

## Radiative Terms in the Thermal Conduction Equation for Planetary Atmospheres

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(Manuscript received 16 January 1968, in revised form 22 March 1968)

### ABSTRACT

Terms in the thermal conduction equation arising from infrared emissions and absorptions by atomic oxygen and carbon monoxide are investigated. The purpose of the investigation is to develop general expressions for the net emission by O and CO taking into account absorption of planetary radiation from below as well as radiation from regions of the mesosphere and thermosphere. These expressions are valid at all optical depths in the thermosphere. An expression for the net emission from a molecular band is also given.

The radiative terms are developed under the assumption of local thermodynamic equilibrium. The expressions developed for the radiative terms permit the evaluation of net heating as well as cooling in the O and CO emission lines.

The results are compared to the Bates' approximation to the radiative loss terms for a partly dissociated CO<sub>2</sub> atmosphere which is optically thick in both O and CO. For this model it is found that, at high altitudes where the atmosphere is optically thin in O and CO, the net emission differs from the Bates' approximation by about 15% due to the effect of absorption. Near unit optical depth the net emission differs by more than an order of magnitude from the Bates' terms.

### 1. Introduction

An important aspect of the theoretical computation of the thermospheric temperature profile is the effect of radiative cooling in the infrared by constituents present in the thermosphere. The most important radiators in the atmospheres of the terrestrial planets are CO<sub>2</sub>, CO and O. Radiative losses from CO<sub>2</sub> will generally occur near the bottom of the thermosphere below the altitude of solar ultraviolet heating, whereas CO and O may radiate effectively at higher altitudes, depending, of course, on the amount of these constituents present.

The usual practice in studying the effect of these last two constituents in cooling a thermosphere has been to utilize an approximation introduced by Bates (1951). This approximation takes unit optical depth in a constituent as a dividing line above which every emitted photon escapes the thermosphere and is thus effective in cooling, and below which every emitted photon is reabsorbed locally and is thus ineffective in cooling. Such an approximation distorts the functional form of the loss terms in the thermal conduction equation with consequent error in the computed temperature profile. The magnitude of this error is, however, difficult to estimate qualitatively. In addition, the Bates' approximation neglects the possibility of heating in the radiatively active constituents. This heating can occur if the effective temperature of the planet is roughly twice the local temperature at the altitude where O and CO will be formed via photodissociation of CO<sub>2</sub> and O<sub>2</sub>.

Published models of the Martian atmosphere indicate temperatures from about 130K (McElroy, 1967) to as

low as 60K (Fjeldbo *et al.*, 1966) in the altitude region where photodissociation would occur. Since the planetary effective temperature is 230K, it is necessary to consider the effect of heating of the radiative constituents (CO and O) by absorption of radiation from below.

The object of this paper is to develop expressions for radiative losses by O and CO which take account of infrared absorption. The use of such expressions in thermospheric energy balance studies should improve the accuracy of thermal structure calculations for optically thick thermospheres or models having a run of temperatures in the lower thermosphere which are less than the planetary effective temperature.

### 2. The thermal conduction equation

The most important processes determining the thermospheric temperature are the deposition of solar ultraviolet energy and the loss of this energy via thermal conduction and infrared radiation. These processes are described by the thermal conduction equation which we will write in the one-dimensional, time-independent form

$$-\frac{d}{dz} \left( \kappa(T) \frac{dT}{dz} \right) + \sum_i h\nu_i (\pi F_i) = -Q(z), \quad (1)$$

where  $\kappa(T)$  is the thermal conductivity, and  $Q(z)$  the ultraviolet heat source. The net emission of radiation in a specified transition is given by the divergence of the photon flux multiplied by the energy of the transition  $h\nu$ . The summation in (1) is taken over the possible radiative transitions. The factor  $\pi$  in the emission term

arises from the definition of the flux as (Chandrasekhar, 1960)

$$\pi F_\nu = \int I_\nu \mu d\Omega, \tag{2}$$

where  $I$  is the photon intensity,  $\mu$  the cosine of the polar angle, and  $d\Omega$  an element of solid angle. The integral on the right-hand side of (2) gives the number of photons  $\text{cm}^{-2} \text{sec}^{-1}$  crossing an area in the radiation beam, and it is the divergence of this quantity which is of interest.

### 3. Derivation of the radiative terms

The divergence of the radiative flux may be obtained in a straightforward way from radiative transfer considerations once the appropriate transfer equation has been found. To derive this equation we consider a system consisting of two energy levels and assume that the spectral line arising from transitions between these levels is Doppler broadened. Such a system is appropriate to both the ground state triplet of atomic oxygen and to the rotational states of carbon monoxide. There are actually two possible transitions within the oxygen triplet, but the  $O(^3P_1) \rightarrow O(^3P_2)$  will be much more important than  $O(^3P_0) \rightarrow O(^3P_1)$ , since its Einstein coefficient for spontaneous emission is about 5 times greater, the statistical weights of  $^3P_0$  and  $^3P_1$  are 1 and 3, respectively, and the population of the higher-energy  $^3P_0$  state will be smaller than that of  $^3P_1$ . There are a number of excited rotational levels for the CO molecule, but only the dipole transitions between adjacent states will be of importance; hence, the summation indicated in (1) may be taken over the rotational states once the flux divergence arising from transitions between adjacent states has been found. The radiative emission under discussion occurs in planetary thermospheres under conditions of very low pressure and the spectral lines are Doppler broadened. In what follows we denote the upper level of the two-level system by a subscript 2 and the lower level by a subscript 1.

We denote the number density of molecules in the upper state which emit a photon in a frequency interval  $d\nu$  within the line profile by  $n_2(\nu)$  and the number density of molecules in the lower state which absorb photons in this frequency interval by  $n_1(\nu)$ . Using Milne's (1924) definition of the Einstein coefficients, we may equate the increase in the number of photons added to the radiation field to the decrease in the number density of the upper state molecules, i.e.,

$$\int d\Omega \frac{d}{ds} \int_0^\infty I_\nu d\nu = \int_0^\infty [n_2(\nu)A_{21} + n_2(\nu)B_{21}\rho_\nu - n_1(\nu)B_{12}\rho_\nu] d\nu, \tag{3}$$

where  $d\Omega$  is the element of solid angle,  $ds$  an element of path length in the medium,  $I_\nu$  the photon intensity of the

radiation field,  $A_{21}$  and  $B_{21}$  the Einstein coefficients for spontaneous and induced emission,  $B_{12}$  the Einstein absorption coefficient, and  $\rho_\nu$  the radiation density. The integrals of  $n_1(\nu)$  and  $n_2(\nu)$  over all frequencies are the total number densities  $n_1$  and  $n_2$ .

We will assume that the radiation density traversing the medium is a broad function of frequency relative to the local line width. This is certainly a good assumption for the planetary radiation. It is also a reasonable assumption for the ambient radiation field in the mesosphere and lower thermosphere where the temperatures are relatively low and the Doppler line widths correspondingly narrow. We will also assume local thermodynamic equilibrium (LTE); the energy levels are therefore populated according to the Boltzmann distribution.

These assumptions enable us to reduce (3) to the standard form for the first moment of the radiative transfer equation, i.e.,

$$\frac{1}{4} \frac{dF}{dz} = -\sigma_D n \bar{I} + \epsilon_D n, \tag{4}$$

where  $F$  and  $\bar{I}$  are the frequency-integrated flux and mean intensity, and  $n$  is the total number density of the radiating constituent. The quantities  $\sigma_D$  and  $\epsilon_D$  are given by

$$\sigma_D = \frac{1}{8\pi^{3/2}} \frac{g_2 A_{21}}{Z(T)} \frac{1}{\alpha_D} \left(\frac{c}{\nu}\right)^2 \times \exp\left(-\frac{\epsilon_1}{kT}\right) \left[1 - \exp\left(-\frac{\epsilon_{21}}{kT}\right)\right], \tag{5}$$

$$\epsilon_D = \frac{1}{4\pi} \frac{g_2 A_{21}}{Z(T)} \exp\left(-\frac{\epsilon_2}{kT}\right), \tag{6}$$

where  $\alpha_D$  is the Doppler width of the line given by  $(\nu/c)(2kT/m)^{1/2}$ ,  $Z(T)$  the partition function for the system under consideration,  $g_2$  the statistical weight of the upper state, and  $\epsilon_{21}$  the energy difference  $\epsilon_2 - \epsilon_1$  between the states.

The quantity  $\sigma_D$  is the Doppler absorption cross section in the center of the line. It is closely related to the absorption coefficient derived by Mitchell and Zemansky (1961). Aside from notation the differences between (5) and Eq. (35) of Mitchell and Zemansky are the exponential factors. The first of these in (5) results from relating the number density of the absorbing state to the total number density. The second represents the effect of stimulated emission on the excited state population which was assumed to be negligible in Mitchell and Zemansky.

The quantity  $\epsilon_D$  is the emission coefficient. We note that  $\epsilon_D/\sigma_D$  is the integral of the Planck function over the line as it must be since we assume LTE. The frequency is the frequency at the center of the line.

The solution of the radiative transfer equation for  $\bar{I}$  is discussed in standard works such as Chandrasekhar (1960) or Kourganoff (1963). Thus,

$$\bar{I}(\tau) = \frac{1}{2}\bar{I}_0 E_2(\tau_0 - \tau) + \frac{1}{2} \int_0^{\tau_0} J(t) E_1(|t - \tau|) dt, \quad (7)$$

where  $\tau$  is the optical depth in the center of the line defined by

$$d\tau = -n\sigma_D dz, \quad (8)$$

$E_1$  and  $E_2$  are special cases of the integro-exponential function defined by

$$E_n(x) = \int_x^\infty e^{-xt} \frac{dt}{t^n}, \quad (9)$$

$\tau_0$  is the total optical thickness of the atmosphere in the spectral line under consideration and  $\bar{I}_0$  represents the flux incident from below, i.e., from the planetary spectrum.  $J(t)$  appearing under the integral in (7) is the source function, which is the Planck function under the LTE assumption. It is worth noting that in the thermosphere, conditions depart radically from radiative equilibrium, and we cannot assume  $\bar{I} = \epsilon_D/\sigma_D$ , which would make the flux divergence zero.

The energy from the planetary spectrum which interacts locally is that contained in a Doppler width of the spectral line. The mean intensity  $\bar{I}_0$  is thus

$$\bar{I}_0 = \frac{c}{4\pi} \int_0^\infty B_\nu(T_E) \exp[-(\nu - \nu_0)^2/\alpha_D^2(T)] d\nu, \quad (10)$$

where  $B_\nu(T_E)$  is the Planck distribution characteristic of the planet,  $T_E$  being the planetary effective temperature. If we take  $B_\nu$  as approximately constant over the Doppler width of the line, then

$$\bar{I}_0 \simeq \frac{c}{4\pi^{\frac{1}{2}}} B_{\nu_0}(T_E) \alpha_D(T), \quad (11)$$

where  $T$  is the local temperature at the altitude where  $\bar{I}(\tau)$  is being evaluated. The emission represented by the source function in the integrand of (7) has a form similar to  $\bar{I}_0$  except that  $T_E$  is replaced by  $T(t)$ , the local temperature at the emitting altitude.

We may now evaluate the flux divergence for the  $62 \mu$  line of O and the CO rotational lines. Substituting the expression for  $\bar{I}(\tau)$  of (7) into (4), using (11) for  $\bar{I}_0$  and a similar expression for  $B(t)$ , and evaluating  $\sigma_D$  of (5) for the ground state triplet of atomic oxygen, we find the divergence of the energy flux to be

$$\frac{d}{dz}(\pi F)$$

$$= -R_{O_X}(z, T) [1 - A^1_{O_X}(T_E, T) - A^2_{O_X}(T)]. \quad (12)$$

The coefficient of the term in brackets is

$$R_{O_X}(z, T) = A_{21} h \nu_{O_X}(z) \left( \frac{3e^{-228/T}}{5 + 3e^{-228/T} + e^{-326/T}} \right), \quad (13)$$

which is just the radiative loss term given by the Bates' approximation. The terms  $A^1_{O_X}(T_E, T)$  and  $A^2_{O_X}(T)$  are

$$A^1_{O_X}(T_E, T) = \frac{1}{2} \left( \frac{e^{228/T} - 1}{e^{228/T_E} - 1} \right) E_2(\tau_0 - \tau), \quad (14)$$

$$A^2_{O_X}(T) = \frac{1}{2} \int_0^{\tau_0} \left( \frac{e^{228/T(z)} - 1}{e^{228/T(t)} - 1} \right) E_1(|t - \tau(z)|) dt. \quad (15)$$

These absorption terms will be discussed after an expression similar to (12) is obtained for the CO rotational lines.

For the CO lines we are interested in the divergence of the sum of the fluxes arising from all transitions between adjacent rotational states  $J \rightarrow J-1$ , where  $J$  is the rotational angular momentum quantum number of the upper state. The Einstein coefficient for spontaneous emission between these states is (based on a rigid-rotator model)

$$A_{J, J-1} = \frac{4}{3\hbar} (4\pi B)^3 d^2 \left( \frac{J^4}{2J+1} \right), \quad (16)$$

where  $d$  is the electric dipole moment for CO, and  $B$  the rotational constant given by  $B = \hbar/(4\pi cI)$ , where  $I$  is the moment of inertia of the molecule and  $c$  the velocity of light. The partition function for the rotational states is

$$Z(T) = \sum_J (2J+1) \exp\left[-\frac{hcB}{kT} J(J+1)\right] \approx \frac{T}{\theta_r}, \quad (17)$$

where the approximate equality in (17) is obtained by replacing the sum over  $J$  states by an integral, and  $\theta_r$  is the characteristic rotational temperature for CO, i.e.,

$$\theta_r = \frac{hcB}{k} = 2.77\text{K}. \quad (18)$$

The replacement of the summation over  $J$  by an integration is valid for  $T \gg \theta_r$ . Using (22) and (23) we find that the expression for the Doppler absorption cross section in the  $J \rightarrow J-1$  line is

$$\sigma_D = \frac{4\pi^{\frac{1}{2}} d^2}{3 \hbar} \left( \frac{m}{2kT} \right)^{\frac{1}{2}} \frac{\theta_r}{T} \exp[-J^2\theta_r/T] \times \{1 - \exp[-2J\theta_r/T]\}. \quad (19)$$

We may now follow a procedure similar to that used to

find the flux divergence in the 62 μ O line to obtain the flux divergence for a  $J \rightarrow J-1$  rotational transition in CO. The expression so obtained is then summed over  $J$ , but the summation is replaced by an integration as in the evaluation of the partition function, and terms in  $J$  are neglected relative to terms in  $J^2$ . The result we obtain is

$$\pi \frac{d}{dz} \sum_{J=1}^{\infty} F_{J,J-1} = -R_{CO}(z, T) \times [1 - A^1_{CO}(T_E, T) - A^2_{CO}(T)], \quad (20)$$

where

$$R_{CO}(z, T) = \frac{2^{10}\pi^4}{3} cd^2 B^4 n_{CO}(z) \left(\frac{T}{\theta_r}\right)^2 = 2.58 \times 10^{-23} n_{CO}(z) T^2 \quad (21)$$

is the radiative loss (ergs cm<sup>-3</sup> sec<sup>-1</sup>) given in the Bates' approximation, and

$$A^1_{CO}(T_E, T) = \frac{1}{2} \left(\frac{T_E}{T}\right) E_2(\tau_0 - \tau), \quad (22)$$

$$A^2_{CO}(T) = \frac{1}{2} \int^{\tau_0} [T(t)/T(z)] E_1(|t - \tau(z)|) dt. \quad (23)$$

The optical depth  $\tau$  is taken as the optical depth in the strongest line. The  $J$  dependence of the optical depth has not been included in the  $J$  sums.

**4. Comparison with the Bates' approximation**

Bates (1951) wrote the rate of radiative loss in the 62 μ O line as

$$R = \epsilon A n (1 - \sigma/\rho), \quad (24)$$

where  $\epsilon$  is the energy emitted in a transition;  $A$  the Einstein coefficient for spontaneous emission;  $n$  the number density of the emitting state, which is readily related to the total species number density through the partition function; and  $\sigma/\rho$  is the ratio of the energy of the radiation field which lies within the Doppler width of the line to the energy which would lie within this width if the radiation field and gas were in thermodynamic equilibrium. The expressions derived above for the net emission in the O [Eq. (12)] and CO [Eq. (20)] lines are of this form,  $\sigma/\rho$  being the sum of the two terms  $A^1$  and  $A^2$  in these equations.

The first term  $A^1$  in the brackets of (12) and (20) represents absorption in the line or lines from the planetary

spectrum. As noted by Bates, near  $\tau = \tau_0$ , this term is roughly  $T_E/2T$ , where  $T$  is the local temperature at  $\tau_0$ . This follows directly from (22) for the CO lines and holds approximately for the 62 μ O line if the local temperature is greater than 228K, as can be seen by expanding the exponential terms in (14). Thus, if the planetary effective temperature is more than twice the temperature at the altitude where O or CO first appears, there can be a net heating due to this term alone.

The second term  $A^2$  in (12) and (20), represents absorption at a given level of the radiation emitted at all other levels of the atmosphere, the radiation from each emitting layer being attenuated along the optical path between these levels.

This physical interpretation facilitates writing a general expression for the net emission from a molecular band. The flux divergence is

$$\int_0^{\infty} \frac{d}{dz} (\pi F_\nu) d\nu = - \int_0^{\infty} 4\pi \sigma_\nu J_\nu(\tau) \left[ 1 - \frac{1}{2} \frac{\bar{I}_0(\tau_0)}{J_\nu(\tau)} E_2(\tau - \tau_0) - \frac{1}{2} \int_0^{\tau_0} \frac{J_\nu(t)}{J_\nu(\tau)} E_1(|t - \tau|) dt \right] n, \quad (25)$$

the last two terms in the brackets of the integrand on the right-hand side of (25) being the ratio of the energy of the radiation field contained in the band to that which would be contained in the band under equilibrium conditions. The frequency integration in (25) is difficult in general. However, if we again assume that the radiation traversing the medium is a broad function of frequency relative to the widths of the absorbing lines in small band intervals, we have

$$\frac{d}{dz} (\pi F) = -4\pi S J(\tau) \left[ 1 - \frac{1}{2} \frac{\bar{I}_0(\tau_0)}{J(\tau)} E_2(\tau_0 - \tau) - \frac{1}{2} \int_0^{\tau_0} \frac{J(t)}{J(\tau)} E_1(|t - \tau|) dt \right] n \quad (26)$$

for the flux divergence in a given band interval,  $S$  being the band intensity in the interval.

Fig. 1 shows a comparison of the Bates' radiative loss term with the loss given by (12) and (20). These are computed on the basis of a model atmosphere for the planet Mars. This is an optically thick model in both O and CO, unit optical depths in these constituents occurring at 121 and 128 km, respectively. The model assumes

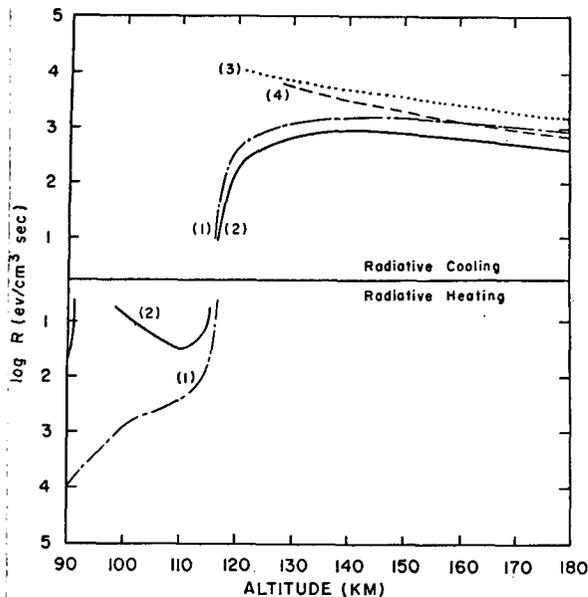


FIG. 1. Comparison of the net emission ( $\text{eV cm}^{-3} \text{sec}^{-1}$ ) in the  $62 \mu$  O line and the CO rotational lines with the radiative losses given by the Bates' approximation. Computed values of the various terms are based on a model Martian atmosphere which is optically thick in both O and CO. The curves are: (1) radiative heating and loss in O; (2) radiative heating and loss in CO; (3) radiative loss in O in Bates' approximation; (4) radiative loss in CO in Bates' approximation. Curves (3) and (4) are terminated at the altitudes of unit optical depth in O and CO.

densities of  $7 \times 10^{11} \text{ cm}^{-3}$  of both O and CO at 90 km. The temperature profile above this point is taken as

$$T(z) = T_m + (T_\infty - T_m) \{1 - \exp[-(z - z_m)^2 / C]\}, \quad (27)$$

where  $T_m$ , the temperature at 90 km, is taken as 125K, and an exospheric temperature  $T_\infty$  of 300K has been assumed. The constant  $C$  may be evaluated by assuming a  $T(z)$  value at any altitude above 90 km. For the computations represented in Fig. 1, we have taken  $T(120) = 160\text{K}$ . The integrals which appear in (15) and (23) have been evaluated with a two-point quadrature formula, the weights and divisions being computed for each value of  $\tau$ . The method is discussed by Chandrasekhar (1960). For the model in Fig. 1 we see that there is a heating in the CO lines which peaks at 110 km and has a magnitude of about  $32 \text{ eV cm}^{-3}$ . This is due entirely to absorption from the surrounding atmosphere, i.e., to the term  $A^2$  in (20). Absorption from the planetary infrared spectrum occurs within the first kilometer above 90 km and is indicated, with exaggerated width, at the extreme left-hand side of the figure. The heat source provided by the term  $A^1$  is of the same magnitude as  $A^2$ . Both of these heating terms are no doubt of trivial importance insofar as determination of the temperature in the 90-

120 km region is concerned. The net heating in the  $62 \mu$  O line is more extensive than that in the CO rotational lines. There is, of course, more energy available for absorption in the planetary spectrum at  $62 \mu$  than in the far infrared CO lines.

For altitudes roughly 15 km above the altitudes of unit optical depth in O and CO, the cooling given by (12) and (20) is less by more than an order of magnitude than that given by Bates' approximation. For several kilometers below the altitudes of unit optical depth there is an actual net cooling where the Bates' approximation gives no cooling. The form of the radiative emission terms, when expressed as the divergence of the radiative fluxes in the emission lines, therefore deviates considerably from the Bates' approximation over a wide altitude interval.

## 5. Summary

Those terms in the thermal conduction equation which represent radiative emission by O and CO have been derived. The thermal conduction equation which includes these terms, as well as  $\text{CO}_2$  loss and ultraviolet heating, is the appropriate one to use in energy balance calculations for the thermospheres of the terrestrial planets. The equation used in this investigation differs from those usually employed in thermospheric investigations by the inclusion of infrared absorption terms. The spontaneous radiative emission at a given altitude is a function only of the local temperature at that altitude, but absorption depends upon the flux originating at all other levels and is thus a function of the run of temperatures throughout the thermosphere, as well as of the planetary effective temperature. The upper atmospheric energy balance is therefore expressed by an integro-differential equation for the temperature profile  $T(z)$  in contrast to the differential equation which expresses energy balance in the Bates' approximation. The net radiative emission as a function of altitude has been compared with that given by the Bates' approximation for a model Martian atmosphere. The differences between the net emission terms and the Bates' approximation are substantial at low altitudes, suggesting that these absorption terms should be included in thermal structure calculations for the terrestrial planets.

*Acknowledgments.* This research was supported by a National Academy of Sciences-National Research Council Research Associateship at the Goddard Institute for Space Studies. I am grateful to Drs. S. I. Rasool, C. Prabhakara, A. Arking, and R. Jastrow for useful discussions regarding this problem.

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