone}} \]

<table>
<thead>
<tr>
<th>Ascent</th>
<th>Effective albedo</th>
<th>Cloud height km</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>II</td>
<td>6.48</td>
</tr>
<tr>
<td>2</td>
<td>III</td>
<td>17.40</td>
</tr>
<tr>
<td>3</td>
<td>IV</td>
<td>0.15</td>
</tr>
<tr>
<td>4</td>
<td>V</td>
<td>6.48</td>
</tr>
<tr>
<td>5</td>
<td>VI</td>
<td>17.40</td>
</tr>
</tbody>
</table>

Figure 4. The solar heating contributed by each absorption band for ascent II.

CH: Chappuis band
HA: Hartley band 240-300 nm
O1: Oxygen absorption 180-200 nm
HB: Hartley band 200-240 nm
O2: Oxygen absorption 200-240 nm
HU: Huggins band 300-350 nm
SR: Schumann Runge bands
T: Total
The heating due to the Chappuis band is increased by 60% in the middle stratosphere, when the effective albedo is increased from 0.2 to 0.9 (Fig. 5). The very low absorption of the band causes this big increase, because it follows from Eqs. (3) and (4) that the reflection term will dominate as \( \tau_L(\phi_0, \phi) \) tends to zero provided that \( a^* \cos \beta > 0.5 \). This condition is readily fulfilled in the tropics, where most of the daily heating occurs when \( \cos \beta \) is close to 1.

As the HA part of the Hartley band produces most of the solar heating and the uncertainties in the solar flux are mainly at wavelengths less than 350 nm, the heating profile for ascent II has been calculated for two alternative estimates of solar flux. Allen's 1958 estimate without modification by Brewer and Wilson's data gives the same heating rates as the modified estimate below the mesosphere. Allen's 1962 estimate gives an increase in total heating, which reaches 7-3% at the level of peak heating.

To check the magnitude of the temperature effect on the heating profile, the heating rates have been calculated for ascent II with the temperature profile replaced by a constant value of \(-40^\circ\text{C}\). This is the approximate mean for the substandard profile between 0 and 89 km. The differences between the results for \(-40^\circ\text{C}\) and the substandard profile are barely significant within the overall accuracy. Thus errors caused by the simple linear temperature correction of the ozone absorption coefficients and by errors in the temperature profile can both be ignored.
To show clearly the effect of the ozone profile, the mixing ratio for ascent II has been multiplied by 0.5, 1.5, and 2.0 at all levels. Fig. 6 shows that this increases the peak heating by about 3°C per day for each step. In the middle and upper stratosphere, the uncertainty bounds for the ozone profile are 0.5 to 1.5 of the selected one. This result emphasises the need for more knowledge of ozone concentrations in the rocket region.

7. An Absorption Curve

The small differences between the heating rates obtained using the substandard temperature profile and those using a constant temperature of -40°C, suggest that a single absorption curve can be easily calculated using this constant temperature. Following Eq. 2, the total instantaneous absorption rate for ozone \( G(u) \) has been calculated by integrating across the ozone bands for a range of \( u \) values.

\[
G(u) = -\int \frac{\partial F_s(u)}{\partial u} \, d\lambda
\]

The previously selected solar flux values and ozone absorption coefficients have been used.

This total absorption rate is compared with those used by Lindzen and Will, and Schoeberl and Strobel in Fig. 7. All three absorption rates differ by less than 20% provided \( u < 0.1 \) kg m\(^{-2}\). The contribution to daily heating rates from absorption at large solar zenith angles is small, so these differences when \( u > 0.1 \) are relatively unimportant because they occur for \( \beta > 85° \).

8. Conclusions

It is clearly seen that the major parameters controlling the solar heating due to ozone are the ozone concentration profile and the effective albedo. The effect of oxygen absorption can be ignored in comparison with ozone below the mesosphere. The effects of temperature are also small, so the use of a single absorption curve at a fixed temperature is justified. Moreover an absorption curve calculated from the data used in the present work agrees reasonably well with those curves calculated by other workers.
Figure 7. The total instantaneous absorption rate for ozone, $G(u)$, as a function of the mass of absorber, $u$.

A: Calculated by integration over wavelength
B: From Lindzen and Will (1973)
C: From Schoeberl and Strobel (1978)

ACKNOWLEDGMENTS

The author wishes to thank Dr C. D. Walsh for his help and encouragement throughout the work. He also wishes to thank Dr C. D. Rodgers, Dr R. E. Murgatroyd, Mr D. E. Miller and Mr S. G. Cornford, for information and advice.

During the work, the author was supported by maintenance grants from the Science Research Council and the Meteorological Office.

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