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A parameterization for absorption due to the A, B, and γ oxygen bands

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ABSTRACT

A new parameterization for the absorption of visible solar radiation due to O_2 is presented. This broad band parameterization is based on comparison with detailed line-by-line calculations and is shown to be in excellent agreement with laboratory measurements. The importance of solar O_2 absorption to atmospheric heating rates and temperatures is also discussed. Although the heating caused by the solar O_2 bands is small (<0.03 K day^{-1}), its presence warms the tropical tropopause region by as much as 1.1 K. Finally, the importance of correct asymptotic limits for modeling the absorptance of O_2 is illustrated.

1. Introduction

The purpose of this work is to present a formulation which accurately models the three major solar absorption bands of oxygen. Using these broad band absorption formulations, we then assess the importance of oxygen to atmospheric solar heating.

The oxygen molecule has three absorption bands in the visible region of the solar spectrum: the A band at 762 nm, the B band at 688 nm and the γ band at 628 nm. These bands are due to a magnetic dipole electronic transition between $^1\Sigma_{g^+}$ and $^3\Sigma_g$ states and are associated with the (0–0), (1–0), and (2–0) vibrational transitions, respectively. The intensities of these bands are very weak, but the relatively large amount of O_2 in the atmosphere, as well as the fact that the positions of these bands are near the peak of the distribution in incoming solar radiation, makes them contribute significantly to the solar energy budget of the atmosphere.

Absorption due to these oxygen bands has been included in solar radiation calculations by Yamamoto (1962). Sasamori et al. (1972) used Yamamoto's absorption curve to estimate solar heating in the southern hemisphere. However, Yamamoto's calculations were based on the data of Langley and Abbot (1900) and Fowle (1917). These data overestimate the absorption of O_2 by nearly 40% when compared with the more recent results of Miller et al. (1969) and Nakazawa et al. (1982).

The absorption by the A, B and γ bands of O_2 is parameterized using the broad band model of Ramanathan (1976). Kiehl and Ramanathan (1983) have shown that the broad band absorptance formulation used herein gives good agreement with more detailed calculations for the 15 μm band system of CO_2. We will show that the same method applied to the oxygen bands yields excellent agreement with line-by-line calculations and laboratory measurements. Section 2 briefly discusses the line-by-line calculations employed in the present study along with a detailed description of the broad band absorptance model. Section 3 discusses the rôle of these oxygen bands in the radiative energy balance in the earth's atmosphere. Section 4 summarizes the most important features of the present study.

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2. The models

The line-by-line calculations of the total band absorptance were calculated as follows. About 400 lines were taken into account for each band in the wave-number regions 13240–12905 cm^{-1}, 14625–14300 cm^{-1}, and 15980–15685 cm^{-1} for the A, B, and γ bands, respectively. The mixed Doppler-Lorentz (Voigt) profile was employed for all calculations (Nakazawa et al., 1978, 1982). The line intensities of the A band were calculated from the band strength of Miller et al. (1969) which was found to be in good agreement with laboratory measurements (Nakazawa et al. 1982). The line intensities for the B and γ bands were calculated from the band strengths of Giver et al. (1974) and Miller et al. (1976), respectively.

The Lorentz half-widths were derived from Giver et al. (1974). A foreign broadening coefficient of 1.0 was employed in all calculations. The line positions were determined by using the theoretical relation with molecular constants obtained by Babcock and Herzberg (1948). The effects of the isotopes $O^{16}O^{16}$, $O^{16}O^{17}$ and $O^{16}O^{18}$ were taken into account in all calculations. A volume of mixing ratio of 0.21 was assumed for the atmospheric amount of O_2.

The broad band model employed in the present study has been used by Ramanathan (1976), Kiehl and Ramanathan (1983), and Donner and Ramanathan (1980) to model the absorption due to the 15 μm band system of CO_2, and 9.6 μm band of O_3, the 7.7 μm band of CH_4 and 7.8 and 17.0 μm bands of N_2O respectively. The band absorptances for the A, B and γ bands ($j = 1$, 2 and 3), respectively, are given by:

$$A_j = 2A_0(\bar{T}) \ln \left\{ 1 + \sum_{i=1}^{3} \frac{u_{ij}}{\sqrt{4 + u_{ij}(1 + 1/\beta_{ij})}} \right\}, \quad (1)$$

where the dimensionless optical depth is defined by:

$$u_{ij} = q_i \int_z^{\infty} \frac{S_{ij}(T)}{A_0(T)} P_a \, dz \quad (2)$$

and the dimensionless mean line parameter is given by:

$$\beta_{ij} = \frac{1}{u_{ij}} \int_z^{\infty} \frac{4\gamma(T)}{d_{ij}} \frac{P}{P_0} \, du_{ij}. \quad (3)$$

S_{ij} is the band strength in cm^{-2} atm^{-1} for a particular isotope i. q_i is the isotope fraction (see Table 1) for the O_2 model. The three isotopes $O^{16}O^{16}$, $O^{16}O^{17}$ and $O^{16}O^{18}$ are designated by $i = 1$, 2 and 3, respectively. Eq. (1) with subscript j is applied to the A, B, and γ bands separately. P_a is the partial pressure of O_2 which is equal to 0.21 P, where P is the total atmospheric pressure in atmospheres. P_0 is a reference pressure of 1 atmosphere. γ is the mean line half width in cm^{-1}. d_{ij} is the mean line spacing which for O_2 is either 2B or 1B, where B is the rotational constant. The value of the mean line spacing is determined by whether the oxygen atoms composing the O_2 molecule have odd or even nuclear spin. Thus, the $O^{16}O^{16}$ molecule would have every other line missing from its spectra since O^{16} has even spin and $d = 2B$ (see p. 141 of Herzberg, 1950). $A_0(\bar{T})$ is the effective band width in cm^{-1} evaluated using the pressure-weighted temperature along the path. The temperature dependence of A_0 accounts for the fact that as temperature increases, higher energy levels become populated and transitions from these levels become important to the absorptivity and the effective width of the band should increase. It can be shown (Cess and Tiwari, 1972) that $A_0 \propto T^{1/2}$ for a rigid rotor molecule. Thus, all of the broad band model parameters except for A_0 can be obtained from the same spectroscopic data which served as the source for the line-by-line calculations of Nakazawa et al. (1978). The band strengths, positions, mean line spacings, and isotopic fractions are given in Table 1.

Table 1. *Band parameters used in eq. (1) for the A, B and γ bands of oxygen; f is the amount of solar radiation for given band*

Band	Band center (μm)	Band strength (cm^{-2} atm^{-1} STP)	f ($W\ m^{-2}\ (cm^{-1})^{-1}$)
A	0.762	5.32×10^{-3}	6.980×10^{-2}
B	0.688	4.08×10^{-4}	6.642×10^{-2}
γ	0.628	1.52×10^{-5}	6.225×10^{-2}

Isotope	q Isotopic fractional abundance	d Mean line spacing (cm^{-1})
$O^{16}O^{16}$	0.99758	2.829
$O^{16}O^{17}$	0.000373	1.4145
$O^{16}O^{18}$	0.002039	1.4145

The mean line half-width was calculated from the

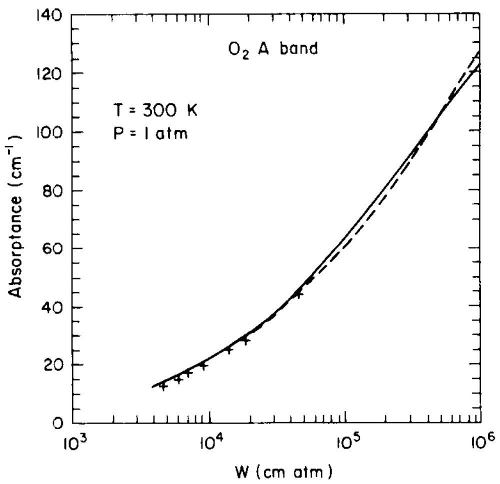

Fig. 1. Absorptance due to the A band of oxygen as a function of amount of O_2 in cm atm. Shown are absorptivities due to the: broad band model of eq. (1) (dashed line), line-by-line calculations (full line), and laboratory measurements (+).

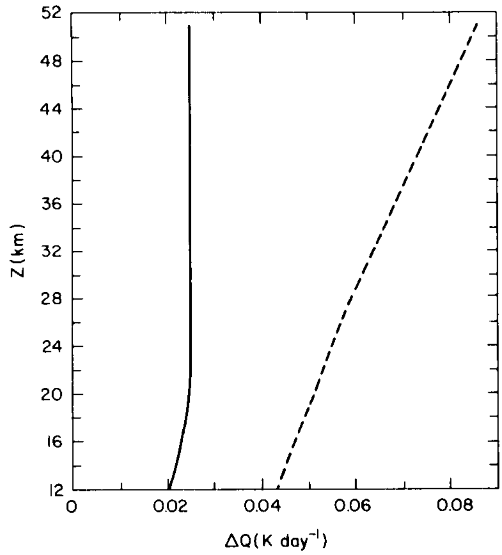

Fig. 2. Stratospheric heating due to the A, B and γ bands of O_2 from eq. (1) (full line), and from the method of Sasamori et al. (1972) (dashed line).

line data available on the AFGL line tape (Rothman et al., 1983). The procedure for calculating the mean line half-width is discussed in Kiehl and Ramanathan (1983). The value obtained for the mean line half width is given by:

$$\gamma(T) = 0.05516\ (300/T)^{1/2}\ \mathrm{cm}^{-1}. \qquad (4)$$

The effective band width parameter, A_0, was obtained by using a least squares routine to minimize the absolute difference between the line-by-line absorptivities and the broad band absorptances. This process yielded the following value for the effective band width:

$$A_0(T) = 46.31\ (T/300)^{1/2}\ \mathrm{cm}^{-1}. \qquad (5)$$

A comparison between the broad band and line-by-line absorptivities for the *A* band are shown in Fig. 1. Also presented in this figure are the laboratory measured O_2 absorptances of Yamanouchi (1977). It is evident that excellent agreement exists between all three results. Similar agreement exists for the *B* and γ bands.

3. The radiative rôle of O_2 in the atmosphere

To assess the radiative rôle of the three solar oxygen bands in the atmosphere, the broad band absorptivity model described in the previous section has been used in the radiation model of Ramanathan and Dickinson (1979). This model employs the formalism of Lacis and Hansen (1974) to account for the solar absorption in the atmosphere. The additional atmospheric heating due to O_2 is shown in Fig. 2. The change in heating shown in Fig. 2 is for 0° N spring conditions: very similar results obtain for mid-latitude conditions. The temperature profile used for the calculations is shown in Fig. 3. The maximum heating due to O_2 occurs above 20 km with a magnitude of 0.026 K day^{-1}, while the heating near the tropopause region is 0.022 K day^{-1}. Also shown in Fig. 2 is the heating due O_2 calculated from the formula of Sasamori et al. (1972). Large differences exist between the present method and those of Sasamori et al. These differences are due to two reasons. First, Sasamori et al. based their absorptances on the results of Yamamoto (1962), which are larger than the current measurements. Secondly, the functional form employed by Sasamori et al. does not possess the correct asymptotic limits for small absorber amounts. In the mid and upper stratosphere, the following limits obtain; $u \ll 1$, $u/\beta \gg 1$

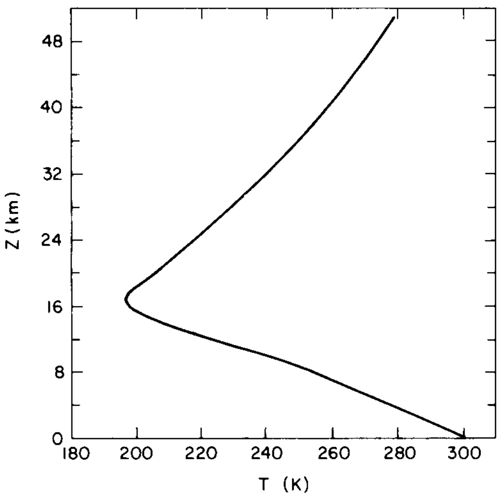

Fig. 3. Temperature profile for 0° N spring conditions.

and $u\beta \ll 1$. Applying these limits to the absorptance expression, eq. (1) reduces to

$$A_j = 2A_0(\bar{T}) \sum_{i=1}^{3} \sqrt{\xi_{ij}} \qquad (6)$$

where,

$$\xi_{ij} = \int_z^\infty \frac{4\gamma(T)}{d_{ij}} \frac{P}{P_0} q_i \frac{S_{ij}(T)}{A_0(T)} \frac{P_a}{\bar{\mu}} \, dz. \qquad (7)$$

$\bar{\mu}$ is the cosine of the mean zenith angle and accounts for the slant path of the direct beam. The direct beam heating for a given band j, which accounts for 94% of the total O_2 heating, is given by,

$$Q_j = \frac{g}{C_p} f_{\text{day}} f_j \bar{\mu} \frac{\partial A_j}{\partial p}, \qquad (8)$$

where g is the acceleration due to gravity, C_p the specific heat of air at constant pressure, f_{day} the fractional amount of daylight. The heating is proportional to the derivative of A with respect to pressure. Examination of (7) indicates that $\xi_{ij} \propto P^2$, where we have used $P_a = 0.21\ P$. Thus, A_j is linearly proportional to the total pressure. This implies that Q_j is constant in height. Using the band parameters listed in Table 1, with $f_{\text{day}} = 0.5$, the total heating due to the A, B and γ bands for the mid to upper stratosphere is,

$$Q = 0.033\sqrt{\bar{\mu}}\ \text{K day}^{-1}. \qquad (9)$$

Table 2. *Solar heating rates in K day*$^{-1}$ *due to* O_2, CO_2 *and* O_3 *for 0° N* spring conditions

Z (km)	O_2	CO_2	O_3
12	0.022	0.051	0.019
16	0.024	0.066	0.046
20	0.025	0.093	0.408
24	0.026	0.118	1.262
28	0.026	0.147	1.872
33	0.026	0.169	3.735
39	0.026	0.197	7.006
45	0.026	0.212	9.513
51	0.026	0.202	7.460

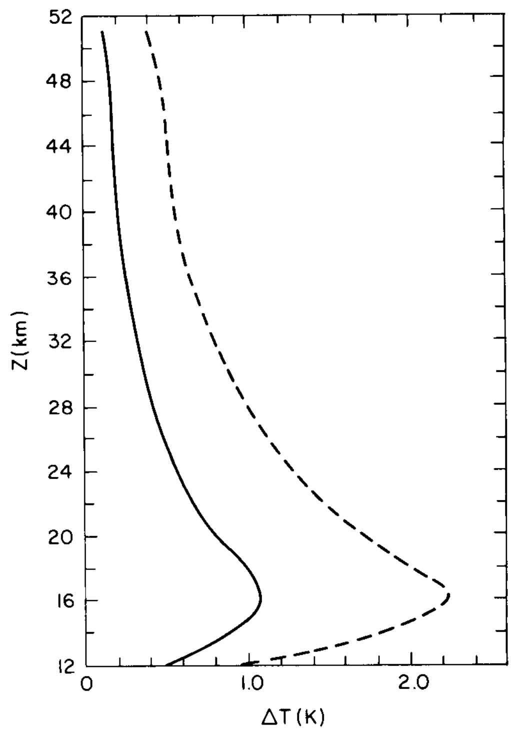

Fig. 4. Change in stratospheric temperatures due to the A, B and γ bands of O_2 for 0° N spring conditions calculated from: broad band model eq. (1) (full line) and the method of Sasamori et al. (1972) (dashed line).

The value for $\bar{\mu}$ in the tropics is 0.63 (Manabe and Möller, 1961) which results in a tropical O_2 heating rate of 0.026 K day^{-1}. The expression given by Sasamori et al. yields a heating rate which is proportional to $p^{-1/8}$, thus leading to increasing heating with decreasing pressure. The magnitude of

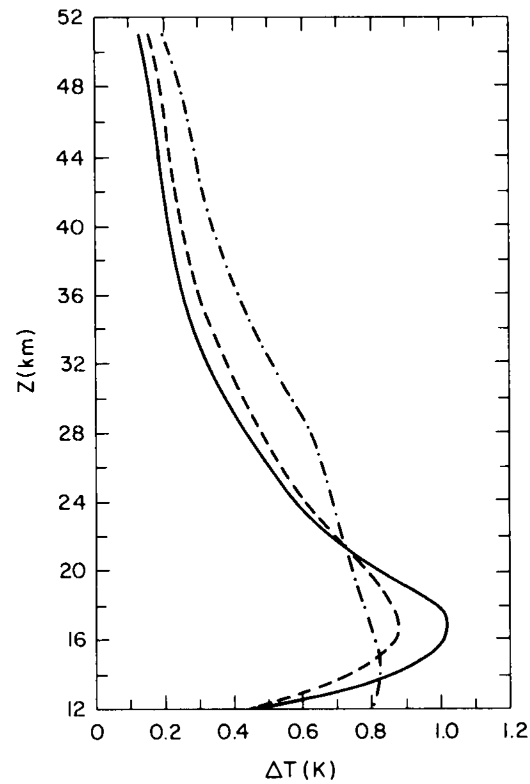

Fig. 5. Change in stratospheric temperatures due to the A, B and γ bands of O_2 calculated from eq. (1) for: 0° N spring (full line), 30° N spring (dashed line) and 70° N summer (dash-dotted line).

O_2 heating is compared with the solar heating due to CO_2 and O_3 in Table 2. Solar O_2 heating is negligible in the middle and upper stratosphere compared to the heating due to ozone. However, near the tropopause region, O_2 heating is approximately equal to O_3 heating. Since the radiative relaxation time is large near the tropopause, especially in the tropics, the temperature change caused by the presence of O_2 can be as large as 1.0 K. This result is illustrated in Fig. 4, where the change in temperature due to the presence of the three solar oxygen bands for 0° N spring is shown. Temperatures are calculated using the fixed dynamical heating assumption discussed by Ramanathan and Dickinson (1979). Also shown is the temperature change obtained from the Sasamori et al. expression. As expected, based upon the heating rate differences, their method overpredicts O_2 temperature effects. The effect of O_2 absorption on atmospheric temperatures at other latitudes is shown in Fig. 5. The behaviour of the temperature change at 70° N exhibits the effect that at high latitudes (i.e., low zenith angles) much of the incoming solar radiation is absorbed in the upper stratosphere.

The presence of the three oxygen bands is found to reduce the planetary albedo by 0.42%. The reduction of incoming solar radiation due to the oxygen bands causes the surface to warm by 0.04 K.

4. Summary

Using the detailed line-by-line calculations of Nakazawa et al. (1978), an efficient and accurate broad band model has been constructed to account for the solar absorption due to O_2. This method is well suited for applications to simple climate models as well as large general circulation models. These bands lead to a small change in stratospheric heating rates (<0.03 K day^{-1}), but because of the large radiative relaxation times near the tropopause, can lead to an increase of tropopause temperatures of from 0.8–1.0 K.

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