INFRARED COOLING BY ATOMIC OXYGEN
IN THE THERMOSPHERE

Gaston Kockarts

Institut d'Aéronomie Spatiale de Belgique, Bruxelles

Belgium

ABSTRACT : The infrared emission of atomic oxygen at 63μ is studied in relation to the heat conduction equation. Below 150 km, a radiative transfer equation has to be used, since the optically thin approximation overestimates the heat loss due to the 63μ emission. The mean net flux and the volume emission are computed and the radiative transfer effect is discussed.

1 - Introduction

In a study of the thermal balance of the upper atmosphere, a knowledge of the heat sources and sinks is of fundamental importance. Numerous satellite drag analyses have confirmed that solar ultraviolet radiation is the principal physical agent for thermosphere heating. Above the mesopause ($\sim$ 85 km), the hydrodynamical regime is such that heat is mainly transported by conduction (Nicolet, 1961). The following hypotheses are adopted as a first approximation:

a) gravity is the only external force acting on the atmosphere;

b) diffusive equilibrium exists among the atmospheric constituents;

c) the mean mass transport velocity is neglected, and the heat conduction equation can then be written (Chapman and Cowling, 1952) :

$$\varrho c_v \frac{\partial T}{\partial t} + \text{div}\,\underline{Q} = P - L \qquad (1)$$

where ϱ is the total density, c_v is the specific heat at constant volume, T is the absolute temperature, t is the time, $\underline{Q}$ is the conduction heat flow, P is the heat production and L is the heat loss.

Nicolet (1961) has clearly shown the effect of heat production P due to the solar ultraviolet radiation, which is mainly absorbed between 100 km and 200 km by atmospheric components such as O, O_2 and N_2. An important factor which is, however, not known is the heating efficiency of the ultraviolet radiation as a function of wavelength and atmospheric components. In practice, the amount of solar energy absorbed in the thermosphere cannot be completely converted into heat. Additional processes, such as atomic and molecular ionization, vibrational and rotational excitation of the molecular species, should be taken into account. Recently, lzakov and Morozov (1971) made an estimate of the heating efficiency and emphasized the effect of the heat input in the Schumann-Runge continuum below 1750 Å.

The loss process compatible with equation (1), is an energy degradation through infrared emission. Atoms or molecules emitting in the infrared must have a permanent magnetic dipole; the transition probability can then be high enough to make the emission important for a heat loss. Among the atmospheric constituents (i.e., O_2, N_2, O, He and H), which can play a role in the total concentration of the upper atmosphere, only atomic oxygen has a permanent magnetic dipole. Nitric oxide, introduced by Nicolet (1945) to explain the D region ionization, can also emit in the infrared. The NO concentration, however, is too small in the thermosphere to affect the heat budget, therefore only the infrared cooling by atomic oxygen emission will be considered in this study. The importance of this effect was first pointed out by Bates (1951), and recen-

tly Feldman and McNutt (1969) and Houck and Harwit (1969) were able
to detect the $63\,\mu$ emission of atomic oxygen.

2 - Excitation and De-Excitation Processes

The ground state of neutral atomic oxygen is a triplet (see Fig.1),
for which the $^3P_0$ and $^3P_1$ levels lie only 226.5 cm^{-1} and 158.5 cm^{-1}
above the ground level $^3P_2$. The excitation potential involved, i.e.,0.028
and 0.020 eV, are of the same order of magnitude as the thermal energy
of the atmospheric constituents. Since collisions are frequent in the
thermosphere, Bates (1951) suggested the following excitation mechanism:

$$X + 0\,(^3P_J) \rightarrow X + 0\,(^3P_{J'}) \tag{2}$$
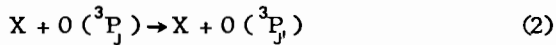
where X is any atmospheric constituent, and the quantum number J is
equal to 2 or 1, and J' is equal to 1 or 0. If process (2) is fast enough,
it is reasonable to assume that the oxygen atoms are distributed at the
levels 0, 1 and 2 according to a Boltzmann distribution. The concentrat
ion $n(0, {}^3P_J)$ is therefore given by:

$$n(0, {}^3P_J) = \frac{n(0)\, g_J \exp(-E_J/kT)}{\sum\limits_{J=0}^{J=2} g_J \exp(-E_J/kT)} \tag{3}$$

where E_J is the excitation energy for the level J, $g_J = 2J + 1$ is the stati
stical weight, k is the Boltzmann constant and n(0) is the total atomic
oxygen concentration. For temperatures ranging from 200°K to 2000°K,
the relative abundance of the $^3P_1$ state varies between 0.16 and 0.31.
The infrared energy emitted by unit volume and in unit time in a transit
ion J'→J is then given by:

$$L = E_{J'} A_{J'-J}\, n(0, {}^3P_{J'}) \tag{4}$$

where $A_{J'-J}$ is the spontaneous transition probability. Using the numeri
cal values given in Fig.1 and equation (3), one immediately obtains:

$$L_{63\mu} = \frac{1.69 \times 10^{-18} n(0) \, e^{-228/T}}{1 + 0.6 \, e^{-228/T} + 0.2 \, e^{-326/T}} \tag{5a}$$

and

$$L_{147\mu} = \frac{4.59 \times 10^{-20} n(0) \, e^{-326/T}}{1 + 0.6 \, e^{-228/T} + 0.2 \, e^{-326/T}} \tag{5b}$$

where $L_{63\mu}$ and $L_{147\mu}$ are both expressed in $\mathrm{erg \, cm^{-3} \, sec^{-1}}$. These relat

O I

Energy

$^3P_0$ ———————————— 226.5 cm^{-1}

$A_{01} = 1.70 \times 10^{-5} \mathrm{sec}^{-1}$
$\lambda = 147\mu$

$^3P_1$ ———————————— 158.5 cm^{-1}

$A_{12} = 8.95 \times 10^{-5} \mathrm{sec}^{-1}$
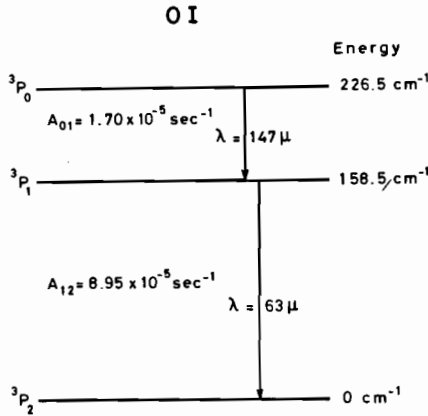$\lambda = 63\mu$

$^3P_2$ ———————————— 0 cm^{-1}

Fig.1 : Energy level diagram of atomic oxygen
ground state.

ions show that, in a first approximation, the 147μ emission is negligible compared to the 63μ emission. The energy rate $R = L/n(0)$ emitted at 63μ and at 147μ is shown in Fig.2 as a function of temperature.

The relations (5a) and (5b) are valid, when the external radiation field is neglected. Before showing the effect of the external radiation field, it is necessary to define the specific intensity I_ν measured in $\mathrm{erg \, cm^{-2} sec^{-1} ster^{-1} Hz^{-1}}$ such that $I_\nu \, d\nu$ is the energy between the frequen cies ν and $\nu + d\nu$ transported across a unit area perpendicular to the beam, in a unit solid angle per unit time. For the transitions between

the two levels 1 and 2., where 1 corresponds to the upper level, the number of absorptions is proportional to $B_{21}I_v$, and the number of emissions is proportional to $A_{12} + B_{12}I_v$ (see Fig.3). The factors B_{21} and B_{12} are the
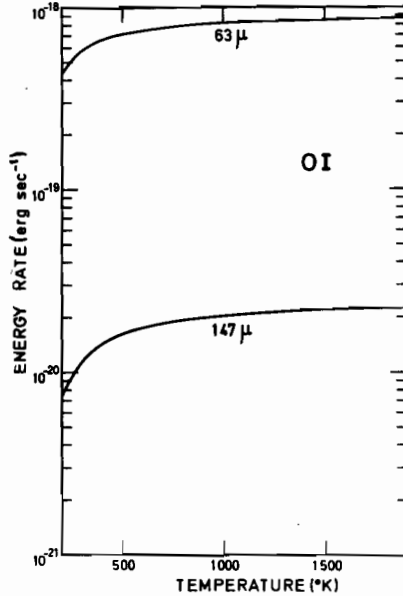

Fig.2 : Emitted energy rate at 63μ and at 147μ as a function of tempe-
rature.

Einstein coefficients of absorption and induced emission, respectively.
The effect of induced emission is to reduce the effective absorption coefficient in the radiative transfer equation presented in section 4. The
Einstein coefficients are related by:

$$g_2 B_{21} = g_1 B_{12} \tag{6}$$

and

$$A_{12} = (2h\nu^3/c^2) B_{12} \tag{7}$$

where g_1 and g_2 are the statistical weights of the levels, h is the Planck
constant, ν is the frequency of the radiation and c the velocity of light.

The amount of absorbed energy is proportional to $n_2 B_{21}I_v$, and the
emitted energy at frequency ν is proportional to $n_1(B_{12}I_v + A_{12})$. The in-

tensity of the radiation field therefore depends on the concentration n_1 and n_2 of the upper and lower level, respectively. It has been assumed that n_1 and n_2 are given by the Boltzmann distribution (3), the subscripts corresponding to the quantum number J. This hypothesis is justified in the terrestrial atmosphere (Bates, 1951; Münch, 1962), since the excitation process (2) takes place much faster than spontaneous photon emission does.

From the preceding discussion, it is clear that relations (5a) and (5b) represent the emitted energy only when absorption and induced emission are neglected. The importance of these processes is, however, di-
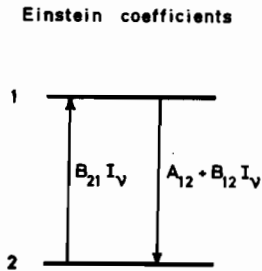
Einstein coefficients

Fig.3 : Einstein relations.

rectly related to the amount of atomic oxygen in the upper atmosphere. It is then intuitively evident that absorption of the 63μ emission becomes important below a certain altitude. This altitude can only be determined by solving the radiative transfer equation discussed in section 4.

3 - Importance of the 63μ Emission

It is possible to show from equation (1) that the vertical heat flow Q due to solar ultraviolet absorption is given by:

$$Q = Q_{uv}\left[1 - \exp\left(-\tau_{uv}\right)\right] \qquad (8)$$

where Q_{uv} is the solar ultraviolet flux at the top of the atmosphere and

τ_{uv} is the optical depth resulting from absorption by all the atmospheric components (Nicolet, 1961). The maximum local heat production occurs approximately at the altitude where the optical depth τ_{uv} is unity. If $\tau_{uv}= 1$ at a height where $n(0) \simeq 10^{10} cm^{-3}$, i.e., around 150 km, the heat flow Q is approximately equal to $1.2 \ erg\, cm^{-2} sec^{-1}$ for a solar flux of $2 \ erg\, cm^{-2} sec^{-1}$. At lower heights Q is, of course, smaller.

When the 63μ absorption is neglected, the vertical infrared flow $Q_{ir}(z)$ at altitude z can be obtained by integrating equation (4):

$$Q_{ir}(z) = E_1 A_{12} \int_z^\infty n(0, {}^3P_1)\, dz \tag{9a}$$

If the atmospheric temperature ranges from $300°K$ to $2000°K$, the ratio $n(0, {}^3P)/n(0)$ varies between 0.2 and 0.3. The infrared cooling flow (9b), evaluated with the numerical data of Fig.1, is then given approximately in $erg\, cm^{-2} sec^{-1}$ by:

$$Q_{ir}(z) \simeq 7 \times 10^{-19} \int_z^\infty n(0)\, dz \tag{9b}$$

In order to make a numerical estimate, it is necessary to adopt a vertical atomic oxygen distribution. Fig.4 shows a possible atomic oxygen distribution briefly discussed by Kockarts and Peetermans (1970). The total contents of atomic oxygen above 120 km and 150 km are respectively $1.8 \times 10^{18} cm^{-2}$ and $5.3 \times 10^{17} cm^{-2}$ for a thermopause temperature of $750°K$. These quantities show that the estimated infrared cooling flow (9b) is of the same order of magnitude, or is even greater than the ultraviolet heating below 150 km. The preceding section indicates that expressions (9a) and (9b) overestimate the infrared loss below a certain height. In theoretical atmospheric models, the lower boundary conditions are usually fixed around 120 km or lower. Any solution of the heat conduction equation (1) should therefore take into account the infrared loss term. It is, however, necessary to know the degree of accuracy given by the approximations (4) or (9b).
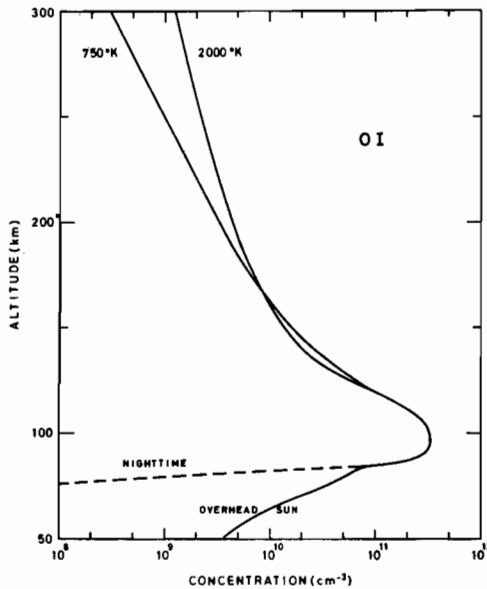
Fig.4 : Vertical atomic oxygen distribution for thermopause temperatu-
res of 750°K and 2000°K.

4 - Radiative Transfer Equation

By counting the gains and losses of a pencil of radiation through a
length of path ds in the atmosphere, the radiative transfer equation can
be written (Chandrasekhar, 1960):

$$\Delta \nu \, dI_v/ds = \left[n_1(A_{12} + B_{12} I_v) - n_2 B_{21} I_v \right] \cdot (h\nu/4\pi) \qquad (10)$$

where $\Delta \nu$ is the total width of the 63μ line and $h\nu = E_1$ is the energy of
the excited level giving rise to the 63μ emission. The introduction of $\Delta \nu$
has been made in order to avoid an integration over frequency. Actually,
this procedure is equivalent to assuming that the emission line has a rec
tangular profile of width $\Delta \nu$. Equation (10) shows the terms due to spon
taneous and induced emission and the absorption term.

If the direction s makes an angle θ with the vertical z, measured
positively from the earth's surface (dz = $\cos \vartheta$ ds = u ds), it is possible
to transform equation (10) into:

$$u \, dI_v/dz = - K_v I_v + \varepsilon_v \tag{11}$$

where

$$K_v = n_2 B_{21} h\nu \left[1 - \exp(- E_1/kT)\right]/4\pi\triangle\nu \tag{12}$$

and

$$\varepsilon_v = A_{12} h_v n_1/4\pi\triangle\nu \tag{13}$$

Relation (12) is obtained by using expressions (3) and (6) to elimate B_{12} and to express n_1 as a function of n_2. From relation (12), the optical depth derivative $d\tau/dz$ is defined by:

$$d\tau/dz = - K_v \tag{14}$$

By using equation (14), equation (11) can finally be written:

$$u \, dI_v/d\tau = I_v - B(T) \tag{15}$$

where

$$B(T) = (2h\nu^3/c^2) \cdot \left[\exp(E_1/kT) - 1\right]^{-1} \tag{16}$$

is the specific intensity at frequency ν of a black body characterized by a temperature T depending on the altitude, i.e., on the optical depth.

It is reasonable in the earth's upper atmosphere to adopt a Doppler profile for the 63μ line. Fig.5 gives the absorption cross section as a function of wave number expressed in Doppler widths. The cross section σ_0 at the center of the line is given in cm^2 by:

$$\sigma_0 = 9.4 \times 10^{-17} T^{-1/2} \tag{17}$$

and it can be obtained in the manner described by Kockarts and Peeter-
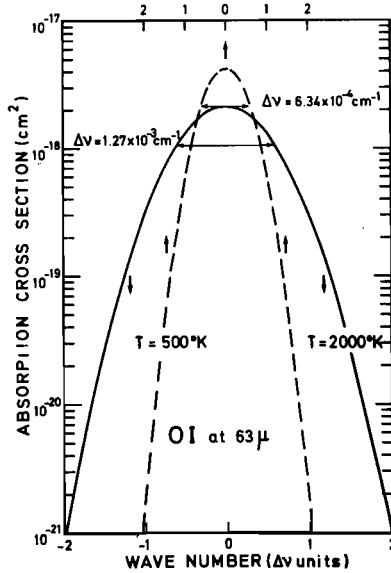mans (1970). As we are mainly interested in the total energy involved in

Fig.5 : Atomic oxygen absorption cross section at 63μ as a function of
wave number expressed in Doppler width units.

the 63μ line, the profiles shown in Fig.5 may be approximated by rect-
angular profiles of width $\Delta\nu$. The total Doppler width changes however
with temperature, i.e., with height, according to:

$$\Delta\nu = 2 \; \frac{\nu_0}{c} \left(\frac{2kT\ln 2}{m} \right)^{1/2} = 8.51 \times 10^5 T^{1/2} \text{ (Hz)} \qquad (18)$$

where ν_0 is the frequency at the centre of the line and m the mass of an
oxygen atom. This factor comes into the optical depth τ and the result of
the integration of equation (14) is shown in Fig.6 (Kockarts and Peeter-
mans, 1970).

     When a value is adopted for the 63μ line width, it is possible to
approximate the frequency integrated intensity $I = \int I_\nu d\nu$ by $I_\nu \Delta\nu$. The

solutions of the radiative transfer equation can therefore be multiplied by
the total Doppler width to obtain a frequency integrated intensity in
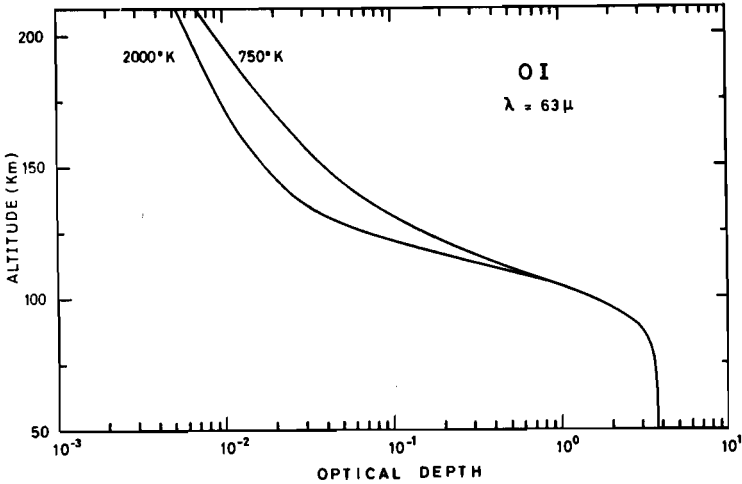$erg\,cm^{-2}sec^{-1}ster^{-1}$.

Fig.6 : Vertical distribution of the optical depth at $63\,\mu$ for thermopause
temperatures of 750 and 2000°K.

5 - Solution of the radiative Transfer Equation

The frequency integrated intensity $I = I_\nu \Delta\nu$ can be obtained from equation (15) in the general form:

$$I = \Delta\nu \left\{ I_0 \exp\left[(\tau - \tau_0)/u\right] - u^{-1} \exp\left[(\tau - \tau_0)/u\right] \cdot \int_{\tau_0}^{\tau} \exp\left[(\tau_0 - t)/u\right] \cdot B(t)\,dt \right\}$$

(19)

In equation (19), I_0 is the specific intensity at the boundary level where
the $63\,\mu$ optical depth is τ_0, and $B(t)$ is the black body specific intensity
which implicitly depends on τ, i.e., on temperature and height.

The intensity can be divided into an upward intensity $(u > 0)$ and a
downward intensity $(u < 0)$. For each case, the boundary condition is different. For the descending radiation, Kockarts and Peetermans (1970)

have shown that the specific intensity due to solar emission at $63\,\mu$ can be neglected at great altitudes, where $\tau_0 = 0$. In this case, the frequency integrated downward intensity is given from (19) by:

$$I_-(\tau,\mu) = -\Delta\nu \int_0^\tau \exp\left[(\tau-t)/u\right]\cdot B(T)\,\frac{dt}{u} \qquad (20)$$

For the ascending radiation, it is necessary to assume a black body emission $B(T_E)$ at $63\,\mu$, coming from the vicinity of the tropopause. Such an emission can correspond to infrared water vapour rotational transitions. In the present study, a tropopause temperature $T_E = 190°K$ is adopted. The choice of this value is not very critical for the infrared emission above 100 km, since the $63\,\mu$ emission above this height comes entirely from the ambient atomic oxygen. Under these conditions, the frequency integrated upward intensity is obtained from equation (19) as:

$$I_+(\tau,\mu) = \Delta\nu \left\{ \int_\tau^{\tau_0} \exp\left[(\tau-t)/u\right] B(T)\,\frac{dt}{u} + B(T_E)\,\exp\left[(\tau-\tau_0)/u\right] \right\}$$

$$(21)$$

where τ_0 is the optical depth at the lower boundary. At 50 km altitude, τ_0 is of the order of 3.7.

The frequency integrated intensities can be experimentally determined and the recent observation by Feldman and McNutt (1969) was discussed by Kockarts and Peetermans (1970) in relation to the radiative transfer process.

6 - Mean net Flux and Volume Emission Rate

For the heat conduction equation, another quantity is, however, useful. It is the mean net flux $F(\tau)$ resulting from an upward and a downward flux

$$F(\tau) = F_+(\tau) + F_-(\tau) \qquad (22)$$

This flux is obtained by integrating I_+ and I_- over one hemisphere for u varying from 1 to 0 and from 0 to -1, respectively. In this way, the mean net flux is written:

$$F(\tau) = 2\pi\Delta\nu\left[\int_0^{\tau_0} B(t)\,E_2(|\tau - t|)\,dt + B(T_E)\cdot E_3(\tau_0 - \tau)\right] \qquad (23)$$

where the exponential integral $E_n(x)$ is defined by:

$$E_n(x) = \int_0^1 u^{n-2}\exp(-x/u)\,du \qquad (24)$$

In the one dimensional heat conduction equation, this mean net flux appears after a first integration over height, which leads to the heat flow transported by conduction. It has, however, been assumed that the atmosphere is stratified in parallel planes and a three-dimensional solution would require a more complex radiative transfer equation.

Fig.7 shows the mean net flux computed for a thermopause temperature of 1000°K. Above 110 km, F is positive and the infrared emission is lost into interplanetary space. Below 90 km, F is positive or negative depending on whether or not a lower boundary emission is introduced. The effect of the lower boundary emission is, however, negligible at altitudes above 100 km. At 300 km, the mean net flux, directed upwards, is equal to 0.1 or 0.2 erg cm^{-2}sec^{-1} for thermopause temperatures of 750°K and 2000°K, respectively.

The volume emission rate L (erg cm^{-3}sec^{-1}), to be used in equation (1) is, in fact, given by the divergence of the mean net flux. L(z) as a function of height is written as follows:

$$L(z) = \frac{dF}{d\tau}\cdot\frac{d\tau}{dz} \qquad (25)$$

By using the expressions (5a) and (23), equation (25) becomes:

$$L(z) = L_{63\mu}\left[1 - X\right] \qquad (26)$$

where:

$$X = 0.5 \left[\exp(228/T) - 1 \right] \left\{ \int_0^{\tau_0} E_1(|t - \tau|) \left[\exp(228/T) - 1 \right]^{-1} dt + \right.$$

$$\left. + E_2(\tau_0 - \tau) \left[\exp(228/T_E) - 1 \right]^{-1} \right\} \tag{27}$$

The term containing the second order exponential integral E_2 in expression (27) is due to the lower boundary emission. A numerical procedure that may be used to evaluate expression (27) has been described by Kockarts and Peetermans (1970).
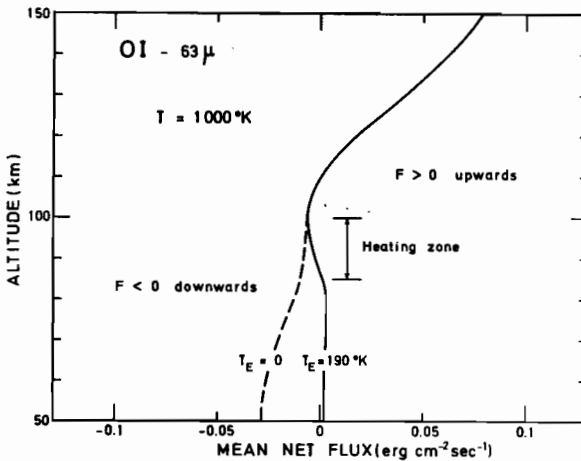

Fig.7 : Mean net flux for a thermopause temperature of 1000°K. The dotted curve ($T_E = 0$) corresponds to the case where no lower boundary emission is present.

The volume emission rate at $63\,\mu$, computed from equation (26), is shown in Fig.8 for a thermopause temperature of 1000°K. The black body temperature T_E for the lower boundary emission was taken to be equal to 190°K. This emission is actually responsible for a sign change of $L(z)$: the cooling process becomes a heating mechanism in a region near the mesopause. The heating region can also be seen in Fig.7, where the slope
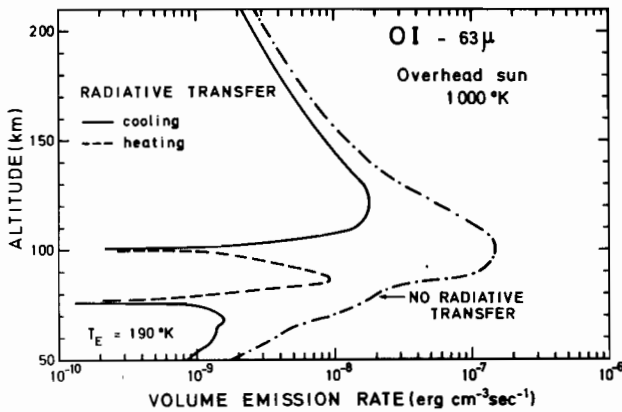
Fig.8 : Volume emission rate for a thermopause temperature of 1000°K.
The heating region is due to the lower boundary emission corre
sponding to a black body temperature of 190°K.

of the mean net flux becomes negative. Above 100 km, the radiative tran
sfer curve in Fig.8 is always below the curve corresponding to the opti
cally thin case, in which absorption and induced emission are neglected.
If the optically thin approximation is used for computing an atmospheric
model, the radiative cooling is overestimated by several orders of magni
.tude in the region around 100 km. The departure from an optically thin
layer is indicated in Fig.9, where the reduction factor 1 - X of expres
sion (26) is shown for two models corresponding to thermopause tempera
tures of 750°K and 2000°K. The effect of radiative transfer is very im-
portant below 150 km and even at greater heights the infrared loss is
decreased by 10-20 per cent compared to the case of the optically thin
layer.

7 - Conclusion

The atomic oxygen emission at 63μ has been analyzed in the upper
atmosphere in relation to the heat conduction equation. Since the infra-
red emission is an important cooling mechanism, the physical processes
involved have been described. Absorption and induced emission are im-
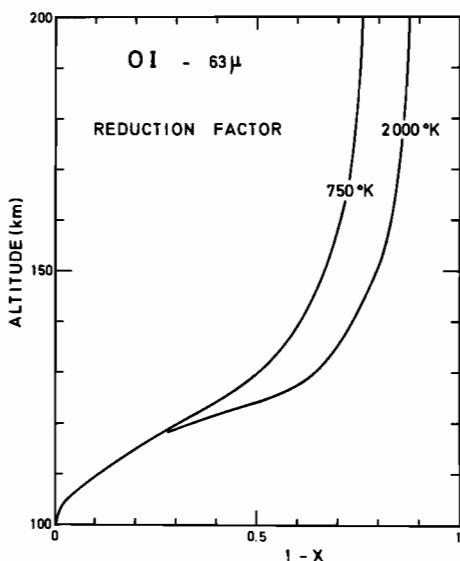portant and should be taken into account. A radiative transfer equation

Fig.9 : Reduction factor 1 - X showing the departure from an optically thin atmosphere.

has, therefore, been solved and the results indicate that the optically thin approximation is no longer valid below 150 km. The volume emission rate obtained by solving the radiative transfer equation is always smaller than in an optically thin layer. Actually, the volume emission rate can change its sign, leading in this way to a heating mechanism around the mesopause.

A detailed solution of the heat conduction equation should take into consideration an infrared loss computed under radiative transfer conditions. If a three dimensional solution is attempted, the problem is even more complex, since the plane parallel geometry must be modified.

References

Bates, D.R., The temperature of the upper atmosphere, Proc.Phys.Soc., 64B, 805-821, 1951.

Chandrasekhar, S., Radiative transfer, 392 pp., Dover, New York,1960.

Chapman, S., and T.G.Cowling, The mathematical theory of non-uniform gases, second ed., 431 pp., Cambridge University Press,1952.

Feldman, P.D., and D.P.McNutt, Far infrared nightglow emission from atomic oxygen, J.Geophys.Res., 74, 4791-4793, 1969.

Houck, J.R., and M.Harwit, Far infrared observations of the night sky, Science, 194, 1271-1273, 1969.

Izakov, M.N., and S.K.Morozov, The heating function of thermosphere by solar radiation in Schumann-Runge continuum, Space Research XI, Akademie-Verlag, Berlin, in press, 1971.

Kockarts, G., and W.Peetermans, Atomic oxygen infrared emission in the earth's upper atmosphere, Planet.Space Sci., 18, 271-285, 1970.

Münch, G., The intensity of forbidden emission lines, Astrophys.J., 136, 823-831, 1962.

Nicolet,M., Contribution à l'étude de l'ionosphère, 162 pp., Mémoires Inst.Roy.Météor.de Belgique, vol.19, 1945.

Nicolet, M., Structure of the thermosphere, Planet.Space Sci., 5, 1-32, 1961.