UJJ-7

National Aeronautics and Space Administration
Goddard Space Flight Center
Contract No.NAS-5-12487

ST-AM-SPS-10847

THE THERMAL EFFECT OF RADIATIVE TRANSFER IN THE ATOMIC OXYGEN LINE NEAR 63μ

by

G.M. Shved

&

A.F. Nerushev

(USSR)

FACILITY FORM 602

N69-28246	1
(ACCESSION NUMBER)	(THRU)
11	
(PAGES)	(CODE)
CR-101426	13
(NASA CR OR TMX OR AD NUMBER)	(CATEGORY)

18 JUNE 1969

ST-AM-SPS-10847

THE THERMAL EFFECT OF RADIATIVE TRANSFER IN THE ATOMIC OXYGEN LINE NEAR 63μ

Fizika Atmosfery i Okeana
Vol ~~Tom~~ 4, No.5, pp 473 - 479
Izd-vo "Nauka", Moscow 1969

by
G.M. Shved and
A.F. Nerushev

SUMMARY

The computation of energy fluxes resulting from the emission in the atomic oxygen line near 63μ is made on the basis of the numerical solution of radiative transfer equation for the lower thermosphere. As compared with the approximation of the optically thin atmosphere, usually applied for oxygen emission, the solution of the transfer equation leads to essentially different values of energy fluxes below 130 km. The most probable thermal effect of oxygen emission below 100 km is heating. Under ordinary conditions this emission does not constitute the essential factor of the thermosphere's thermal conditions below 150km and in the first approximation can be disregarded in the theory of this layer's thermal regime.

* * *

The idea about the cooling effect of atomic oxygen emission near 63μ in the upper atmosphere was introduced by Bates [1]. The calculation of the cooling was always done in the approximation of optically thin atmosphere which is justified for a considerable thermosphere thickness. However, in the lowest layers of the thermosphere, having a maximum concentration of atomic oxygen, the optical thickness of the atmosphere at the center of the line is found to be no less than several units, and the optically thin atmosphere approximation cannot be used. The present paper is dedicated to the estimate of radial energy influxes on the basis of the solution of the radiative transfer equation.

STATEMENT OF THE PROBLEM

The basic term ^3P of atomic oxygen splits in three levels (Fig.1), between which the optical magneto-dipole transitions are possible. Only the $^3P_1 \rightarrow {}^3P_2$ transition which yields the line in 63.2μ [2] is taken into account in the thermal regime of the thermosphere. The lines pertaining to the remaining two transitions are much weaker than the investigated one. In comparison with oscillating molecule transitions, the probability of spontaneous transition $^3P_1 \rightarrow {}^3P_2$ is small, $A_{12} = 8.9 \cdot 10^{-5}$ sec^{-1}. However, atomic oxygen could yield a perceptible thermal effect in the thermosphere where it becomes one of the basic atmospheric components.

If the Kirhoff's law is valid for the study, the radial energy influx per unit of volume, conditioned by radiative transfer in the Doppler line is determined by the following formula [3,4]:

$$H(\tau) = -4\pi B(\tau) S(\tau) + 2\sqrt{\pi \ln 2}\,\frac{S(\tau)}{\alpha_D(\tau)} \times$$
$$\times \left\{ \int_0^{\tau} d\tau' B(\tau') \int_{-\infty}^{\infty} dy\, f(y,\tau) f(y,\tau') E_1\left[\int_{\tau'}^{\tau} f(y,\tau'')\, d\tau''\right] + \right.$$
$$+ \int_{\tau}^{\tau^*} d\tau' B(\tau') \int_{-\infty}^{\infty} dy\, f(y,\tau) f(y,\tau') E_1\left[\int_{\tau}^{\tau'} f(y,\tau'')\, d\tau''\right] +$$
$$\left. + B(0) \int_{-\infty}^{\infty} dy\, f(y,\tau) E_2\left[\int_0^{\tau} f(y,\tau'')\, d\tau''\right] \right\}. \quad (1)$$

Here τ is the optical thickness of atmosphere's layer at the center of the line, counted upward from a certain initial level; τ^* is the optical thickness of the total atmosphere above the ground B is the intensity of absolute blackbody radiation for the frequency of line's center; α_D is the half-width of the Doppler line; S is the line intensity;

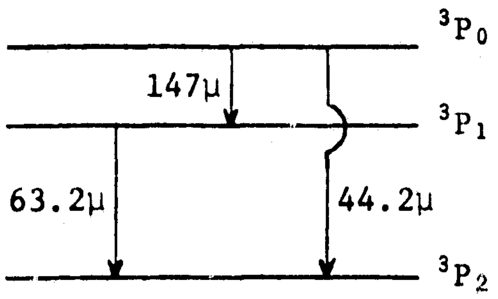

Fig.1

Diagram of energetic levels of the basic term of O atom

$$f(y,\tau) = \exp\left[-\frac{y^2 \ln 2}{\alpha_D^2(\tau)}\right], \quad E_l(x) = \int_1^{\infty} \frac{dt}{t^l}\, e^{-tx}. \quad (2)$$

The terms of the right-hand part of (1) have the following physical sense. The first term describes the proper thermal radiation of the investigated level. The addends of the second term describe respectively the heating of the investigated level by the radiation arriving from the overlying and underlying layers and from the initial level ($\tau = 0$). In approximation of optically thin atmosphere ($\tau^* \ll 1$), the thermal effect is described by the first term.

To be thermal the emission of O (the Kirhoff's law was satisfied) the populations of lower and upper states of transition must be subject to Boltzman's law at temperature equal to kinetic temperature of the gas. It is fulfilled, if

$$\theta_r \gg \theta_c \tag{3}$$

where θ_r is the radiational lifetime of the upper state; θ_c is the effective time between collisions, leading to de-excitation. Inasmuch as

$$\theta_r \approx A_{12}^{-1}, \quad \theta_c \sim [\sigma_{12} v n]^{-1} \tag{4}$$

(σ_{12} is the de-excitation cross-section at the expense of collissions, $\underline{v}$ is the mean thermal motion velocity of molecules; $\underline{n}$ is the molecule concentration in the gas), the condition (3) for the considered situation will be reduced to the inequality

$$\sigma_{12} n \gg 10^{-9}\ \mathrm{cm}^{-1}. \tag{5}$$

The transition ${}^3P_1 \rightarrow {}^3P_2$ cross-section was not measured. Therefore we must make use of available laboratory measurements for other atoms at comparable transition energies [5]. In the worst case the collision cross section with de-excitation will be by four orders less than the kinetic cross section. Then the applicability of the Kirhoff law is guaranteed to the altitude of 150 km, and Eq. (1) is valid for the radiation transfer in the lower thermosphere. On the strenght of resonance, at collisions of identical atoms the de-excitation cross-section may even exceed the kinetic cross-section. Inasmuch as O is one of the basic components of the thermosphere, the main role in de-excitation will apparently, be played by the O-O collisions. Therefore, it seems most probable that the Boltzman distribution by levels takes place for the entire thermosphere. At thermospheric temperatures we have for the investigated line $\alpha_D \approx (2\text{-}4)\cdot 10^{-4}$ cm^{-1}. The use of Doppler contour is justified, if, in the first place, $\alpha_D >> \alpha_L$, say the Lorentz line's half-width, and secondly, if the optical density of the atmosphere is not as great as to realize the radiative transfers in the far-away parts of line's wings having the Lorentz form. For the investigated line measurements of α_L were not performed. The estimates obtained on the basis of the impact theory of widening in the assumption of Van der Vaals interaction between the colliding p rticles [6] lead to $\alpha_L \sim 0.1 - 1$ cm^{-1} at normal conditions, whereupon the lower value is the most probable. In view of relatively great concentration of 0 in the thermosphere, the line's self-widening must be taken into account. As a result of resonance effect, the widening is, as a rule, by one order greater than the widening conditioned by the collision with molecules of other kind. Taking into consideration the proportionality of α_L of the perturbing particles concentration, and knowing the vertical profile of relative concentration of 0 in the thermosphere, it is possible to assume for the upper limit at the mesopause (about 85 km) $\alpha_L \sim 10^{-5}$ cm^{-1}. With the increase of altitude the value of the upper limit of α_L drops. Thus, the condition $\alpha_D >> \alpha_L$ is valid in the thermosphere.

For the more rigorous estimate of the validity of Doppler line approximation the second derivatives from the absorption function for the Doppler and the real Lorentz-Doppler contours were compared. These derivatives characterize the contribution of proper radiation of certain levels and the atmosphere heating in other levels [4]. Comparison has shown that for oxygen concentration used in the work, the Doppler contour is a good approximation in the computation of radial energy fluxes in the thermosphere.

The optical density of the atmosphere layer, embedded between the original level at the altitude z_0, and certain superincumbent level at the height $\underline{z}$, for the center of Doppler line is determined by the expression

$$\tau(z) = \sqrt{\frac{\ln 2}{\pi}} \int_{z_0}^{z} \frac{S(z')}{\alpha_D(z')} dz', \qquad (6)$$

whereupon for the investigated transition

$$S = \frac{A_{12}n}{8\pi\nu^2} \cdot \frac{3\left(1 - e^{-\frac{E_1}{kT}}\right)}{5 + 3e^{-\frac{E_1}{kT}} + e^{-\frac{E_0}{kT}}} . \tag{7}$$

Here $\underline{k}$ is the Boltzman constant; T is the temperature; ν is the transition's $^3P_1 \to {}^3P_2$ frequency in cm^{-1}; E_0 and E_1 are respectively the energies of levels $^3P_0$ and $^3P_1$; $\underline{n}$ is the concentration of O.

COMPUTATION METHOD

The integration in the argument of functions E_1 is conditioned by the dependence of α_D on T ($\alpha_D \propto \sqrt{T}$). In order to avoid this integration, we introduced for each interval (τ,τ) the mean half-width $\overline{\alpha}_D$, determined by the relation

$$\frac{2}{\overline{\alpha}_D^2(\tau,\tau')} = \frac{1}{\alpha_D^2(\tau)} + \frac{1}{\alpha_D^2(\tau')} . \tag{8}$$

The insignificance of α_D variation in the investigated atmospheric layer speaks in favor of such an approximation. Controlled accurate computations of radial energy influxes were performed for a series of levels' approximation (8) assures a good precision in the computation of influxes, if H is of the same order as the term describing the proper thermal radiation of the investigated level. The order of magnitude of the influx can be guaranteed only if the order of magnitude of H is smaller than that of the mentioned term.

Using (8) and introducing a new variable

$$x = \frac{\sqrt{2\ln 2}}{\overline{\alpha}_D\ (\tau,\tau')}\, y, \tag{9}$$

we may write (1) in the following form:

$$H(\tau) = -4\pi B(\tau)S(\tau) + 2\pi\frac{S(\tau)}{\alpha_D(\tau)}\left\{\int_0^{\tau} d\tau' B(\tau')\,\overline{\alpha}_D(\tau,\tau')\,N_{21}(\tau-\tau') + \right.$$
$$\left. + \int_{\tau} d\tau' B(\tau')\,\overline{\alpha}_D(\tau',\tau)\,N_{21}(\tau'-\tau) + B(0)\,\overline{\alpha}_D(\tau,0)\,N_{12}(\tau)\right\}, \tag{10}$$

where

$$N_{kl}(\mu) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-kx^2} E_l(\mu e^{x^2})\, dx, \tag{11}$$

We shall break down the atmosphere into n layers, considering in each of them B and $\bar{\alpha}_D$ as constants. Then each integral in (10) may be represented in the form of a sum by layers

$$\sum_i (\bar{\alpha}_D)_i B_i \int_{\tau_{i-1}}^{\tau_i} d\tau' N_{21}, \tag{12}$$

whereupon the i-th layer is embedded between the levels, characterized by optical densities τ_{i-1} and τ_i ($\tau_0 = 0$). Performing integration in (12) we shall obtain a final computation formula for radial energy influx in the j-th level.

$$\begin{aligned} H(\tau_j) &= -4\pi B(\tau_j) S(\tau_j) + \\ &+ 2\pi \frac{S(\tau_j)}{\alpha_D(\tau_j)} \Big\{ \sum_{i=1}^{j} (\bar{\alpha}_D)_i B_i [N_{12}(\tau_j - \tau_i) - N_{12}(\tau_j - \tau_{i-1})] + \\ &+ \sum_{i=j+1}^{n} (\bar{\alpha}_D)_i B_i [N_{12}(\tau_{i-1} - \tau_j) - N_{12}(\tau_i - \tau_j)] + B(0)\, \bar{\alpha}_D(\tau_j, 0)\, N_{12}(\tau_j) \Big\}. \end{aligned} \tag{13}$$

For the computation of N_{12} when $\mu < 2$ the expansion in series

$$\begin{aligned} N_{12}(\mu) &= \frac{\gamma - 1/4}{\sqrt{2}} \mu + \frac{1}{\sqrt{2}} \mu \ln \mu + \\ &+ \sum_{k=0}^{\infty} (-1)^k \frac{\mu^k}{k! \sqrt{1+k}} + \sum_{k=1}^{\infty} (-1)^k \frac{\mu^{k+1}}{k k! \sqrt{2+k}}. \end{aligned} \tag{14}$$

is used, where $\gamma = 0.577216$ is the Euler constant. For $\mu \gtrsim 2$ quadratic interpolation was performed of the values N_{12}, tabularly compiled in [7]. The error in the computation of N_{12} does not exceed 10^{-3}.

The solution of radiation transfer equation was carried out for the atmosphere thickness from z_0 = 50 km to 200 km. The initially indicated thickness was broken down into 5 km-layers. The doubling of the number of layers was performed m times so long as the relative difference between the steps

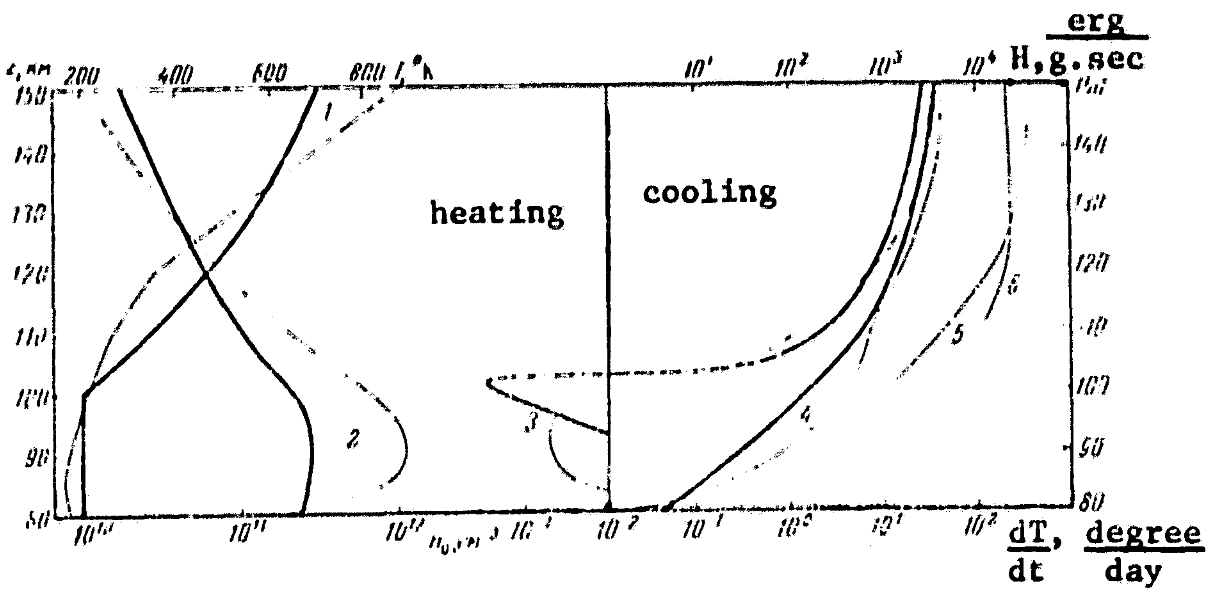

Fig.2

Altitude distributions: of temperature (curves 1); of oxygen concentration (curves 2); of energies of radial influxes, conditioned by radiation transfer of O in the line near 63μ (curves 3 corresponding to H at the solution of radiation transfer equation and curves 4 - at utilization of optically thin atmosphere approximation); of frequencies of solar heating (curves 5 and 6 respectively for the distribution of O_2 from the works [11] and [12]).

m-1-M and m-M did not become less than 10^{-2}. Thus the computation of sums with a precision to 1% is practically assured.

DISCUSSION OF RESULTS

For the lack of measurements of oxygen concentration, the computation of the energy of radial influxes for the layers lower than 120 km, were performed for characteristic profiles of O (fig.2) obtained by theoretical means [8,9]. To the distribution of O from work [8] corresponds $\tau^* = 3$, and from work [9] $\tau^* = 9$. The distributions of T (fig.2) were taken identical as those used at plotting of O profiles in the works referred to. Because of scarcity of observations and of probable variation of atmospheric conditions, one cannot consider that the used distributions of O and T encompass all characteristic conditions of lower thermosphere. Nevertheless, it is possible to assume that the performed computations yield not only the correct qualitative course of radial energy influxes, but also a correct order of magnitudes.

The computed values of H in $erg \cdot g^{-1} \cdot sec^{-1}$ and $deg \cdot day^{-1}$ (specific heat capacity $cp \approx 10^7$ $erg \cdot deg^{-1} \cdot mole^{-1}$) are presented in Fig.2. Presented in Fig.3 is the characteristic vertical course of the heat rate, conditioned by the radiation absorption below and above incumbent layers of atmosphere computed by the distributions of O and T borrowed from the work [9]. From formula (1) it is obvious that the approximation $\tau^{*} << 1$ always underrates ,. This approximation leads to substantial errors in the computation of the heat effect of O below 130 km, increasing the cooling rate by two or more times. At sufficiently high concentration of O, the real H in the 80-100 km layer may be even more than zero, which could have been expected from qualitative consideration of [4]. During the computations of H, it is possible to obtain in the regions of powerful breaks of model distributions of T an unreal atmosphere heating. This effect apparently explains the anomalous heating near 100 km for the distribution of O and T resulting from [8].

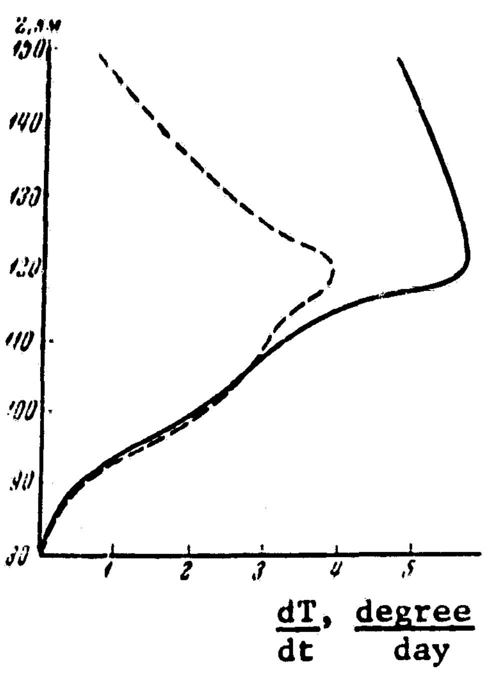

Fig.3. The dependence on altitude of heating rate caused by absorption of radiation, incoming from the overlying and underlying atmosphere layers is respectively represented by solid and dashed lines.

The oxygen emission may constitute a significant factor of thermal regime only if the corresponding absolute values of energy influxes are comparable by order of magnitude with the energy influxes conditioned by a basic factor of the thermal regime. Such a factor is the heating by molecular oxygen at the expense of solar ultraviolet radiation. Taking into account the energy transfer in chemical form by atomic oxygen [4,10], solar heating in the layer from the mesopause to 105 km exceeds the absolute values of radial energy influxes at the expense of oxygen emission by no less than two orders. For higher levels, solar heating is presented in Fig.2. In present case the calculations are carried out for the two measured distributions of O_2 [11,12] of Sun's average zenith angle $\vartheta = 1$ and of the 12 hour day's duration. It is possible to conclude that in the normal conditions the oxygen emission in the entire investigated layer of lower thermosphere, is not an essential factor of the thermal regime.

However, in some anomalous conditions the oxygen emission sould still constitute an important factor of the thermal regime. First of all, one naturally may expect this in the case of anomalous increase of the relative concentration of O and of the temperature. The increase of O concentration is possible, for example, at well regulated downward motions of the atmosphere. The performed calculations tend to favor the following idea: for the oxygen emission to become substantial in the thermal regime of the atmosphere below 100 km, an increase of relative concentration at these levels by no less than one order is necessary by comparison with the distribution utilized in computations. Secondly, the oxygen emission could become an essential factor of the thermal regime above 100 km in the conditions of polar night, beginning from the altitudes, where the cooling effect in 63μ of the line O becomes of the same order as the cooling effect in 15μ of the CO_2 band [4].

CONCLUSIONS

1. The solution of the transfer equation at computations of radial energy influxes conditiond by oxygen emission in the line near 63μ, becomes indispensable below 130 km.

2. The most probable thermal effect of oxygen emission below 100 km is heating.

3. The oxygen emission does not constitute the essential factor of the thermospheric regime below 150 km and can be discounted in the first approximation in the theory of the heat regime of this atmospheric layer.

* * * * THE END * * * *

Leningrad State
University

Manuscript received
10 June 1968.

REFERENCES

1. BATES, D.R. The Temperature of the Upper Atmosphere. Proc. Phys. Soc., Sec. B. 64, No.381, 1951

2. KAPLAN, S.A. PIKEL'NER S.B. Interstellar Medium, Fizmatgiz, 1963

3. GUDI, R.M. Atmospheric Radiation. 1. Foundations of Theory. "Mir", 1966.

4. SHVED, G.M. Thermal Effect of Radiation and its Determinating Factors in Atmosphere Layers from 30 to 100 km (Review) "Problemy Fiziki Atmosfery", No.5, Izd-vo LGU, 1967

5. KRAUSE, L. Collisional Excitation Transfer between the $^2P_{1/2}$ and $^2P_{3/2}$ Levels in Alkali Atoms. Appl. Optics, 5, No.9, 1966.

6. SOBEL'MAN, I.I. Introduction to the Theory of Atomic Spectra. Fizmatgiz, 1963.

7. IVANOV, V.V. SCHERBAKOV, V.T. Tables of Functions Encountered in Theory of Resonance Radiation Transfer. II. Astrofizika. 1, vyp.1, 1965.

8. SHIMAZAKI, T. Dynamic Effects on Atomic and Molecular Oxygen Density Distribution in the Upper Atmosphere: a Numerical Solution to Equations of Motion and Continuity. J. Atmos. and Terr. Phys., 29, No.6, 1967.

9. HESSTVEDT, E. On the Effect of Vertical Eddy Diffusion on Atmospheric Composition in the Mesosphere and Lower Thermosphere. Institute of Geophysics, University of Oslo, 1967.

10. KOPASHENOK, V.N., SHVED, G.M. On Physical Conditions near the Mesopause. Izv. AN SSSR, Fizika Atmosfery i Okeana, 4, No.5, 1968.

11. POKHUNKOV, A.A. Gravitational Subdivision, Composition and Structural Parameters of the Night Atmosphere in 100 to 210 km Altitude Range. ISZ (AES) vyp. 13, 1962.

12. NIER, A.O., HOFFMAN, J.H., JOHNSON, C.Y., HOLMES, J.C. Neutral Composition of the Atmosphere in the 100-to 200 kilometer range. J. Geophys. Res., 69, No.5, 1964.

CONTRACT NO.NAS-5-12487

Volt Information Sciences, Inc.,
1145 - 19th Street, N.W.
Washington, D.C. 20036
Tel: [202] 223-6700 X 36 & 37

Translated by
Ludmilla D. Fedine
13 June, 1969
Revised by
Dr. Andre L. Brichant
16 June, 1969