RADIATIVE TERMS
IN THE
THERMAL CONDUCTION EQUATION

by

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Abstract

Those terms in the thermal conduction equation which arise due to infrared emissions and absorptions by atomic oxygen and carbon monoxide are investigated. The purpose of this investigation is to develop general expressions for the net emission by O and CO which take account of absorption from the planetary black-body spectrum and from other regions of the thermosphere and are thus valid at all optical depths in the thermosphere.

The radiative terms are developed under the assumptions of local thermodynamic equilibrium and an Eddington approximation for the radiation field. The results are compared to the Bates' approximation to the radiative loss terms for a Martian model atmosphere which is optically thick in both O and CO. It is found that the net emission differs from the Bates' expressions by more than an order of magnitude near unit optical depth and that absorption causes the emission to be somewhat less than the Bates' approximation in optically thin regions of the high thermosphere.

The expressions developed for the radiative terms permit the evaluation of net heating as well as cooling in the O and CO emission lines. For the model thermosphere used to compare the net emission with the Bates' cooling terms it was found

that near the mesopause there was a heat source of about 10^4 ev/cm^{3}sec due to heating in the O 62μ line and a lesser source of about 10-100 ev/cm^{3}sec due to heating in the CO rotational lines.

The recent advent of direct observation of planetary atmospheres by fly-by space probes has given great impetus to theoretical studies of the upper atmospheres of the terrestrial planets. The occultation experiment carried out by the Mariner IV spacecraft on the Martian atmosphere has generated a great deal of discussion concerning the physical conditions which exist in that atmosphere. Since the data obtained fall far short of strictly delimiting these conditions, there has been wide latitude for theoretical speculations. The observed ionization profile has variously been interpreted as an E, F_1, or F_2 layer, and calculated exospheric temperatures have been published ranging from 130° to 400°K (Fjeldbo et al., 1966; McElroy, 1967; Chamberlain and McElroy, 1966).

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_2, CO, and O. Radiative losses from CO_2 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 would, however, be 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_2 and O_2.

Published models of the Martian atmosphere indicate temperatures from about 130^oK (McElroy, 1967) to as low as 60^oK (Fjeldbo <u>et</u> <u>al</u>., 1966) in the altitude region where photodissociation would occur. Since the planetary effective temperature is 230^oK, the possible effect of heating in the radiative constituents must be considered.

The object of this paper is to develop expressions for the radiative losses by O and CO which take account of absorption in the emission lines. The use of such expressions in thermospheric energy balance studies should alleviate doubts which may arise concerning the accuracy of such calculations when the Bates' approximation is employed in optically thick thermospheres or in models having a run of temperatures in the lower thermosphere which are less than the planetary effective temperature.

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 following one-dimensional, time-independent form:

$$\frac{d}{dz}\left(\varkappa(T)\,\frac{dT}{dz}\right) + \sum_{i} h\nu_i\,\frac{d}{dz}\left(\pi F_i\right) = -Q(z) \qquad (1)$$

$\varkappa(T)$ 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 π in the emission term arises from the definition of the flux as (Chandrasekhar, 1960)

$$\pi F_\nu = \int I_\nu \mu \, d\Omega \qquad (2)$$

where I is the photon intensity, μ 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/cm^{2}sec crossing an area in the radiation beam, and it is the divergence of this quantity which is of interest.

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.

The number of molecules which undergo transitions 2 → 1 and emit a photon in the frequency interval $d\nu$ will be denoted by $\delta_\nu N_2$, where N_2 is the upper state population. The net decrease in the upper state population in a time interval dt is $-d(\delta_\nu N_2)$. Equating this to the corresponding number of photons added to the radiation field we have

$$-d(\delta_\nu N_2) = \int d\Omega \left(dI_\nu \, d\sigma \, dt \, d\nu \right) \tag{3}$$

where dI_ν is the increase in photon intensity in the frequency interval $d\nu$, $d\sigma$ is an elementary area across which the radiation flows, and the integration is over solid angle. If we multiply and divide by an element of path length in the medium, ds, on the right hand side of (3) and integrate over frequency we obtain

$$-\frac{dn_2}{dt} = \int d\Omega \; \frac{d}{ds}\int_0^\infty I_\nu d\nu \tag{4}$$

which relates the rate of change of number density in the upper state to the change in intensity of the radiation field. For a two-level system we may also write

$$-\frac{dn_2}{dt} = n_2 A_{21} + n_2 B_{21}\rho_\nu - n_1 B_{12}\rho_\nu \tag{5}$$

where ρ_ν is the density of the radiation field traversing the medium, A_{21} and B_{21} are the Einstein coefficients for spontaneous and induced emission, B_{12} is the Einstein absorption coefficient, and n_1 and n_2 are the number densities in the lower and upper energy levels. Since we have assumed Doppler broadening, the intensity may be written

$$I_\nu = I_{\nu_0}\; e^{-(\nu-\nu_0)^2/\alpha_D^2} \tag{6}$$

where I_{ν_0} is the intensity at the center of the line (at frequency ν_0), and $\alpha_D = (\nu_0/c)(2kT/m)^{\frac{1}{2}}$ is the Doppler width of the line.

We now introduce the assumption of local thermodynamic equilibrium (L.T.E.). If the radiation field and the gas are nearly in equilibrium, the population of the various energy states are related through the Boltzmann distribution. In particular we have

$$\frac{n_1}{n_2} = \frac{g_1}{g_2} e^{-\epsilon_{21}/kT} \quad ; \quad n_2 = \frac{g_2}{Z(T)} e^{-\epsilon_2/kT} n \tag{7}$$

where g_1 and g_2 are the statistical weights of the corresponging states, ϵ_{21} is the energy difference, $\epsilon_2 - \epsilon_1$, between states 2 and 1, ϵ_2 is the energy (above the ground state) of state 2, n is the total number density of the gas, and Z(T) is the partition function for the system under consideration. The relations between the Einstein coefficients are

$$\frac{B_{21}}{A_{21}} = \frac{c}{8\pi}\left(\frac{c}{\nu}\right)^2 \quad ; \quad \frac{B_{12}}{B_{21}} = \frac{g_2}{g_1} \tag{8}$$

Finally, the radiation density and intensity are related by

$$\rho_\nu = \frac{1}{c}\int I_\nu \, d\Omega = \frac{4\pi}{c}\bar{\bar{I}}_\nu \tag{9}$$

where $\bar{\bar{I}}_\nu$ is the mean intensity of the radiation field. We now write the element of path length in the medium as $ds = \mu dz$, where dz defines the vertical direction. Equating the right hand side of (4) and (5), performing the integration over frequencies using (6), and making use of (2), (7), (8) and (9), we obtain, after some algebraic manipulation,

$$\frac{1}{4}\frac{dF_\nu}{dz} = -\sigma_D n \bar{\bar{I}}_\nu + \mathcal{E}_D n \tag{10}$$

where

$$\sigma_D = \frac{1}{4\pi^{1/2}} \frac{g_2 A_{21}}{Z(T)} \left(\frac{m}{2kT}\right)^{1/2} \left(\frac{c}{\nu}\right)^3 e^{-\epsilon_1/kT}\left(1 - e^{-\epsilon_{21}/kT}\right) \tag{11}$$

is the Doppler absorption cross section in the line, and

$$\mathcal{E}_D = \frac{1}{2\pi^{1/2}} \frac{g_2 A_{21}}{Z(T)} \left(\frac{m}{2kT}\right)^{1/2} \left(\frac{c}{\nu}\right) e^{-\epsilon_2/kT} \tag{12}$$

is the emission coefficient. The ratio ϵ_D/σ_D is the Plank distribution (for photons), as it must be since L.T.E. has been assumed. The frequency appearing in (10) - (12) is the frequency at the center of the line. Equation (10) is the standard form of the first moment of the radiative transfer equation. The solution of the radiative transfer equation for the mean intensity $\bar{I}_\nu$ and flux F_ν are discussed in standard works such as Chandrasekhar (1960) or Kourganoff (1963) and need not be re-derived here. If we assume the adequacy of the Eddington approximation, i.e., that the radiation field may be divided into upward and downward moving streams of radiation having different intensities, then the solution for the mean intensity is

$$\bar{I}_\nu(\tau) = \frac{1}{2} I_0 E_2(\tau_0 - \tau) + \frac{1}{2}\int_0^{\tau_0} B(t)\, E_1(|t-\tau|)\, dt \tag{13}$$

where τ is the optical depth in the line defined by

$$d\tau = -n\,\sigma_D\,dz \tag{14}$$

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

$$E_n(x) = \int_1^\infty e^{-xt}\,\frac{dt}{t^n} \tag{15}$$

The total optical thickness of the atmosphere in the spectral line under consideration is denoted by τ_0. $\bar{I}_0$ represents the flux incident from below, i.e., from the planetary spectrum. B(t) appearing under the integral in (13) is the source function, which is the Planck function under the L.T.E. assumption. It is worth noting that in the thermosphere conditions depart radically from radiative equilibrium, and we cannot assume $\bar{I} = B$, 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

$$\bar{I}_0 = \frac{c}{4\pi}\int_c^\infty \rho_\nu(T_E)\,e^{-(\nu-\nu_0)^2/\alpha_D^2(T)}\,d\nu \tag{16}$$

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

$$\bar{I}_0 \simeq \frac{c}{8\pi^{1/2}} \rho_{\nu_0}(T_E) \, \alpha_0(T) \tag{17}$$

where T is the local temperature at the altitude where $\bar{I}_\nu(\tau)$ is being evaluated. The emission represented by the Plank function in the integrand of (13) has a form similar to 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 O 62μ line and the CO rotational lines. Substituting the expression for $I_\nu(\tau)$ of (13) into (10), using (17) for $\bar{I}_0$ and a similar expression for B(t), and evaluating σ_D of (11) for the ground state triplet of atomic oxygen, we find the divergence of the energy flux to be

$$\frac{d}{dz}(\pi F_\nu) = - R_{ox}(z,T)\left[1 - A^1_{ox}(T_E,T) - A^2_{ox}(T)\right] \tag{18}$$

The coefficient of the term in brackets is

$$R_{ox}(z,T) = A_{21}\, n_{ox}(z) \, \frac{3e^{-228/T}}{5 + 3e^{-228/T} + e^{-326/T}} \tag{19}$$

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

$$A^1_{ox}(T_E,T) = \frac{1}{2}\, \frac{e^{228/T} - 1}{e^{228/T_E} - 1}\, E_2(\tau_0 - \tau) \tag{20}$$

$$A_{ox}^{2}(T) = \frac{1}{2}\int_{0}^{\tau_0} \frac{e^{22\nu/T(\bar{\tau})}-1}{e^{22\nu/T(t)}-1} E_1\left(|t-\tau(\bar{\tau})|\right) dt \qquad (21)$$

These absorption terms will be discussed after an expression similar to (18) 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 → 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)

$$A_{J,J-1} = \frac{4}{3\hbar}(4\pi B)^3\, d^2\, \frac{J^4}{2J+1} \qquad (22)$$

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

$$Z(T) = \sum_{J} (2J+1)\, e^{-\frac{hcB}{kT}J(J+1)} \approx \frac{T}{\theta_r} \qquad (23)$$

The approximate equality in (23) is obtained by replacing the sum over J states by an integral. θ_r is the characteristic rotational temperature for CO

$$\theta_r = \frac{hcB}{k} = 2.77\,^\circ K \tag{24}$$

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

$$\sigma_D = \frac{8\pi^{3/2}}{3}\frac{d^2}{\hbar}\left(\frac{m}{2kT}\right)^{1/2}\frac{\theta_r}{T}\;J\;e^{-\frac{\theta_r}{T}J^2}\left(1 - e^{-2\frac{\theta_r}{T}J}\right) \tag{25}$$

We may now follow a procedure similar to that used to find the flux divergence in the 62μ O line to obtain the flux divergence for a J → 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

$$\pi\frac{d}{dz}\sum_{J=1}^{\infty} F_{J,J-1} = -R_{CO}(z,T)\left[1 - A^1_{CO}(T_i,T) - A^2_{CO}(T)\right] \tag{26}$$

where

$$R_{CO}(z,T) = \frac{2^{10}\pi^4}{3}c\,d^2B^4 n_{CO}(z)\left(\frac{T}{\theta_r}\right)^2 = 2.58\times10^{-18}\,n_{CO}(z)\,T^2 \tag{27}$$

is the radiative loss (in ergs/cm^{3}sec) given in the Bates' approximation, and

$$\mathcal{A}^{1}_{co}(T_{\varepsilon}, T) = \frac{1}{2}\left(\frac{T_{\varepsilon}}{T}\right) E_{2}(\tau_{0} - \tau) \tag{28}$$

$$\mathcal{A}^{2}_{co}(\tau) = \frac{1}{2}\int_{0}^{\tau_{0}} \left[T(t)/T(z)\right] E_{1}(|t - \tau(z)|)\,dt \tag{29}$$

The optical depth, τ, 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.

Comparison with the Bates' Approximation

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

$$R = \epsilon A n(1 - \sigma/\rho) \tag{30}$$

where ε is the energy emitted in a transition, A the Einstein coefficient for spontaneous emission, and n the number density of the emitting state, which is readily related to the total species number density through the partition function. σ/ρ 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, (18), and CO, (26), lines are of this form. σ/ρ is the sum of the two terms A^1 and A^2 in these equations.

The first term in the brackets of (18) and (26), A^1, represents absorption in the line or lines from the planetary spectrum. As noted by Bates, near $\tau = \tau_o$ this term is roughly $T_E/2T$, where T is the local temperature at τ_o. This follows directly from (28) for the CO lines and holds approximately for the 62μ O line if the local temperature is greater than 228°K, as can be seen by expanding the exponential terms in (20). 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 in (18) and (26), A^2, 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.

If the atmosphere is optically thick, the term representing absorption from the planetary spectrum rapidly approaches zero at short distances above the CO_2 dissociation level. There may thus be a large peak of heating due to this absorption near the dissociation level, but none of the energy from the planetary spectrum will penetrate far into the thermosphere. The term representing absorption at a given level due to radiation from all other levels does not vanish even at high altitudes. If we denote by T_x the temperature high in the thermosphere where $\tau \approx 0$, and by T_M a mean temperature at the levels from which absorption occurs, then this second term is of the order of

$$\mathcal{A}^2 \approx \frac{T_M}{2T_x} E_2(\tau_M) \qquad (31)$$

where τ_M is a mean optical depth from which absorption occurs. In practice, for optically thick atmospheres, we may have $T_M/T_x \approx 1$, and τ_M is surely < 1. Thus, this absorption term should attain some value between, roughly, .08 and .50 at high altitudes. The first figure follows from setting $\tau_M = .7$, the second from $\tau_M = 0$. The radiative losses given by (18) and (26) therefore do not approach the Bates' approximation exactly at high altitudes, but are somewhat less due to the effects of reabsorption.

If the atmosphere is optically thin in the radiating constituents, the effect of absorption from the planetary spectrum will be felt higher in the thermosphere and thus constitutes a heat source which should be included in thermal calculations. The second absorption term will be less important at high altitudes in this case since T_M will refer to a temperature nearer the mesopause, and we will have $T_M/T_x < 1$.

Figure 1 shows a comparison of the Bates' radiative loss term with the loss given by (18) and (26). 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 densities of 7×10^{11} cm^{-3} of both O and CO at 90 km, which results in optical thicknesses of about 6 and 49, respectively. The temperature profile above this point is taken as

$$T(z) = T_m + (T_\infty - T_m)\left[1 - e^{-(z-z_m)^2/C}\right] \tag{32}$$

where T_m, the temperature at 90 km, is taken as 125°K, and an exospheric temperature $T_\infty = 300^\circ$K 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 Figure 1, we have taken $T(120) = 160^\circ$K. The integrals which appear in (21) and (29) have been evaluated with a two-point quadrature formula, the weights and divisions being computed for each value of τ. The method is discussed by Chandrasekhar (1960). For the model in Figure 1 we see that there is a heating in the CO lines which peaks at 110 km and has a magnitude of about 32 ev/cm^3. This is due entirely to absorption from the surrounding atmosphere, i.e., to the term A^2 in (26). 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 this 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 62μ 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 62μ 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 (18) and (26) 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.

A model atmosphere which is optically thin in O and CO has also been studied. The same temperature profile as that given by (32) was used, but a number density of $7 \times 10^9 \text{ cm}^{-3}$ was assumed for both O and CO at 90 km. The net emission in this model was, at high altitudes, about 30% less than that given by the Bates' approximation, due to the absorption terms. At lower altitudes there was again a net heating.

Summary and Conclusions

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 CO_2 loss and ultraviolet heating, is the appropriate one to use in energy balance calculations for the thermospheres of the terrestrial planets. The difference between the equation given in this paper and that which is usually employed in thermospheric investigations is the inclusion of infrared absorption terms in the former. 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 integrodifferential 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 magnitude of the deviation of the net emission terms from the Bates' approximation strongly suggests that the efficacy of this type of approximation be tested by including the absorption terms in thermal structure calculations for the thermospheres of the terrestrial planets.

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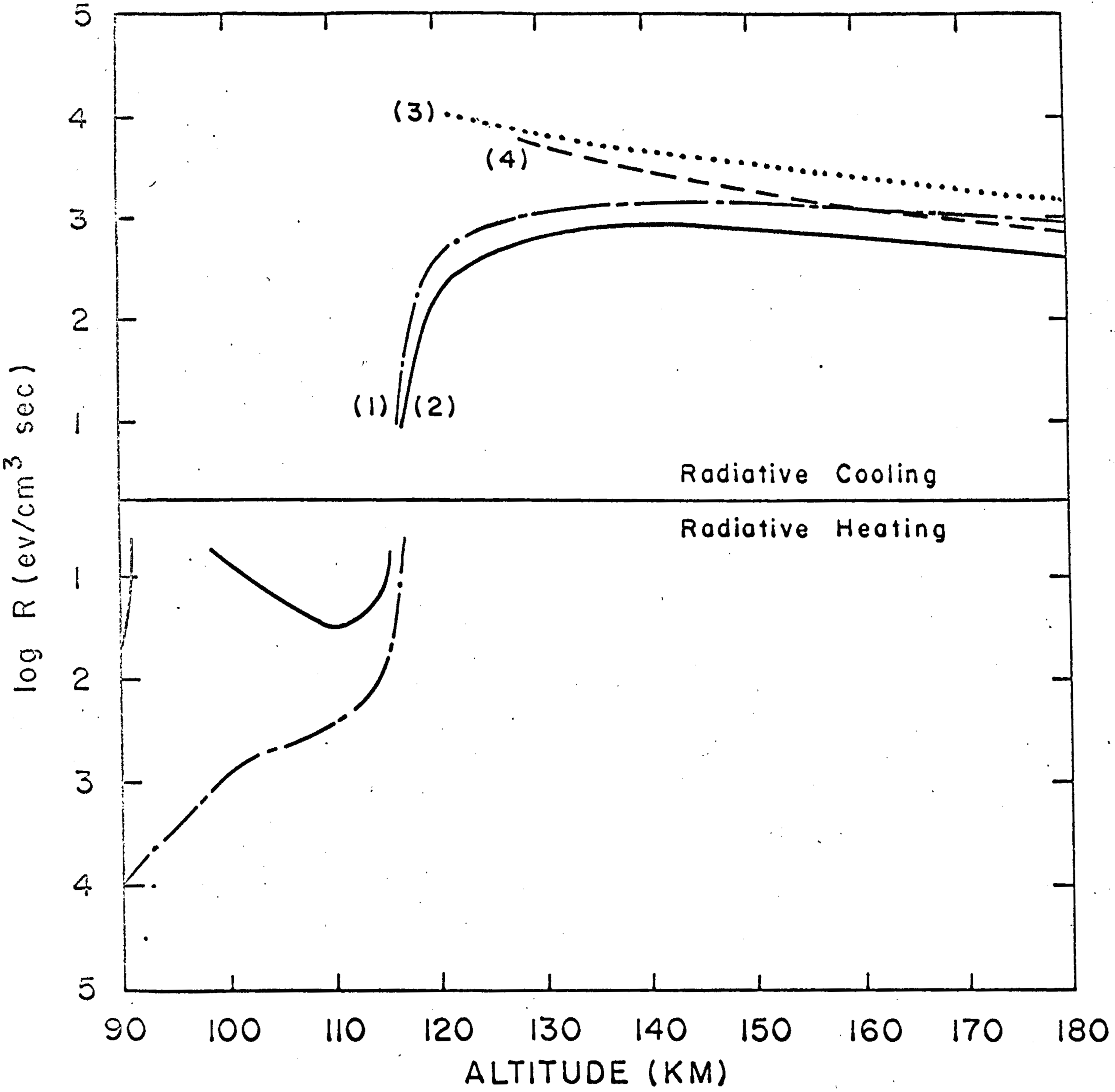
Figure Caption

Fig. 1. Comparison of the net emission, in ev/cm^{3}sec, in the O 62μ 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.



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log R (ev/cm³ sec)
(3)
(4)
(1)
(2)
Radiative Cooling
Radiative Heating
90
100
110
120
130
140
150
160
170
180
ALTITUDE (KM)