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NEW FINE STRUCTURE COOLING RATE

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ABSTRACT

One of the dominant electron cooling processes in the
ionosphere is caused by electron impact induced fine struc-
ture transitions among the ground state levels of atomic
oxygen. This fine structure cooling rate is based on theo-
retical cross sections. Recent advances in the numerical
cross section determinations to include polarization effects
and more accurate representations of the atomic target re-
sult in new lower values. These cross sections are em-
ployed in this paper to derive a new fine structure cooling
rate which is between 40% and 60% of the currently used
rate. A new generalized formula is presented for the cool-
ing rate (from which the fine structure cooling rate is de-
rived), valid for arbitrary mass and temperature difference
of the colliding particles and arbitrary inelastic energy
difference.

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INTRODUCTION

Electron energy balance is an important aspect of a total understanding of the ionosphere and thermosphere. Solar EUV and energetic particle heating of electrons is balanced by thermal conduction and by cooling to ions and neutrals. Dalgarno and Degges (1968) have shown that the dominant electron cooling process in the lower thermosphere is due to electron impact collisions with the ground state of atomic oxygen which produce transitions among the spin multiplets: the fine structure levels ^3P_J, $J = 0, 1, 2$. A number of analytical formulas for this fine structure cooling rate have appeared: Dalgarno (1969), Lejeune and Petit (1969), and Rees and Roble (1975). Recent articles by Schunk and Walker (1973) and Swartz and Nisbet (1973) used the Dalgarno cooling rate formula. All of these cooling rates are based on the original fine structure cross section calculation of Brieg and Lin (1966).

Recently, three new fine structure cross section calculations have been published; Saraph (1973), Tambe and Henry (1974, 1976), and LeDourneuf and Nesbet (1976). The importance of the fine structure cooling rate relative to other electron cooling rates, warrants a comparison of the cooling rates calculated with the four independent theoretical cross sections, respectively designated BL, S, TH, and LN for Brieg-Lin, Saraph, Tambe-Henry, and LeDourneuf-Nesbet.

This paper briefly summarizes the differences in the cross section calculations and then identifies the most accurate ones. A least square fit of the

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theoretical cross sections is made to a simple power law for use in the cooling

rate formula. The fine structure cooling rates are evaluated for each of the

cross sections employing a generalized formula for the inelastic cooling rate,

which has been derived from the inelastic Boltzmann collision operator using no

approximations. Use of the general formula, Eq. 3, limits errors in the cooling

rates to errors in the cross sections or in the approximate analytical represen-

tation of the cross sections, Eqs. 1 and 2. The four cooling rates are compared

in Figure 1 to the widely used cooling rate (Dalgarno, 1969).

THEORETICAL CROSS SECTIONS

The cross sections for fine structure transitions among the triplet $J = 0, 1, 2$

levels of the atomic oxygen ground state ^3P_j have been computed independently

by BI, S, TH, and LN. The square of the transition matrix elements is a di-

mensionless pure number, Ω, first employed by Hebb and Menzel (1940) and

called collision strength (in analogy to line strength for radiative transitions) by

Seaton (1953). The symmetry of Ω in initial and final labels $\Omega(J, J') = \Omega(J', J)$

expresses the rule of detailed balancing, relating collisions with their inverse.

The cross section for the transition $J \rightarrow J'$ is obtained from the collision strength

(matrix elements) by

$$\sigma_{JJ'} = \frac{\pi a_0^2 \Omega(J,J')}{g_J k_J^2} \ cm^2 \qquad (1)$$

where $a_0 = 5.29167 \times 10^{-9}$ cm is the Bohr radius, $g_J = 2J + 1$ the statistical weight,

and k_J the initial wave number of the colliding electron, $k_J = 6.3335 \times 10^{-6} \times E/k$,

k is Boltzmann's constant and E_J the initial electron energy in ergs. The triplet level energies are $E_2 = 0$, $E_1 = 0.02\,eV$ and $E_0 = 0.028\,eV$. Therefore the energy differences – the level splittings, when expressed in units of °K are 228°K, 326°K, and 98°K for the transitions 1-2, 0-2, and 0-1 respectively. A discussion of the four collision strength calculations follows.

Breig and Lin made the first atomic oxygen fine structure collision strength calculation which led to a realization of the importance of the fine structure cooling rate. Their calculation used a single configuration for the atomic wave function, $1s^2 2s^2 2p^4$. They found that inclusion of level splitting (accounting for energy differences of the triplet ground state levels) increased the value of Ω. Saraph used a multiconfiguration representation of the atomic wave function – the configurations $1s^2 2s^2 2p^4$ and $1s^2 2s 2p^4 3d$ for the ground state. In the wave function expansion, Saraph included the bound state $1s^2 2s^2 2p^5$ to correctly treat p waves. The numerical difference between the BL and S calculations is primarily due to the absence of this important bound state in the BL calculation. All calculations after BL include the bound state $1s^2 2s^2 2p^5$. The effect of using the multiconfiguration representation rather than the single configuration representation is to slightly increase the collision strengths.

Tambe and Henry (1974) demonstrated that polarization effects (not included in the S calculation) as well as level splitting decrease the collision strengths,

but they did not use the $1s^2 2s2p^4$ 3d configuration used by Saraph. The contradiction with BL on the direction of the level splitting effect is explained by the incorrect p wave calculation of BL. Tambe and Henry (1976) used a different multiconfiguration representation than Saraph and demonstrated that at energies > 3000° K, the collision strengths are not sensitive to the multi- versus single representation, but instead are more affected (lowered) by inclusion of a polarization potential.

LeDourneuf and Nesbet (1976) used a more complete multiconfiguration representation (including polarization) than TH, but did not include level splitting. They made an approximate perturbation correction to account for level splitting and consequently found good agreement with the combined Tambe and Henry results (1974 and 1976).

The nearly identical TH and LN calculations are the best to date. They include the most terms in the target atom representation and in the wave function expansions; however the low energy TH calculation should be extended to include a multiconfiguration representation, and the LN calculation should be modified to explicitly include level splitting. Although there are no measured fine structure cross sections available for comparison, agreement has been found (within experimental scatter) between measured and calculated elastic electron-oxygen cross sections (Tambe and Henry, 1976).

COLLISION STRENGTH FITS

Evaluation of the cooling rate requires the integral of the product of the cross section and the particle distribution functions over all energies. In order to carry this out, the collision strengths of BL, S, TH, and LN are represented analytically by a least square fit of the calculated points to a linear function of $\ln \Omega$ versus $\ln T$, with fit parameters A and B

$$\Omega = AT^B \tag{2}$$

where T is the final electron energy (in °K) in an excitation transition and is the initial energy in a deexcitation transition. This insures that $\Omega \rightarrow 0$ as the energy approaches the threshold energy (LeDourneuf and Nesbet, 1976). An alternate analytical fit, an expansion in T and T^2, was used by LN to represent their calculated points, however their fit gives too much weight to the high energy Ω points, thus modifying some of the low energy values. Hence the fit of Eq. 2 was used to represent all four sets of calculations. We consider Eq. 2 to be an approximation to a form completely symmetric in the initial and final energies T_i, T_f where T of Eq. 2 would be replaced by $\sqrt{T_i T_f}$.

One problem in applying the fit of Eq. 2 to the theoretical Ω values is in determining how the authors define their energy parameter. Representing the energy parameter T as the initial energy of the excitation transition instead of the deexcitation transition could produce differences in the cross sections of 60% at 500° K and 20% at 3000° K. All four calculations are consistent with the

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assumption that initial and final energies refer to the excitation transitions. The fit values of A and B are listed in Table 1.

COOLING RATE

The electron impact fine structure cooling rate is calculated from the integral over all energies of the product of the fine structure cross section with the electron and oxygen velocity distribution functions. The formula for this integral is obtained from the energy moment of the inelastic Boltzmann collision operator (Desloge and Matthyse, 1960). In performing this energy moment, the only assumption is that of Maxwellian velocity distributions. The result is a formula for the inelastic, non-ionizing cooling rate, valid for arbitrary masses m and M and temperatures t and T of the colliding particles of number densities n and N respectively.

$$
\frac{dU}{dt} = nN \frac{2}{\sqrt{\pi}} \frac{M}{m+M} \sqrt{\frac{2kT}{M} + \frac{2kt}{m}} \sum_{IJ} \int_{0,Th}^{\infty} dx e^{-x}
$$

$$
\cdot \Big| \epsilon_{IJ} x \sigma_{I \to J} (x \mathcal{T}) + \frac{m}{m+M} 2k(T-t) x^{3/2}
$$

$$
\cdot \Big(\sqrt{x + \epsilon_{IJ}/k \mathcal{T}} \; \sigma^{M}_{I \to J} (x \mathcal{T})
$$

$$
+ \Big(\sqrt{x + \epsilon_{IJ}/k \mathcal{T}} - \sqrt{x} \Big) \sigma_{I \to J} (x \mathcal{T}) \Big) \Big|
$$

(3)

where the lower integration limits are the thresholds Th, 0 for excitation, de-excitation transitions respectively, σ is the total inelastic cross section, σ^M is the inelastic momentum transfer cross section, and

$$\mathcal{J} = (mT + Mt)/(m + M)$$

a_1 determines the relative concentration of the I th level, N_1,

$$N_I \quad = \quad N a_1$$

$$a_1 \quad = \quad g_1 \, Z^{-1} \, \exp \, (-E_1 /kT_1)$$

$$g_1 \quad = \quad \text{statistical weight}$$

$$Z \quad = \quad \text{partition function}$$

$$E_1 \quad = \quad \text{level energy}$$

$$T_I \quad = \quad \text{level temperature, characteristic of the Boltzmann distribution of the levels}$$

$$\epsilon_{IJ} \quad = \quad E_I - E_J \, , \text{ energy level difference.}$$

Since Eq. 3 was derived with no approximations, it is applicable for any neutral-neutral excitation collisions, where m ~ M as well as electron impact excitation collisions, where m ≪ M. For purely elastic collisions, Eq. 3 reduces to the standard formula for elastic cooling rates, (Banks and Kockarts, 1973), while for inelastic collisions it contains an extra term proportional to the temperature difference, T-t.

The electron cooling rate is obtained from Eq. 3 upon substitution of the fine structure cross section, Eqs. 1-2, neglecting higher order terms in m/M,

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where m, t, n are replaced by the electron parameters m_e, T_e, n_e, and M, T, N by the oxygen parameters M, T_g, $n(0)$, and by assuming equality of the momentum transfer and total cross sections (no differential scattering cross sections have been published):

$$\frac{dU_e}{dt} = 8.629 \times 10^{-6} \frac{n_e n(0)}{Z} \Sigma \ AB! \ T_e^{B-\frac{1}{2}}$$

$$\cdot \left| \ \epsilon(D_x - E_x) + 5.91 \times 10^{-9} (T_g - T_e) \right. \tag{4}$$

$$\left. \cdot \left((1 + B)D_x + (E/T_e + 1 + B)E_x \right) \right| \ , \ \frac{eV}{cm^3 s}$$

where the sum is over the three transitions 12, 02, 01 and in respective order the terms are:

$$\epsilon = 0.02, 0.028, 0.008$$

$$D_x = \exp(-228/T_1), \exp(-326/T_0), \exp(-326/T_0)$$

$$E_x = \exp(-228/T_e), \exp(-326/T_e), \exp\left(-\left(\frac{98}{T_e} + \frac{228}{T_1}\right)\right)$$

$$E = 228, 326, 98$$

$$Z = 5 + 3 \exp(-228/T_1) + \exp(-326/T_0),$$

and A and B are given in Table 1.

Using Eq. 4, the fine structure cooling rates for the TH and LN collision strengths are plotted in Figure 1 as ratios with respect to the Dalgarno (1969) cooling rate

$$D = 3.4 \times 10^{-12} \, n_e n(0) \, \frac{(T_e - T_g)}{T_g} \, (1 - 7 \times 10^{-5} \, T_e).$$ (5)

for the condition $T_0 = T_1 = T_g = 800°K$ and for different values of T_e. Throughout the temperature range $T_e = 800°K$ to $6000°K$ it is seen that the LN derived cooling rate is $\sim 10\%$ higher than the TH rate; this small difference demonstrates the good agreement between their cross section calculations as noted by LeDourneuf and Nesbet (1976). The 800°K gas temperature is typical for minimum solar conditions. The ratio of cooling rates is nearly independent of T_g, therefore Figure 1 may be applied to a wide range of T_g values from $\sim 500°K$ to $\sim 1500°K$. (Cooling rates based on the BL and S collision strengths are not shown since they did not include some important terms in their calculations.)

Note that the fine structure cooling rate formula depends on the four temperatures T_e, T_g, T_0, and T_1. It cannot always be assumed that the level temperatures T_0 and T_1 are equal to the gas kinetic temperature T_g. For example, Tohmatsu (1965) found that the observed line intensity ratios of the 1300A dayglow could only be explained when T_0 and T_1 were significantly greater than T_g. To produce this temperature inequality, Tohmatsu showed that the reaction rate for the neutral-neutral fine structure transition would have to be orders of magnitude less than the rate estimated by Bates (1951), in such a case the electron

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impact collisions would be sufficiently rapid to elevate T_0 and T_1 above T_g. Hence the full functional dependence of the cooling rate on all the temperatures has been retained in Eq. 4. Further discussion of this is deferred to a second paper. The term in Eq. 4 which explicitly contains T_g is of the order of magnitude of the elastic electron-oxygen cooling rate.

CONCLUSION

The original cross section calculation by Breig and Lin (1966), although it neglected some important target representations, was instrumental in bringing fine structure cooling into electron heat balance study. Recent advances in the quantum mechanical collision strength calculations by S, TH, and LN have made possible reliable determinations of the atomic oxygen fine structure cross sections. The calculations of Tambe and Henry (1974 and 1976) and LeDourneuf and Nesbet (1976) together represent the best calculation to date since they include most of the effects which have been shown to be important - polarization, multiconfiguration representation of the target atom, and level splitting. Their calculations should be redone, however at energies below 3000°K to simultaneously include energy level splitting and all the states considered by TH and LN, in order to improve the accuracy of the fine structure cooling rate. Their calculations above 3000°K are in good agreement and may be considered very reliable since they are practically independent of level splitting. The discrepancy of the Saraph (1973) calculation from Tambe-Henry and LeDourneuf-

Nesbet can probably be attributed to the neglect of polarization effects and a different variational procedure used to determine the multiconfiguration representation of the target atom.

The fine structure cooling rate has been evaluated with the new cross sections and is given in a form, Eq. 4, applicable to the most general non-equilibrium condition of the ionosphere. Numerically, the new cooling rate is 40% to 60% of the widely used Dalgarno cooling rate. Consequently, the net ambient electron cooling rate is reduced by almost a factor of two in the lower thermosphere. Thus a re-examination of previous electron heat budget studies is warranted by the new smaller cooling rate. Brace et al. (1976) have applied the new cooling rate (with level temperatures T_0 and T_1 equal to T_g) to Atmosphere Explorer C satellite electron heating and cooling calculations and have demonstrated an over all improvement in the heat budget.

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Table 1

Parameters in Fit of $\Omega = AT^B$ to Theoretical Collision Strengths

Source	A(12)†	A(02)	A(01)	B(12)	B(02)	B(01)
BL	2.531(-6)*	2.46(-7)	2.708(-7)	1.272	1.377	1.414
S	1.561(-5)	7.476(-6)	3.166(-6)	1.001	0.9411	1.052
TH	7.883(-6)	9.466(-6)	1.037(-8)	1.021	0.8458	1.633
LN	8.58(-6)	7.201(-6)	2.463(-7)	1.019	0.8998	1.268

*The numbers in parentheses denote powers of ten.
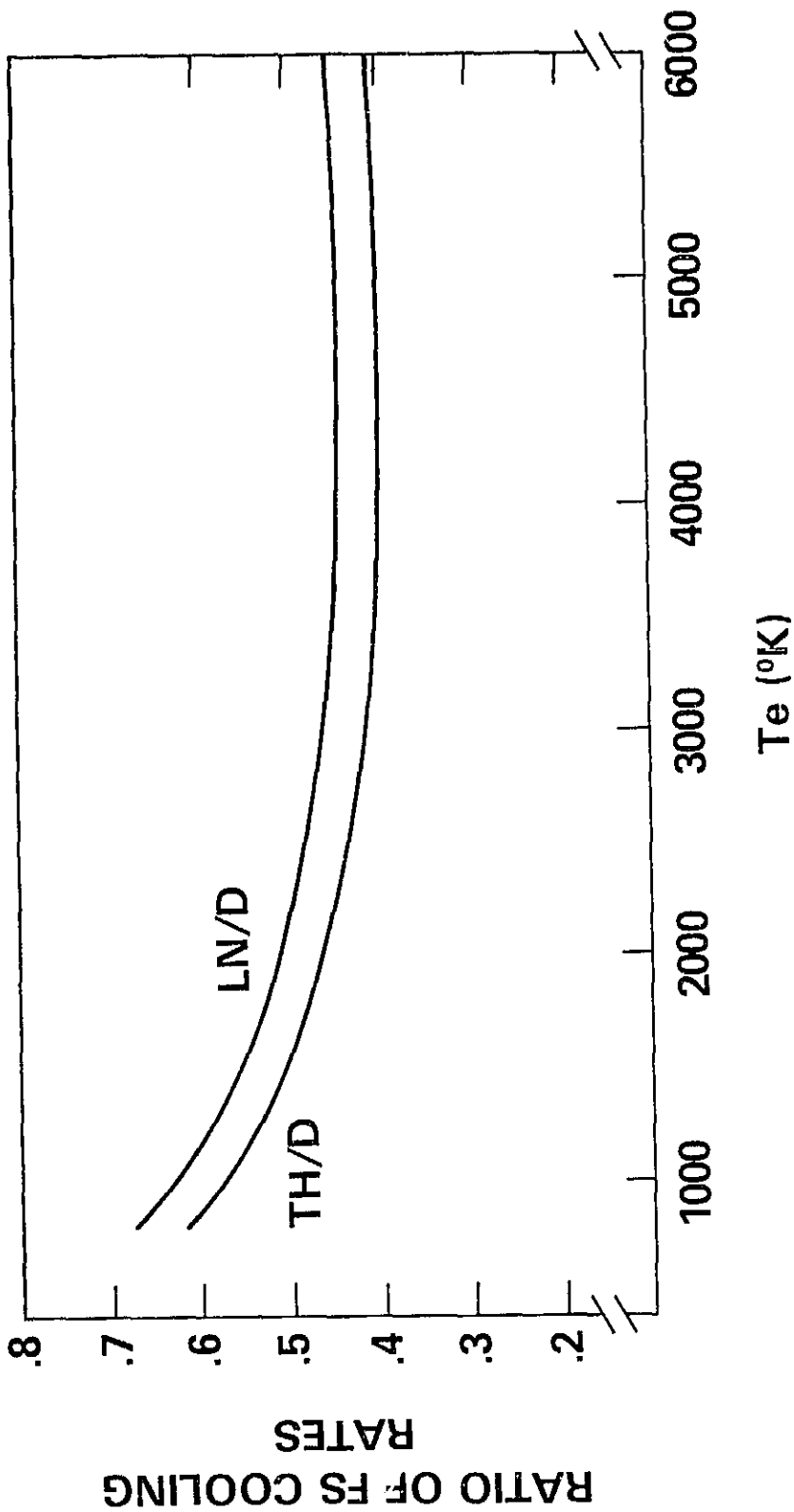†The numbers denote initial and final J levels 0, 1, and 2.

Figure 1. Ratios of atomic oxygen fine structure cooling rates with respect to the Dalgarno rate (D) for the collision strength calculations of Tambe-Henry (TH) and LeDourneuf-Nesbet (LN), for

$T_0 = T_1 = T_g = 800°K.$