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THEORETICAL CALCULATION OF X RADIATION FROM NON-EQUILIBRIUM ALUMINUM PLASMAS

THESIS

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THEORETICAL CALCULATION OF X RADIATION FROM NON-EQUILIBRIUM ALUMINUM PLASMAS

THESIS

Presented to the Faculty of the School of Engineering

of the Air Force Institute of Technology

Air University

in Partial Fufillment of the

Requirements for the Degree of

Master of Science

by

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First Lieutenant USAF

Graduate Engineering Physics

June 1972

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Preface

This thesis is the result of my attempt to create a useful computer code for the Simulation Branch of the Technology Division, Air Force Weapons Laboratory. While the theory on which this code is based is not new, I found very little in the way of published results of calculations like those performed here. Consequently, I ended up doing much more application of theory than critical evaluation of results, either mine or others'. There is something lacking in theory which remains untested, so hopefully more careful evaluation of these calculations can come at a later date.

In the meantime, I would like to thank all of the people in the Simulation Branch with whom I had contact during my very enjoyable stay there. Particularly, I am indebted to the individuals I worked most closely with: Tom McCann, Bill Baker, and Pete Turchi. Also, I want to thank Steve Patterson for his numerous critical inquiries and Cliff Rhoades for his time when time was growing short.

R. W. Boyd

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Notation

A . . . . . surface area of the plasma, in m^2.

$A(z,q,p)$. . . spontaneous radiative transition probability for the transition $I(z,q) \rightarrow I(z,p)$, in sec^{-1}.

$\alpha(z,p)$. . . . recombination coefficient for recombination of $I(z+1,g)$ to $I(z,p)$, in sec^{-1}.

E_e. . . . . total thermal energy of the electrons, i.e., $E_e = \frac{3}{2}N_e T_e$, in eV.

E_i. . . . . total thermal energy of the ions, i.e., $E_i = \frac{3}{2}N_i T_i$, in eV.

E_{pot}. . . . . total potential energy of the ions, in eV.

E_r. . . . . energy of radiation, i.e., $E_r = h\nu$ where ν is the frequency of the radiation, in eV.

$I(z,p)$. . . . ion or atom of charge z in state p (g for ground state).

$N(z,p)$. . . . total number of $I(z,p)$ in the plasma.

$n(z,p)$. . . . number density of $I(z,p)$, in cm^{-3}.

N_e. . . . . number of free electrons in the plasma.

n_e. . . . . number density of free electrons, in cm^{-3}.

N_i. . . . . number of atoms and ions, i.e., $N_i = \sum_z N(z,p)$.

n_i. . . . . number density of atoms and ions, in cm^{-3}.

P_{rad} . . . . total power radiated by the plasma, in $\frac{eV}{sec}$.

$S(z,p)$. . . . collisional ionization coefficient for ionization of $I(z,p)$ to $I(z+1,g)$, in sec^{-1}.

T_e. . . . . electron kinetic temperature, in eV.

T_i. . . . . ion kinetic temperature, in eV.

V . . . . . volume of the plasma, in cm^3.

$X(z,p,q)$. . . coefficient for excitation of $I(z,p)$ to $I(z,q)$, in sec^{-1}.

$Y(z,q,p)$. . . coefficient for deexcitation of $I(z,q)$ to $I(z,p)$, in sec^{-1}.

$\chi(z,p)$. . . . ionization potential of $I(z,p)$, in eV.

Abstract

TORCH, a computer code which calculates the spectrum arising from the radiation of a metallic plasma, is described. The population of each ionic species is determined from a time-dependent corona model which includes three-body recombination. Both time-resolved and time-integrated spectra are obtained, showing the contributions from bremsstrahlung, recombination radiation, and line radiation. Ion and electron temperatures are allowed to differ, with radiative losses causing continuous electron cooling. Energy may be added to the electrons and/or ions at arbitrary rates, for arbitrary times, and TORCH will compute the temperatures based on the rates of radiation, ionization, and electron-ion energy exchange. Calculations are included for aluminum plasmas with electron densities of 10^{18} to $10^{21}/cm^3$ and electron temperatures of 10 eV to several KeV. Also included are calculations of radiation from a deuterium plasma with 5% aluminum impurities.

THEORETICAL CALCULATION OF X RADIATION FROM NON-EQUILIBRIUM ALUMINUM PLASMAS

I. Introduction

The calculation of the radiation emitted by a metallic plasma is a very complex problem if handled in its entirety. The first part of this work is concerned primarily with identifying aspects of the problem which can be eliminated without seriously harming the credibility of the results. There are two fundamental assumptions which are made at the outset to limit the scope of the problem. It is assumed that the plasma is optically thin to its own radiation, that is, all radiation originating within the plasma escapes without further interaction with the plasma volume. Also, it is assumed that the electrons and ions can be described by a Maxwellian velocity distribution function at all times. There are many other assumptions which must be made, the validity and applicability of which are examined in some detail in what follows.

This model is fairly easily applied to any metal, and aluminum is used here because of the availability of atomic data as well as interest in this specific metallic plasma. The model has been programmed into a code called TORCH which computes the ionic species populations, species energies, and the radiation spectrum.

II. The Atomic Model

In order to calculate the radiation emitted by a metallic plasma, one must determine which ionic species are present and in what proportions. This, in turn, specifies the number of electrons present, both of which are important inputs to the calculation of the overall distribution of energy among the plasma particles. This energy distribution is, of course, needed to determine the kinetic temperatures of the particles which, when combined with all of the other data, enable one to calculate the radiation emitted by the plasma. Finally, the radiative power loss is a major factor affecting the overall plasma energy distribution.

Populations of Ionic Species

The first step necessary in specifying the ionic species populations is to select the atomic processes that are likely to be important in the ionization and recombination of the various ions. The model implied by these processes may then be used to predict which ions are being produced, which are being lost, and at what rate this is occuring. From such a model, and sufficient initial conditions, the population of each species can be calculated at future times by simply integrating the rate equations of the model.

Atomic Processes Considered. There are some atomic processes which are probably not important in any plasma of interest in the production of radiation. For example, collisional ionization cross sections depend on the velocity, as opposed to the energy, of the colliding particle. For a plasma in which ion and electron energies are similar, ionization by ion collision is generally negligible in comparison with ionization by electron collision. Also, there are processes which are not allowed under the

assumption of optical thinness. These include photoionization and stimulated emission, both of which could greatly affect the microscopic nature of an optically thick plasma. Finally, there are processes which may or may not be important in a given plasma, depending on the range of number density and temperature that is considered.

Plasmas of interest in the present work typically have electron temperatures of from 100 eV to 2000 eV and electron densities of about 10^{21} /cm^3. For high-Z plasmas in these ranges, there are two main questions to be answered in developing a suitable model. One is that of the relative importance of collisional and radiative processes in the recombination; the other concerns the handling of ions in excited states.

Collisional recombination, in which an ion combines with two electrons (the second electron being necessary for energy and momentum conservation), is represented by:

$$e + e + I(z,g) \rightarrow I(z-1,p) + e \qquad (1)$$

and is clearly proportional to N_e^2. Radiative recombination (in which a photon is emitted to conserve momentum and energy), however, is proportional to N_e:

$$e + I(z,g) \rightarrow I(z-1,p) + \text{photon} \qquad (2)$$

Because of the extra power of N_e in the rate of the collisional process, the radiative process only becomes important at low electron densities. Bates, Kingston, and McWhirter have shown, however, that even at the high electron densities of interest here, radiative recombination is important due to the temperatures and high-Z materials considered (Ref 3). Their criteria will be presented in Section V, but the result is that, while

radiative recombination is probably dominant, three-body recombination is important also. For this reason, both processes are considered in the present model.

The effect of the above is that processes (1) and (2) combine to give a total recombination coefficient $\alpha(z,p)$, in sec^{-1}, such that:

$$N_e N(z+1,g)\alpha(z,p) \quad sec^{-1} \tag{3}$$

is the number of recombinations occuring per second from $I(z+1,g)$ to $I(z,p)$.

The ionization process included in the model is collisional ionization:

$$e + I(z,p) \rightarrow I(z+1,g) + e + e \tag{4}$$

with ionization coefficient $S(z,p)$, in sec^{-1}, such that:

$$N_e N(z,p) S(z,p) \quad sec^{-1} \tag{5}$$

is the number of ionizations occuring per second from $I(z,p)$ to $I(z+1,g)$.

<u>Treatment of Excited States in Ions</u>. In general, the population of an excited state of an ion is determined by the processes of collisional excitation and spontaneous radiative decay as well as collisional deexcitation. That is:

$$e + I(z,g) \leftrightarrow I(z,p) + e \tag{6}$$

and

$$I(z,p) \rightarrow I(z,g) + \text{photon} \tag{7}$$

Process (6) has rate coefficients $X(z,g,p)$ and $Y(z,p,g)$ for the forward and reverse reactions, respectively, and process (7) has transition

probability $A(z,p,g)$, with all three coefficients in units of sec^{-1}. These three processes lead to a very complicated model if many excited states are considered for each ion. For the present work, one excited state is allowed for each ion (with certain exceptions discussed in Section III), but even this doubles the number of equations necessary to describe the ionization and excitation state of the plasma.

Fortunately, considerable simplification of the atomic model can be achieved if the following statements are true about these excited states:

(1) Spontaneous radiative decay is a much more important process than collisional deexcitation.

(2) Compared with the ground state, only negligible numbers of ions are in their excited states.

(3) The time to establish excited-level populations is much shorter than the intrinsic relaxation time for the plasma to approach steady state.

The validity of the first statement is determined by straightforward evaluation of the rates of the two processes. In general, the radiative process is important at low electron densities; the collisional process being dominant for high densities. McWhirter (Ref 10) gives an analytic expression for determining the minimum density necessary to insure that collisional deexcitation dominates. This will be presented in Section V and will show, as will other data discussed there, that statement (1) is true for the most important transitions considered in this work.

The second statement is really only true for those levels which have excitation energies much greater than the mean thermal energy of the plasma. Thus, it is probably valid for the high energy (>1 KeV) transitions but not for the low energy transitions. In Section V, it will be argued that the

effect of assuming statement (2) to be true for all excited states most likely does not detract from the calculations made here. By assuming the excited-level populations are small, however, one can ignore processes involving these excited states, such as ionization and recombination from and to excited states, as well as transitions that do not involve the ground state.

Statement (3) leads to the greatest simplification of all. If it is also true, then one need never be concerned with the actual populations of excited states. The effect of the third statement is that at any time the rate at which an excited level is being populated is exactly balanced by the rate at which it is being depleted. This will be the case regardless of the actual population of the state, but if this population is small, the rate of population of excited level I(z,p) is given by:

$$N_e N(z,g) X(z,g,p) \quad \text{sec}^{-1} \tag{8}$$

where N(z,g) may be taken to be the sum of all ions of charge z. The validity of the third statement is addressed by McWhirter (Ref 10), as will be shown in Section V.

<u>Rate Equations</u>. Based on the preceding remarks, it is only necessary to calculate the total number of each ionic species as a function of time. Since all ions are considered to be in their ground states, the only processes included are collisional ionization from the ground state, three-body recombination to the ground state, and radiative recombination to the ground state. The rate of change of N(z,g) is then given by:

$$\frac{dN(z,g)}{dt} = N_e\{N(z-1,g)S(z-1,g) + N(z+1,g)\alpha(z+1,g)\}$$
$$- N_e N(z,g)\{S(z,g) + \alpha(z,g)\} \tag{9}$$

For aluminum, which has atomic number 13, there are fourteen of these equations to be solved simultaneously. Together with them the energy and radiation equations developed below must be solved.

Radiation Equations

There are two reasons for considering radiation in the model. The first is to predict the spectrum being emitted by the plasma, which is the main goal of this work. The second reason is the importance of the total radiative power loss, particularly its effect on the plasma temperature. The total power being radiated can be easily obtained by integrating over the spectrum, so it is the spectrum which the model must supply, not simply the total radiative loss.

The radiation calculations performed here consider only atomic processes, that is, those due to transitions involving bound or free states of ions or atoms. Nonatomic mechanisms, such as cyclotron or synchrotron radiation, are not treated by the model. All of these radiative processes are discussed in detail in the literature so will only be described in brief here (Ref 5, 14,15 for example).

Bremsstrahlung. Bremsstrahlung is the radiation which sometimes occurs with the scattering of a free electron by a heavy charge center, typically an ion. Stratton (Ref 15:388) gives the intensity of bremsstrahlung per cubic centimeter per second, in a unit frequency interval, due to n_i ions/cm^3 of effective charge Z_i in a plasma with electron temperature T_e, in eV, as:

$$\frac{dP_{ff}}{d\nu} = 1.7\times10^{-40} n_e n_i Z_i^2 \sqrt{\chi_H/T_e}\; g_{ff} \exp[-h\nu/T_e] \quad \frac{erg}{cm^3} \tag{10}$$

where χ_H is the hydrogen ionization potential and g_{ff} is the free-free

Gaunt factor representing the departure of the quantum-mechanical calculation from the classical result (the handling of Gaunt factors is discussed in Section IV).

Converting this to intensity in watts per unit energy range of radiation, and summing over all ionic species, gives:

$$\frac{dP_{ff}}{dE_r} = 4.11\times10^{-33} V\, N_e \sqrt{\chi_H/T_e}\; g_{ff} \exp[-E_r/T_e] \cdot \sum_z N(z,g) z^2 \quad \frac{\text{watt}}{\text{eV}} \tag{11}$$

where V is the volume of the plasma in cubic centimeters.

Recombination Radiation. Recombination radiation is the radiation that sometimes accompanies the capture of a free electron into a bound state of an ion. The radiation due to recombination to I(z,g) is of energy $E_r = E_e + \chi(z,g)$, where E_e is the kinetic energy of the electron before capture and $\chi(z,g)$ is the ionization potential of I(z,g). This radiation is continuous above $\chi(z,g)$ and clearly must be zero below $\chi(z,g)$. Stratton (Ref 15:388) gives the intensity of radiation per cubic centimeter per second, in a unit frequency interval, due to recombination into shell n of a hydrogenlike ion of charge z as:

$$\frac{dP_{bf}}{d\nu} = 1.7\times10^{-40} n_e n(z+1,g) \sqrt{(\chi_H/T_e)^3}\, \left(\chi(z,g)/\chi_H\right)^2 \cdot \frac{\zeta_n}{n}\, g_{bf} \exp[(\chi(z,g)-h\nu)/T_e] \quad \frac{\text{erg}}{\text{cm}^3} \tag{12}$$

where ζ_n is the number of places in shell n which can be occupied by the captured electron and g_{bf} is the bound-free Gaunt factor. Of course, this expression only applies for frequencies greater than $\chi(z,g)/h$. It is assumed here, and generally elsewhere, that this expression is reasonably valid for other than hydrogenlike ions, although the cross sections are not well known.

Again, conversion to intensity in watts per unit energy range of radiation and summing over all ions yields:

$$\frac{dP_{bf}}{dE_r} = 4.11\times10^{-33} V\, N_e \sqrt{\{\chi_H/T_e\}^3}\, g_{bf}\, H[\chi(z,g)-E_r]$$

$$\cdot \sum_z N(z+1,g)\left(\chi(z,g)/\chi_H\right)^2 \frac{\zeta_n(z)}{n(z)} \exp[\{\chi(z,g)-E_r\}/T_e] \quad \frac{\text{watt}}{\text{eV}} \qquad (13)$$

where:

$$H(d) = \begin{cases} 0 \text{ for } d > 0 \\ 1 \text{ for } d \leq 0 \end{cases}$$

Line Radiation. The calculation of line radiation involves consideration of the intensities of the lines on the one hand and of spectral line shapes on the other. Calculation of the former follows in a very straightforward manner from the model for excitation described above. The broadening of a spectral line, however, is a very complicated function of the interaction of the radiating atom or ion with its environment. The main need for detailed line broadening calculations is not in predicting spectra, however, but in analyzing experimentally obtained spectra to determine particle densities and temperatures. Consequently, only limited line broadening calculations are performed in this work.

Under the assumptions discussed above, the rate at which transitions occur from ions in excited state I(z,p) to their ground state I(z,g) is equal to the rate at which transitions are occuring in the opposite direction. This rate is given by Eq. (8) which, when multiplied by the energy of the transition, gives the total rate at which energy is being radiated by this transition. The power radiated in the line is then:

$$N_e N(z,g) X(z,g,p)[\chi(z,g) - \chi(z,p)] \quad \frac{\text{eV}}{\text{sec}} \qquad (14)$$

and is, of course, all radiated at the energy of the transition if there is no line broadening. In nearly all plasmas, however, there is considerable line broadening, the two major causes of which are the Doppler effect and the interatomic Stark effect. This broadening does not change the total power radiated by a given transition, but only causes the radiation to be emitted over a range of frequencies.

Doppler broadening results from the random motions of the radiating particles toward or away from the observer. The randomness of the particle motions leads to a Gaussian line shape which Wiese (Ref 16:268) gives as:

$$\frac{dP_l}{d\lambda} = \frac{P_t}{\sqrt{\pi}\,\Delta\lambda_D} \exp[-\{(\lambda - \lambda^\circ)/\Delta\lambda_D\}^2] \quad \frac{\text{watt}}{\text{Å}} \tag{15}$$

where P_t is the total power radiated by the line, λ° is the unshifted wavelength, and $\Delta\lambda_D$ is the Doppler width, given by:

$$\Delta\lambda_D = (v/c)\lambda^\circ \quad \text{Å} \tag{16}$$

where:

$$v = \sqrt{2RT_i/m} \tag{17}$$

is the most probable velocity of the radiating ions. Here, R is the gas constant, m the atomic weight, and T_i the ion temperature. Converting Eq. (15) to intensity in watts per unit energy range of radiation gives:

$$\frac{dP_l}{dE_r} = \frac{6.996\times10^3 P_t}{E_r^2\,\Delta\lambda_D} \exp[-\{1.24\times10^4(1/E_r - 1/E^\circ)/\Delta\lambda_D\}^2] \quad \frac{\text{watt}}{\text{eV}} \tag{18}$$

where E° is the unshifted energy of the radiation, that is, the energy of the transition.

Unlike Doppler broadening, Stark broadening requires detailed analysis of the interaction of the radiating ion with the other particles in the plasma. While this effect is probably large for the densities of interest here, there is no suitable theory which can be readily applied to all transitions in all ions. It is worth mentioning, however, that Baranger (Ref 2) gives a detailed discussion of the theory involved in Stark broadening and Wiese (Ref 16) concerns himself mainly with the use of available data. Calculations have been made for a number of transitions (Ref 5:445-529), but tabulated data are generally only available for neutral and singly-ionized species which are unimportant here. The exclusion of any Stark broadening from these calculations affects the line shapes, but, as mentioned above, the energy radiated in the lines is generally not changed.

The radiation equations presented above can now be used to calculate the total intensity resulting from the three processes considered. By calculating this intensity for a range of radiation energies, the spectrum is produced from which the total radiative energy loss may be obtained by integration. The next step, then, is to examine the effect of this energy loss on the plasma.

Distribution of Energy

One requirement of a theoretical model for a plasma is that it not only conserve the internal energy of the plasma, but that it describe how that energy is distributed among the various energy modes throughout the plasma. The present model assumes the plasma energy to exist in the following forms: potential energy of the ions, thermal energy of the ions, and thermal energy of the electrons.

Ionization, Excitation, and Radiation. The potential energy of the

ions refers to the total ionization energy of the plasma, that is, the amount of energy that has been used in removing the free electrons. This is given in terms of the ground state ionization potentials by:

$$E_{pot} = \sum_{z} N(z,g) \sum_{j=1}^{z-1} \chi(j,g) \tag{19}$$

Since it is assumed that the populations of excited states are small, energy which has been used in populating these states is not accounted for. However, the radiation that results from excitation and subsequent radiative decay must certainly be removed from the plasma, so the model subtracts it from the thermal energy of the electrons, since it is primarily the free electrons which give up energy in the exciting collisions.

Electron-Ion Energy Exchange. The thermal energies of the ions and electrons are given by the ideal gas law as:

$$E_i = \frac{3}{2} N_i T_i \tag{20}$$

and

$$E_e = \frac{3}{2} N_e T_e \tag{21}$$

respectively. In the model, it is the energies which are integrated in time, so Eqs. (20) and (21) are actually used in the reverse sense to calculate the temperatures at specific times. Since the ion [illegible]ntial energy can be readily calculated from the species populations [illegible] 9), it is only necessary to have expressions for the derivative [illegible] ion and electron thermal energies.

The rate at which the ions and electrons are exchanging thermal energy may be written as:

$$\frac{dE_i}{dt} = \frac{3}{2}(T_e - T_i)\nu_{ei} \tag{22}$$

where ν_{ei} is the total electron-ion energy exchange rate and is developed below.

Now, since N_i is constant in time by the requirement of mass conservation, from Eq. (20) one can write:

$$\frac{dE_i}{dt} = \frac{3}{2} N_i \frac{dT_i}{dt} \tag{23}$$

From the Fokker-Planck equation, Spitzer (Ref 14:135) derives:

$$\frac{dT_i}{dt} = \frac{T_e - T_i}{t_{eq}} \tag{24}$$

where t_{eq} is the temperature equipartition time, due to electron-ion collisions. Eq. (23) thus becomes:

$$\frac{dE_i}{dt} = \frac{3}{2} N_i \frac{T_e - T_i}{t_{eq}} \tag{25}$$

with

$$t_{eq} = \frac{5.87\ A_e A_i}{n_i Z_i^2 \ln\Lambda_i} \sqrt{(T_e/A_e + T_i/A_i)^3} \tag{26}$$

where, here only, T_e and T_i are in °K. Folding the N_i in Eq. (25) into t_{eq}, summing over all ionic species, and converting T_e and T_i to eV, gives:

$$\nu_{ei} = \frac{\sum_z N^2(z,g) z^2 \ln\Lambda_z}{1.08\times10^5 \sqrt{(T_e/A_e + T_i/A_i)^3}} \tag{27}$$

where in all of these equations, the A's are the atomic weights. Spitzer (Ref 14:127) also gives the following expression for Λ_z:

$$\Lambda_z = \frac{3}{2ze^3}\sqrt{k^3T_e^3/\pi n_e} \cdot \min[1, \sqrt{4.2\times10^5/T_e}\,] \tag{28}$$

with $e=4.803\times10^{-10}$e.s.u., $k=1.38\times10^{-16}$erg/°K, and where T_e is again in °K. Removing the constants and allowing for the temperature in eV yields:

$$\Lambda_z = \frac{1.54\times10^{10}}{z}\sqrt{T_e^3/n_e} \cdot \min[1, \sqrt{36.2/T_e}\,] \tag{29}$$

This completes the description of the variables used in Eq. (22).

For the same reason as was given for line radiation, the loss due to Bremsstrahlung may be considered to remove energy from the electrons only. Recombination radiation, however, removes energy from both the electrons and the potential energy of the ions. Therefore, in the absence of any external processes adding energy to the system,

$$\frac{d}{dt}(E_e+E_{pot}) = -P_{rad} - \frac{dE_i}{dt} \tag{30}$$

where P_{rad} is the total radiative power loss and $\frac{dE_i}{dt}$ is given by Eq.(22). Rewriting this as:

$$\frac{dE_e}{dt} = -P_{rad} - \frac{dE_i}{dt} - \frac{dE_{pot}}{dt} \tag{31}$$

and noting that, by Eq. (19):

$$\frac{dE_{pot}}{dt} = \sum_z \frac{dN(z,g)}{dt} \sum_{j=1}^{z-1} \chi(j,g) \tag{32}$$

the derivative of the electron thermal energy is easily evaluated.

In summary, the species rate equations and energy equations described above constitute a self-consistent model for following in time the variables that define the radiation from a metallic plasma. Of course, the simultaneous solution of these equations requires a considerable amount of

information which has not yet been discussed. In particular, one must have some fundamental atomic data about the particular metallic plasma of interest. Also, the various rate coefficients must be available, preferably through analytic formulae. In the next sections, these topics will be presented and adjustments will be made in the model to account for some special cases.

III. Corona Model Applied to Aluminum

The equations developed in the previous section to describe the rate of ionization are generally known as the corona model equations. The only important difference is the inclusion of three-body recombination in this work. The difference is a minor one, both in the mechanics of adding it to the model and in the change it makes in the results. Certainly, one could proceed from here to apply this model to a specific problem and material without making any changes. Kolb and McWhirter, though, point out the necessity of handling metastable states and low-lying states in some ions a bit more carefully than they would be treated in the normal corona model (Ref 7). The only ions requiring modified treatment here are the heliumlike Al XII ion and the Lithiumlike Al XI ion. All other ions are described by the equations developed in the previous section.

Heliumlike Al XII

For the heliumlike Al XII ion (z=11), a more complete model is used to describe the ionization and radiation processes. The reason for this is the existence o the 2^3S metastable level. Since this level can not radiatively decay to the ground level very rapidly, a significant population could be produced. It might be mentioned that this does not seem to happen, however. For the combinations of parameters considered in this work, only about 1% (and at most 10%) of the Al XII ions are in the metastable state.

Since the corona model ignores several processes on the assumption of small excited-level populations, it is necessary to consider some of these

for the Al XII ion. They are illustrated schematically in Fig. 1 and are numbered there according to the following scheme:

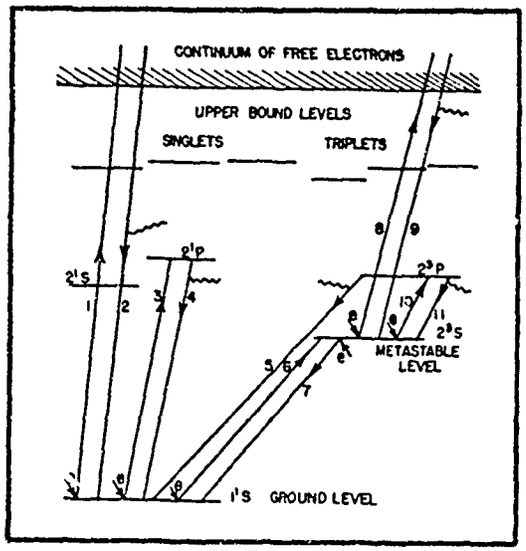


Fig. 1. Schematic representation of the collisional and radiative processes included in the ionization and radiation models for the Al XII ion (From Ref 7:522).

(1) Collisional ionization from the ground level.

(2) Collisional-radiative recombination to the ground level.

(3) Collisional excitation from the ground level to the 2^1P excited level.

(4) Radiative decay of the 2^1P level.

(5) Radiative decay of the 2^3S metastable level via the 2^3P level.

(6) Collisional excitation of the 2^3S level.

(7) Collisional deexcitation of the 2^3S level.

(8) Collisional ionization of the 2^3S level.

(9) Collisional-radiative recombination to the 2^3S level.

(10) Collisional excitation of the 2^3P level from the 2^3S metastable level.

(11) Radiative decay of the 2^3P level to the 2^3S level.

To account for these processes, the population of the metastable 2^3S level is explicitly calculated in time, just as the ground states of other ions are. The 2^1P level is handled the same as excited levels in other ions, that is, under the assumption of small level population. Lastly, the 2^3P level is assumed to have approximately the same population as the 2^3S level.

The rate equations which result from the inclusion of the above are given here for the ground state, I(11,g), and the metastable state, I(11,m).

They are:

$$\frac{dN(11,g)}{dt} = N(10,g)N_eS(10,g)$$

$$- N(11,g)N_e[S(11,g)+X(11,g,m)+\alpha(11,g)]$$

$$+ N(11,m)[A(11,2^3P,g)+N_eY(11,m,g)]$$

$$+ N(12,g)N_e\alpha(12,g) \tag{33}$$

and

$$\frac{dN(11,m)}{dt} = N(12,g)N_e\alpha(12,m)$$

$$+ N(11,g)N_eX(11,g,m)$$

$$- N(11,m)[A(11,2^3P,g)+N_e\{Y(11,m,g)+S(11,m)\}] \tag{34}$$

Because the metastable state is considered to be interacting with the ground state of the Al XIII ion (z=12), the rate equation for that ion must also be changed from that given by Eq. (9). The equation then becomes:

$$\frac{dN(12,g)}{dt} = N(11,g)N_eS(11,g)$$

$$+ N(11,m)N_eS(11,m)$$

$$- N(12,g)N_e[S(12,g)+\alpha(12,g)+\alpha(12,m)]$$

$$+ N(13,g)N_e\alpha(13,g) \tag{35}$$

The singling out of the heliumlike ion for more detailed treatment is possibly of questionable value. Increasing the accuracy of an isolated segment of a model seldom leads to the same increase in the accuracy

of the entire model. In this instance, however, it happens that this particular ion is nearly always the most highly populated ion in calculations for plasmas of interest in X ray production. Because of this fact, the more sophisticated model appears to be justified.

Lithiumlike Al XI

In the lithiumlike Al XI ion (z=10), the 2P level has an excitation potential of only 22.3 eV above the 2S ground level. This is much lower than the ionization potential of this species which is 2085.5 eV. Because this first-excited level is so low lying, the Al XI ion is likely to be a very efficient radiator. Also, step-wise excitation, in which an ion undergoes another exciting collision before radiatively decaying, is relatively more important here than in other ionic species. To account for some of these processes, the model is modified somewhat, although notably less than for the Al XII ion.

Because the radiative lifetime of the 2P state is short, it is assumed that the population of the 2P level is given by the steady-state value. This is defined by the processes which affect this level. They are:

$$e + I(10,g) \leftrightarrow I(10,2P) + e \tag{36}$$

and

$$I(10,2P) \rightarrow I(10,g) + \text{photon} \tag{37}$$

The rate equation for the population of the 2P level is then:

$$\frac{dN(10,2P)}{dt} = N_e[N(10,g)X(10,g,2P)-N(10,2P)Y(10,2P,g)] - N(10,2P)A(10,2P,g) \tag{38}$$

For the steady-state value, the left side of Eq. (38) is zero and:

$$\frac{N(10,2P)}{N(10,g)} = \frac{N_e X(10,g,2P)}{N_e Y(10,2P,g) + A(10,2P,g)} \tag{39}$$

is the ratio of the 2P excited level population to the ground level population.

For purposes of solving the ionization rate equations, it is assumed that all of the ions are in the ground state. The error introduced by this should be negligible because of the small excitation potential, even if the 2P level is fairly highly populated. Only in calculating the line radiation from the ion is it necessary to separate the population of the 2P state from that of the ground state.

The Al XI ion is considered to have five energy levels (four excited levels and the ground level) which give rise to the emission of four spectral lines. The transitions included in the model are listed in Appendix A, along with the remainder of the atomic data used below for aluminum.

IV. TORCH: A Time-Dependent Corona Model Computer Code

In this section, the method used to apply the model discussed above is presented. The computer code resulting from this work has been designated TORCH and is listed in Appendix B. Although the model must obviously be used as a whole, it is convenient to separate the integration of the rate equations from the consideration of the energy equations.

Integration of the Rate Equations

The integration of the rate equations is certainly a very straightforward process. The equations are coupled through the ionic species populations, but there are very adequate standard programs available to handle this. Some attention must be given to the conservation of heavy particles (ions and atoms) as well as the calculation of the number of electrons, but these are at most minor problems. The major difficulty arises in choosing the atomic rate coefficients.

Rate Coefficients. The rate coefficients used here are those used by Kolb and McWhirter (Ref 7:524). The exact choice of which coefficients to use is made somewhat arbitrarily due to the lack of any good comparison between experiment and theory in this area. Throughout the literature, Seaton's (Ref 13:374) ionization and excitation cross sections are generally accepted, and are the basis of the coefficients used here. All of these coefficients have reportedly been adjusted to give the best agreement with measured data or other theoretical calculations. The uncertainties in these expressions will be discussed in Section V.

The ionization coefficient is the result of integrating the expression given by Seaton for the excitation cross section of an ion, over a Maxwellian electron velocity distribution. The analytical expression this gives

is the following:

$$S(z,p) = \frac{1.64\times10^{-6}}{\chi(z,p)\sqrt{T_e}\,V} \exp[-\chi(z,p)/T_e] \quad \text{sec}^{-1} \tag{40}$$

This equation neglects the detailed behavior of the ionization cross section near the threshold, so the dependence on the temperature is probably not very accurate.

The formula used for the recombination coefficient includes the contributions of both radiative and three-body recombination. The radiative portion is due to Seaton and the three-body coefficient is that used by Bristow, et al. (Ref 4). The total coefficient used here is:

$$\alpha(z,p) = \frac{5.2\times10^{-14} z\sqrt{R}}{V}[.429+.5\ln R+.469/\sqrt{R}] + \frac{1.4\times10^{-31} N_e R^2}{V\, z^6}\exp[R] \quad \text{sec}^{-1} \tag{41}$$

where

$$R \equiv \chi(z-1,p)/T_e \tag{42}$$

This expression was obtained specifically for recombination of an electron with an ion to form a hydrogenlike ion, but is used here for all ions as is generally done elsewhere. The first term is the coefficient for radiative recombination and the second is the collisional term.

The same expression which was used to give the ionization coefficient has been used to derive a value for the excitation coefficient. If $f(z,g,p)$ is the absorption oscillator strength of the transition, the excitation coefficient is:

$$X(z,g,p) = \frac{6.0\times10^{-6} f(z,g,p)}{\chi_e(z,g,p)} \exp[-\chi_e(z,g,p)/T_e] \quad \text{sec}^{-1} \tag{43}$$

where

$$\chi_e(z,g,p) = \chi(z,g) - \chi(z,p) \tag{44}$$

is the excitation potential of level p above the ground level.

The deexcitation coefficient is obtained by the principle of detailed balance of inverse processes and is:

$$Y(z,p,g) = \frac{\omega(g)}{\omega(p)} X(z,g,p) \exp[\chi_e(z,g,p)/T_e] \quad \text{sec}^{-1} \tag{45}$$

where the ω's are the statistical weights of the levels.

For those lines which did not have transition probabilities available in the literature, the following formula was used (Ref 7:525):

$$A(z,p,g) = .43\times10^8 \frac{\omega(p)}{\omega(g)} f(z,g,p)\chi_e^2(z,g,p) \quad \text{sec}^{-1} \tag{46}$$

This completes the coefficients required to integrate the ionization equations.

Conservation of Ions. If the coefficients were all perfect, or their errors were properly correlated, the number of heavy particles would be constant in the absence of any external effect acting on the plasma to change this number. Because of the cumulative nature of this lack of particle conservation, substantial numbers of ions can be created or destroyed simply due to error in the coefficients. TORCH prevents this as follows. If the rate equations are written as:

$$\frac{dN(z,g)}{dt} = \sum_j B(z,j)N(j,g) \tag{47}$$

then the total number of ions, $\sum_z N(z,g)$, will remain constant if it is required that $\sum_z B(z,j) = 0$ for all j. TORCH does this by defining the

diagonal of the B matrix by:

$$B(j,j) = -\sum_{k \neq j} B(k,j) \qquad \text{for all } j \tag{48}$$

If the ions are conserved in this manner, a consistent number of electrons may be calculated simply as:

$$N_e = \sum_z N(z,g)z \tag{49}$$

<u>DFEQ</u>: <u>A Differential Equation Solver</u>. To integrate the ionization equations, as well as the necessary energy equations, a subroutine called DFEQ was obtained from the Computer Science Center at Wright-Patterson AFB, Ohio. The routine was written by P.J. Nikolai and has two entry points, SET and STEP. SET is called once with the initial conditions, in order to define various control variables and begin the integration. STEP is then called each time another step is to be integrated. STEP integrates three steps using a classical Runge-Kutta method. For the initial value problem:

$$\frac{dy}{dx} = f(x,y) \qquad \text{with} \qquad y(x_0) = y_0 \tag{50}$$

the method gives:

$$y(x+h) = y(x) + \frac{h}{6}\,[k_1 + 2k_2 + 2k_3 + k_4] \tag{51}$$

where

$$\begin{aligned} k_1 &= f[\,x\,,\ y(x)\,] \\ k_2 &= f[\,x + \tfrac{h}{2}\,,\ y(x) + \tfrac{h}{2}k_1\,] \\ k_3 &= f[\,x + \tfrac{h}{2}\,,\ y(x) + \tfrac{h}{2}k_2\,] \\ k_4 &= f[\,x + h\,,\ y(x) + hk_3\,] \end{aligned} \tag{52}$$

The fifth and succeeding points are determined by a four point Adams-Bashforth - Adams-Moulton predictor-corrector method. The predicted value is given by:

$$y_p(4h) = y(3h) + \frac{h}{24}\left(55\frac{dy}{dx}\bigg|_{3h} - 59\frac{dy}{dx}\bigg|_{2h} + 37\frac{dy}{dx}\bigg|_{h} - 9\frac{dy}{dx}\bigg|_{0}\right) \quad (53)$$

and the corrected value by:

$$y_c(4h) = y(3h) + \frac{h}{24}\left(9\frac{dy}{dx}\bigg|_{4h} + 19\frac{dy}{dx}\bigg|_{3h} - 5\frac{dy}{dx}\bigg|_{2h} + \frac{dy}{dx}\bigg|_{h}\right) \quad (54)$$

The variable step size is then adjusted depending on the relative error, ERR, which is determined by:

$$\mathrm{ERR} = \max_i \left(|y_{ci}(x) - y_{pi}(x)|/14 \max[\mathrm{XSIG}, y_{ci}(x)]\right) \quad (55)$$

where XSIG is some specified fraction of the total number of particles. The effect of this parameter is to ignore the error introduced in species with very small populations. In a typical calculation, N_i is about 10^{17} and XSIG is set at 10^2. Running the same problem with XSIG set to unity (as in the original DFEQ) makes no noticeable difference in the populations of the more highly populated ions, but significantly reduces the run time.

Another modification is made to DFEQ to help maintain physical reality and also to decrease the numerical noise. This change prohibits the ionic species populations from being negative. Again, the overall effect is not detrimental to the results for the more populous species, but does help to avoid large oscillations about zero in the populations of the ions which are not very highly populated. Besides the species equations, DFEQ is used to integrate the electron and ion thermal energies as described above. Also, the power radiated in each energy range of interest is integrated in time to give the total energy radiated in that range.

Energy Equations

The radiation and temperature equations have all been presented above. TORCH goes a bit beyond these equations in some cases, either for the sake of speed, accuracy, or experiment. An example of the latter is in the use of Gaunt factors to make classical radiation calculations agree with the quantum-mechanical results.

Radiation Calculations. Karzas and Latter (Ref 6) give a great deal of graphical and tabular data for free-free and bound-free Gaunt factors. Some of this data has been put into more useable form for inclusion in TORCH. The graphical data for temperature-averaged free-free Gaunt factors are given in Appendix C in a form suitable for use with a two-dimensional table look-up routine. Also in Appendix C are the results of integrating the bound-free Gaunt factors over a Maxwellian electron energy distribution, to give averaged factors for recombination into any of the first four shells. These results are also suitable for use with a table look-up routine. In general, the free-free Gaunt factors exhibit a greater range of values than do the bound-free Gaunt factors. The use of the free-free Gaunt factors, however, made no detectable difference in the overall results. Consequently, bound-free Gaunt factors were simply set equal to unity for all calculations.

In an attempt to approximate the effect of optical thickness on the radiation, the spectrum is at all energies limited to that of a blackbody with the same temperature and surface area as the plasma. At every radiation energy, the computed intensity is compared to the intensity of a blackbody which is given by Reif as (Ref 12:388):

$$\frac{dP_{bb}}{d\omega} = \frac{\hbar\omega^3}{4\pi^2c^2}\left(\exp[\hbar\omega/kT] - 1\right)^{-1} \frac{\text{joule}}{\text{m}^2} \tag{56}$$

Converting this to intensity in watts per unit energy range of radiation gives:

$$\frac{dP_{bb}}{dE_r} = \frac{2\pi A E_r^3}{c^2 h^3} \left(\exp[E_r/T_e] - 1\right)^{-1} \frac{\text{watt}}{\text{eV}} \tag{57}$$

where A is the surface area of the plasma in m^2. If the radiation intensity exceeds this blackbody limit, the intensity is equated to that of the blackbody and TORCH proceeds to calculate the radiation at the next energy.

It should be stated that any time this procedure substantially changes the radiation spectrum, a great deal of uncertainty is added to the results. Indeed, such a situation probably indicates that the particular plasma under consideration is not adequately described by the optically thin corona model. As will be shown by the results obtained in Section VI, only under conditions of high number density and relatively low temperature does this occur. For higher-temperature plasmas, even though the density may be very high, the assumption of optical thinness appears to be justified by the results obtained.

After the spectrum is developed by adding the intensities due to line radiation, recombination radiation, and bremsstrahlung, it is necessary to obtain the total power loss by integrating across the spectrum. TORCH does a very simple trapezoidal rule integration. To save time, however, the radiation energies at the high end of the spectrum (>3KeV) are spaced very far apart since there is usually little radiation at these energies. This creates problems in integrating past the last energy with nonzero intensity. Consequently, the assumption is made that since there are no lines present at these energies, the continuum radiation is given by:

$$\frac{dP}{dE_r} = I^\circ \exp[-(E_r - E^\circ)/T_e] \qquad \frac{\text{watt}}{\text{eV}} \tag{58}$$

where I° is the last nonzero intensity and occurs at energy E°. The total power radiated at energies greater than E° is then given by :

$$P = \int_{E^\circ}^{\infty} I^\circ \exp[-(E_r - E^\circ)/T_e] dE_r \quad \text{watt} \tag{59}$$

which results in

$$P = I^\circ T_e \quad \text{watt} \tag{60}$$

TORCH simply stops the numerical integration with E° and adds the factor $I^\circ T_e$ to complete the total radiative power loss.

Finally, TORCH computes, and continually updates, the time integrated spectrum. At each time, the time resolved spectrum is multiplied by the time step length, thus assuming the spectrum to be constant over a step length. This is certainly a crude approximation, but the time steps are usually very short and, more importantly, this spectrum is only used for graphical display where the resolution is probably more limiting than the error introduced here.

Temperature Calculations. In order to increase the utility of the code, TORCH has the capability of adding energy to the electrons, ions, or both at arbitrary power levels for arbitrary times. It is accomplished by simply changing Eq. (22) to read:

$$\frac{dE_i}{dt} = \frac{3}{2}(T_e - T_i)\nu_{ei} + P_i \tag{61}$$

where P_i is power input to the ions from an external source, in eV/sec. Equation (31) must be similarly modified so that:

$$\frac{dE_e}{dt} = -P_{rad} - \left(\frac{dE_i}{dt} - P_i\right) - \frac{dE_{pot}}{dt} + P_e \tag{62}$$

where P_e is analogous to P_i.

A feature added to TORCH to speed up the code is the capability to change to a one-temperature model under some circumstances. If the two temperatures satisfy the condition:

$$|T_e - T_i| < .01 \min[T_e, T_i, 100] \tag{63}$$

and there are no external energy sources, it is assumed that the temperatures are equal and no net flow of energy is occuring between the electrons and the ions. Under these conditions, it is reasonable to expect that the electron and ion temperatures are changing at the same rate. Thus, there are two equations to be satisfied:

$$\frac{dT_e}{dt} = \frac{dT_i}{dt} \tag{64}$$

and

$$\frac{d(E_e+E_i+E_{pot})}{dt} = -P_{rad} \tag{65}$$

Upon substituting for the temperatures in Eq. (64), one finds:

$$\frac{dE_i}{dt} = \frac{N_i}{N_e}\frac{dE_e}{dt} - \frac{N_i E_e}{N_e^2}\frac{dN_e}{dt} \tag{66}$$

Equation (65) then becomes:

$$\frac{dE_e}{dt} = \frac{N_e}{N_i+N_e}\left(-P_{rad} + \frac{N_i E_e}{N_e^2}\frac{dN_e}{dt} - \frac{dE_{pot}}{dt}\right) \tag{67}$$

and these two equations are the ones used in TORCH under the conditions specified. Once again, this feature does not alter the results appreciably, but does allow DFEQ to take larger time steps, thus shortening the run time.

Finally, it might be pointed out that nowhere in TORCH is the total plasma energy explicitly conserved. The reason for this is that it was discovered that such a constraint tends to introduce numerical noise into the results. The approach used in TORCH is to integrate the total energy in time and compare it to the sum of its parts throughout the run. The difference between the two has never been within ten orders of magnitude of the total energy, so obviously, energy conservation is handled by the code implicitly to an adequate degree.

V. Validity Requirements

A very important aspect of this work is the ability to quantitatively discuss criteria which must be met in order to be within the area where reasonable results may be expected. The limits of this area arise primarily from two sources. The first of these is the set of processes which constitute the corona model as discussed in Section II. The second is the computer code TORCH, in that the rate coefficients used can only be expected to give good results within certain temperature ranges.

Requirements of the Corona Model

The question of radiative versus three-body recombination is not too important here since both processes have been included in the model. Bates, Kingston, and McWhirter (Ref 3:307-310) have performed extensive calculations of the recombination coefficient for the formation hydrogenlike ions. The results are in terms of their reduced values of the electron temperature and number density, defined as:

$$\Theta \equiv T_e/z^2 \quad {}^\circ K \qquad \text{and} \qquad \eta \equiv n_e/z^7 \quad cm^{-3} \tag{68}$$

By comparing their collisional-radiative recombination coefficient (their table 6.A) for different values of η with the value for the limit as η approaches zero, a pattern is observed. As Θ increases, η must be ever larger to cause the same percentage increase in the recombination coefficient over the value as η approaches zero. This illustrates that higher electron densities are needed to cause significant three-body recombination at higher temperatures. Picking the value of η at which the coefficient has increased by about 20%, the following expression fits the points

reasonably well.

$$\eta = 10^{2\log_2[2\Theta/10^3]} \tag{69}$$

For z = 13 at 1 KeV (1.[illegible]×10[illegible] K), this says that the maximum n_e to cause less than a 20% contribution from the collisional process is about 1.2×10^{22} cm^{-3}.

It is more instructive, however, to look at the population levels predicted by the steady-state corona model equations:

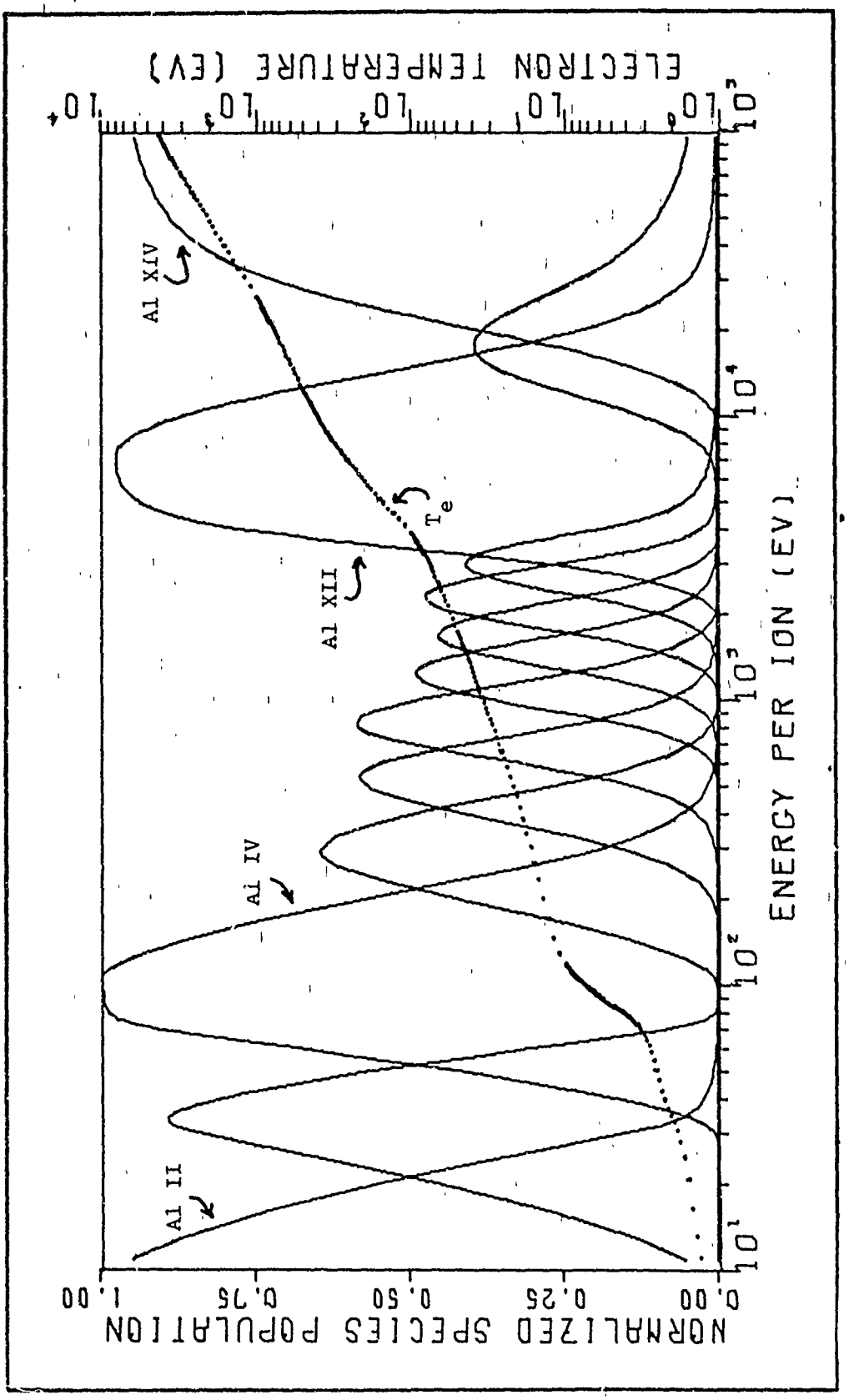
$$N(z,g)/N(z+1,g) = \alpha(z+1,g)/S(z,g) \tag{70}$$

Figure 2 shows the populations, normalized to unity, versus the total plasma energy per ion. The inclusion of three-body recombination makes almost no difference for temperatures above about 100 eV, but the same is not true for lower temperatures.

McWhirter (Ref 10:205-206) gives a criterion for determining how low the electron density can be before radiative decay will cause 10% of the transitions of an excited state to the ground state. Changing his expression to give the reverse information results in:

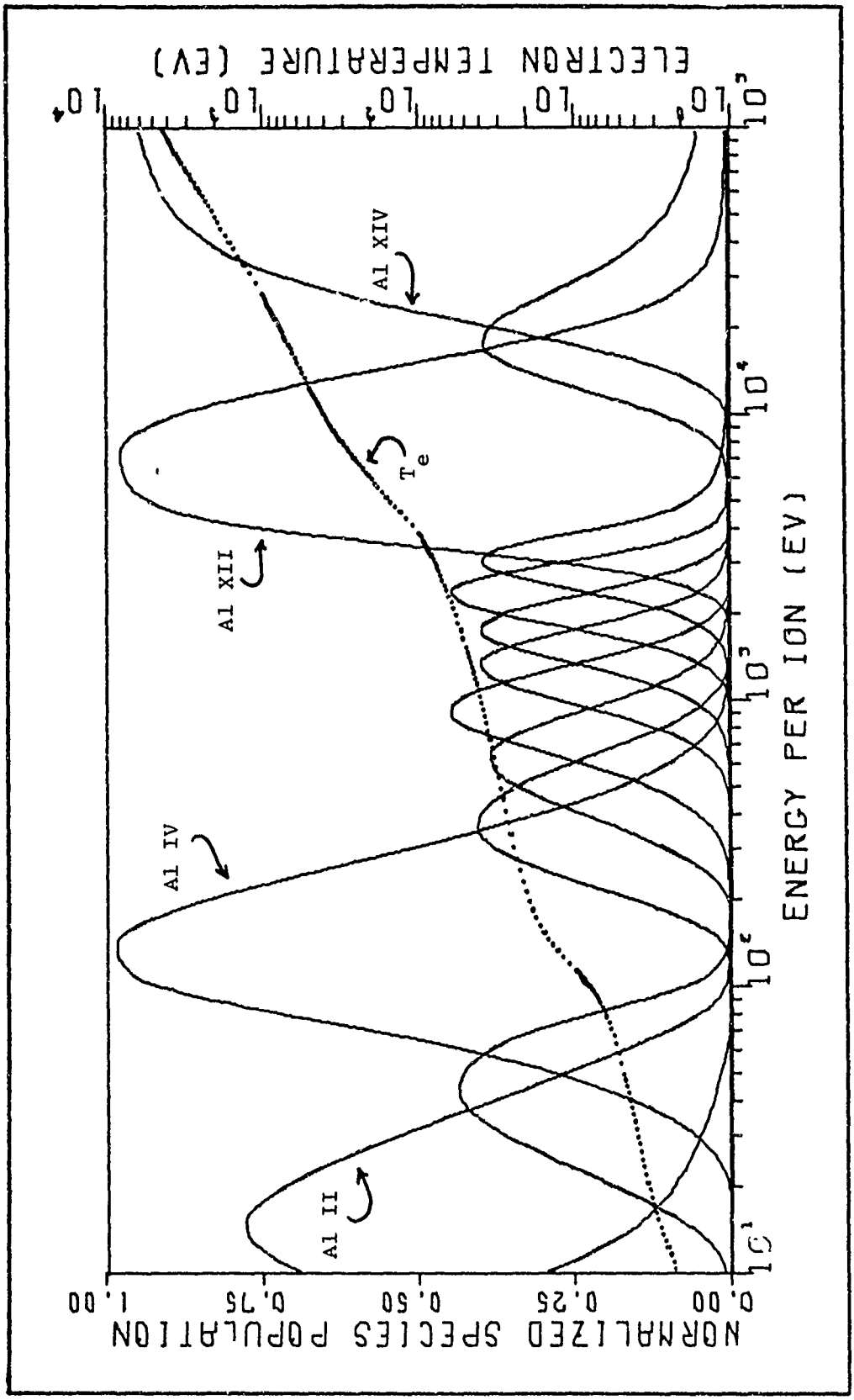
$$n_e \leq 1.6\times10^{10} \sqrt{T_e}\, \chi(z,p,g) \quad cm^{-3} \tag{71}$$

If this is satisfied, less than 10% of the transitions will be due to collisional deexcitation. This must be evaluated for every transition under consideration to determine whether or not radiative decay does indeed dominate. For example, with $n_e = 10^{21} cm^{-3}$ and T_e = 1KeV, only transitions with excitation energies below about 1.2 KeV will have more than 10% of the transitions be collisional.



(a) Model without three-body recombination. Populations are the same for any density.

Fig. 2. Steady-State Corona Model Species Populations



(b) Model with three-body recombination for $n_i = 10^{20}$ cm.$^{-3}$.

Fig. 2. (continued)

By looking at the coefficients used in TORCH, for almost all conditions of interest the transitions above 1 KeV are dominated by radiative decay. This being the case, neglecting collisional deexcitation can only make the results pessimistic as far as X ray production is concerned. By neglecting the collisional process, the low energy lines will have their intensities overestimated, thus leading to a colder plasma with less X radiation.

The assumption that ions are mainly found in the ground state is admittedly bad. However, the same comments as were made for the previous question apply here also. That is, as long as the excitation potential is somewhat greater than the mean thermal energy of the plasma, the assumption is good. For the lower-energy transitions, this is severely violated, but the result should be a tendency to overestimate low-energy radiation and consequently underestimate the X radiation.

This, of course, does depend on the premise that the excited levels attain steady-state populations in times much shorter than other times of interest in the plasma. McWhirter (Ref 10:216) concludes that the atomic relaxation time for a corona model plasma is given, to an order of magnitude, by:

$$\tau \simeq 10^{12}/n_e \quad \text{sec} \tag{72}$$

By comparing this with the inverse of the spontaneous radiative transition probabilities, one finds that even for n_e as great as 10^{21}cm^{-3}, only a very few transitions have lifetimes within an order of magnitude of τ. Even the low energy transitions have lifetimes which are in the range of $<10^{-10}$ sec.

Requirements of TORCH

For all of the atomic coefficients presented in Section IV, the accepted range of validity is about $.1 < \{T_e/\chi\} < 10$. While this appears to be somewhat restrictive for aluminum, for example, which has ionization coefficients from about 6 eV to 2.3 KeV, it actually is not. If some ions have populations five or ten orders of magnitude below the total number density, it does not matter if the rate coefficients are not valid for those ions at that particular moment.

For the more highly populated ions, $\{T_e/\chi\} \gtrsim .5$, almost always. Even allowing for the time-dependence of the ionization, the temperature requirements should generally be met. In any event, it is doubtful how accurate the coefficients are - even in the specified range. Both the ionization and deexcitation coefficients are claimed to agree with the Coulomb-Born approximation to within a factor of three to ten. The recombination coefficient is probably good to within 50% for hydrogenlike ions, but a factor of five is probably the best that can be expected in using it for other ions.

VI. Results

There are three different problems to which TORCH has already been applied. All are experiments oriented toward the production of soft X rays from metallic plasmas, but they differ in the manner through which energy is deposited in the plasma. While it is not the purpose of this work to analyze the experiments, brief descriptions of their natures are included here. Although no detailed attempt has yet been made to compare any of these results with experimental data, in the SHIVA experiment the calculations have been used to guide the diagnosticians by providing them with detailed expected radiation spectra. Because TORCH contains no hydrodynamics, it was necessary to approximate the actual experimental plasmas by using appropriate constant-volume configurations. This may well be where the greatest uncertainty lies in these results, but since the calculations only extend over times on the order of tens of nanoseconds, an approximation of no hydrodynamic expansion may be very reasonable.

SHIVA Project

The first problem examined was the SHIVA project. This is an experiment in which a thin ($\approx .5\mu$), cylindrical, aluminum foil is used to join two electrodes that are attached to a high-energy capacitor bank. When the bank is discharged, the current flows longitudinally through the foil cylinder creating azimuthal magnetic fields. The $\vec{J} \times \vec{B}$ force points radially inward, causing the cylinder to collapse. Hydrodynamic calculations indicate that immediately before the plasma collides with itself, it has 250 KJ of kinetic energy and is at a temperature of 30 eV. TORCH computes the steady-state species populations based on the 30 eV temperature and

assumes that at the time of total collapse (t=0), all of the kinetic energy is converted to ion thermal energy. This results in an ion temperature of 5.53 KeV while the electron temperature is still 30 eV.

The hydrodynamic calculations also indicate that the $\vec{J} \times \vec{B}$ force is sufficient to yield a diameter of ≈1 cm for the cylindrical plasma which has a length of 1 cm - the separation of the electrodes. Since N_i is 1.89×10^{20}, n_i becomes $2.4\times10^{20}cm^{-3}$. Table I gives a breakdown of the radiation output, and Fig. 3 illustrates selected spectra computed by TORCH as well as a temperature vs. time plot.

It is interesting to note the short time (≈.1 nsec) necessary for the electron and ion temperatures to become equal in this instance. This typifies many of the calculations made but not included here, although, as expected, this time lengthens appreciably as the density is lowered. A somewhat disturbing aspect of the results for this problem is the fact that at later times, when the temperature has fallen to about 100 eV, the spectrum is severely limited by the blackbody curve. This would seem to indicate that the plasma is not optically thin under these conditions and requires a more complete model to describe it properly.

Laser-Heating Experiment

The second problem illustrates the capability of heating the electrons with some external source of power. A number of experiments are currently underway to heat plasmas with medium-to-high-powered lasers. The configurations range from focusing the laser on a solid target, such as a metal foil, to the heating of a plasma formed by some other means. While it is beyond the scope of this work to discuss the details of the absorption mechanisms, the most commonly assumed one appears to be that of inverse

bremsstrahlung. This being the case, and for 1.06 μ light, an electron density of about $10^{21}cm^{-3}$ is desired to provide optimum absorption (Ref 8:4).

The problem begins with the temperatures at 10 eV and a spherical plasma of radius 10^{-2}cm. For n_i equal to $10^{20}cm^{-3}$, there are 4.19×10^{14} total ions. At time zero, TORCH begins inputting a square power pulse so that 50 joules of energy are added to the electrons in 30 nanoseconds. After the pulse has been applied for about 1 nsec., the temperature has increased to the point (≈500 eV) that the radiative power loss just balances the input power so that the temperature remains constant. After 30 nsec., the pulse is switched off. Table II presents the radiation output data and Fig. 4 contains some of the calculated spectra and a temperature plot.

There are a number of comments which can be made concerning this calculation. First, there seems to be no problem with violating the optical thinness assumption. The results, however, indicate extremely high efficiency of conversion of the laser energy to X rays. The optimism of these results probably comes from two sources - the lack of accounting for the energy required for hydrodynamic expansion and the assumption that all of the incident energy is absorbed by the plasma.

Impurity Radiation

The importance of impurity radiation as a source of plasma cooling has long been known to individuals engaged in controlled fusion research. This effect likely occurs in nearly any laboratory plasma, although the results may very often be unimportant. In the operation of the dense plasma focus, researchers have had to account for the radiation due to impurities in the plasma, particularly those resulting from degradation of the walls of the device. More recently, metal targets have been used in attempts to enhance

the radiation production from these machines. Although copper or tungsten are commonly used, the same types of effects are to be expected as are obtained in the aluminum calculations performed here. The parameters chosen for the plasma are once again based on hydrodynamic considerations and seem to be reasonably descriptive of what actually occurs.

The problem considers a spherical plasma of volume $10^{-2}cm^3$. There are a total of 10^{17} ions, of which 5% are aluminum and the rest are deuterium. Initially, the temperatures are both 100 eV, but 50 joules of energy are added to the ions at time zero, raising the ion temperature to 2.18 Kev. It is assumed that the deuterium is always fully ionized which is certainly very reasonable since the electron temperature is never lower than the initial 100 eV. The main effect of the deuterium, then, is its contribution to the bremsstrahlung, although it is also important in electron-ion energy exchange.

Table III and Fig. 5 present the usual output data, and they indicate that fairly high conversion efficiences might be obtained.

Table I
SHIVA Radiation Output

Total input = 2.7×10^5 Joules

Spectral Range (KeV)	Output (Joules)	Output as % of Input	Output as % of Output
<.5	7.81×10^4	28.5	44.13
.5-1.0	7.15×10^4	26.1	40.45
1.0-1.4	6.20×10^3	2.26	3.5
1.4-1.8	7.00×10^3	2.56	3.96
>1.8	1.41×10^4	5.15	7.96
Total	1.77×10^4	64.57	100.00

Table II
Laser-Heating Radiation Output

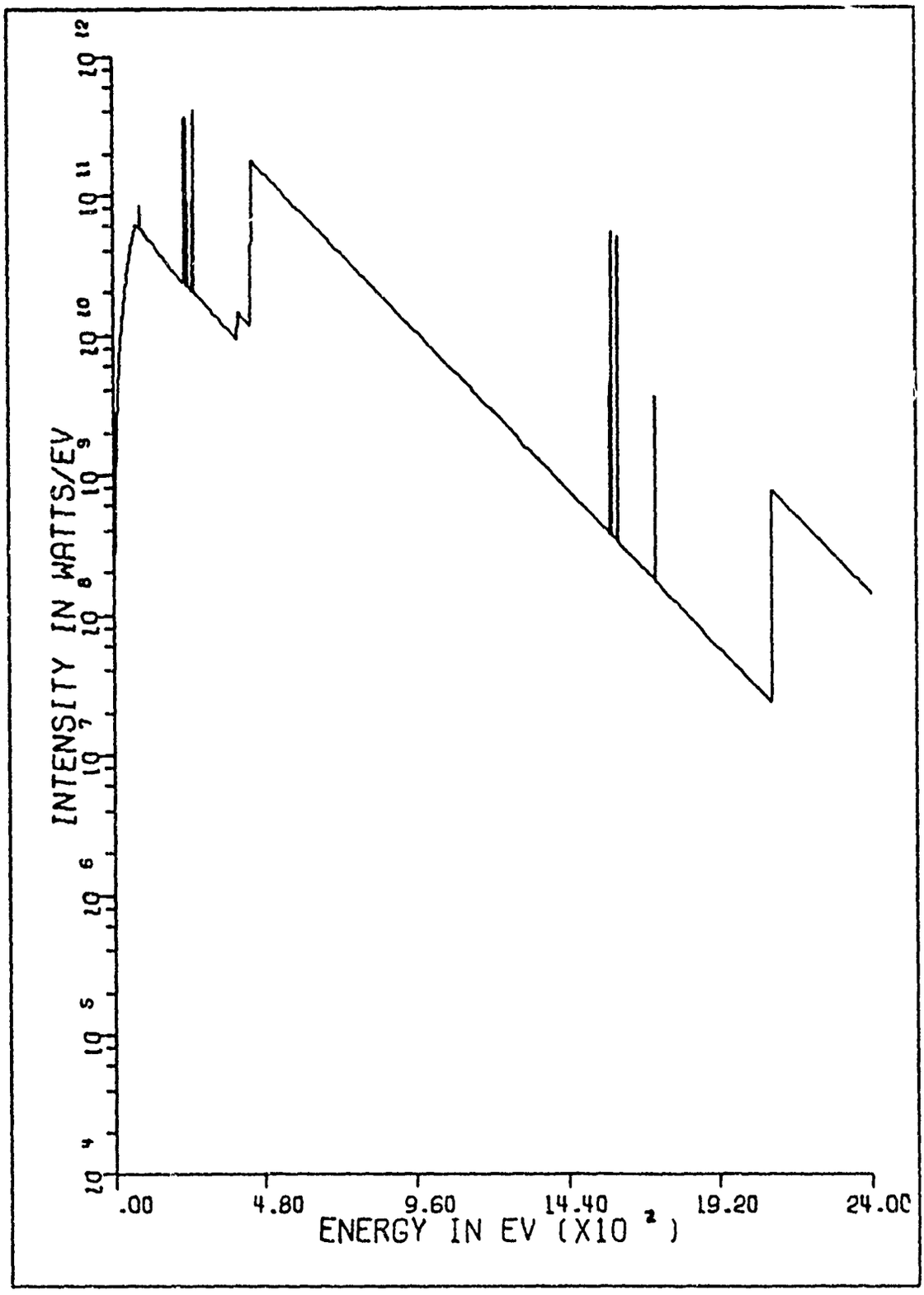
Total input = 50 Joules

Spectral Range (KeV)	Output (Joules)	Output as % of Input	Output as % of Output
<.5	11.68	23.36	23.4
.5-1.0	.42	.84	.85
1.0-1.4	.12	.24	.25
1.4-1.8	21.64	43.28	43.5
>1.8	15.93	31.96	32.
Total	49.97	99.58	100.00

Table III
Impurity Radiation Output

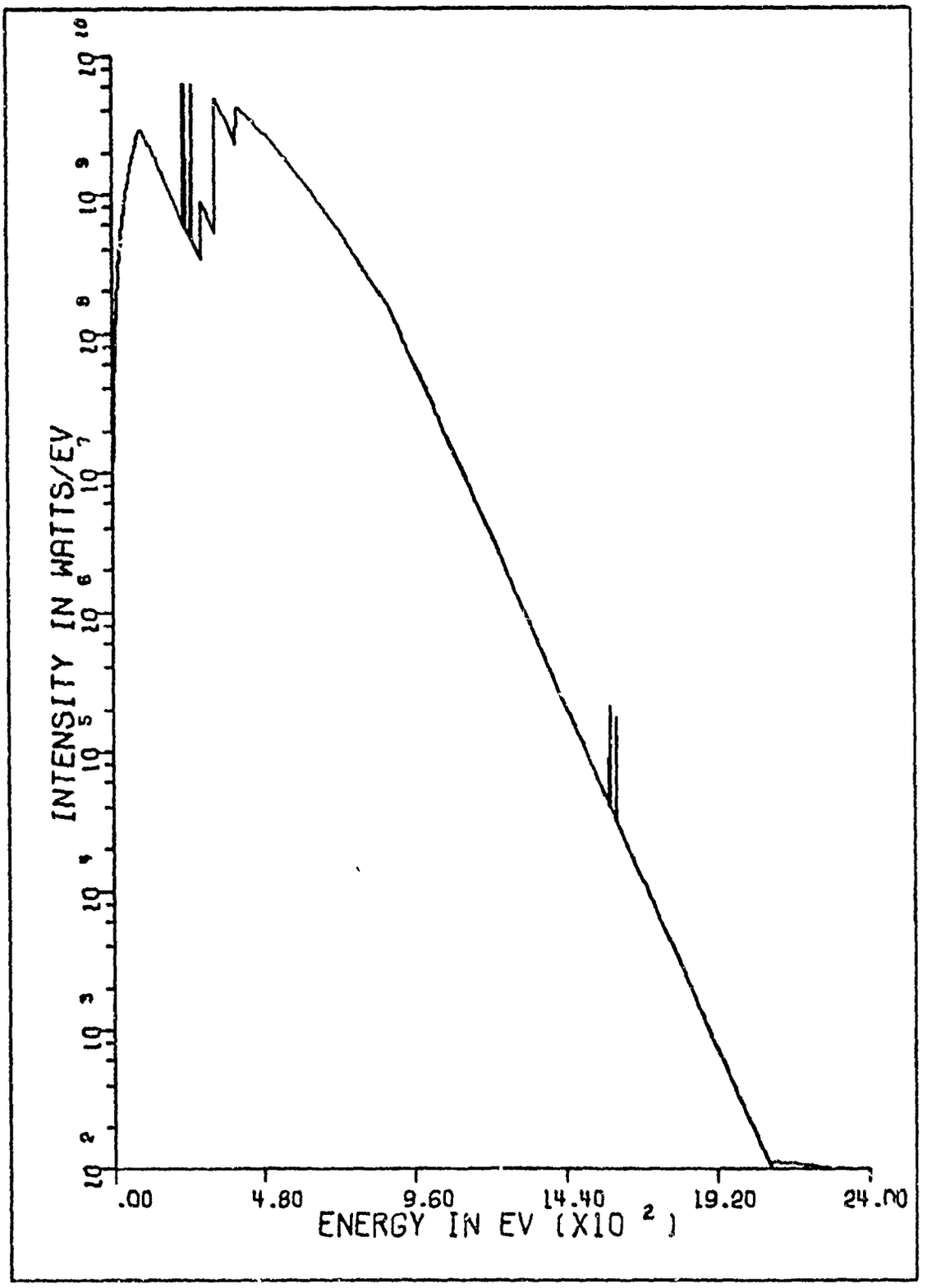
Total input = 57.6 Joules

Spectral Range (KeV)	Output (Joules)	Output as % of Input	Output as % of Output
<.5	11.34	19.73	41.3
.5-1.0	.07	.12	.27
1.0-1.4	.03	.05	.13
1.4-1.8	12.63	21.97	46.1
>1.8	3.35	5.84	12.2
Total	27.42	47.71	100.00



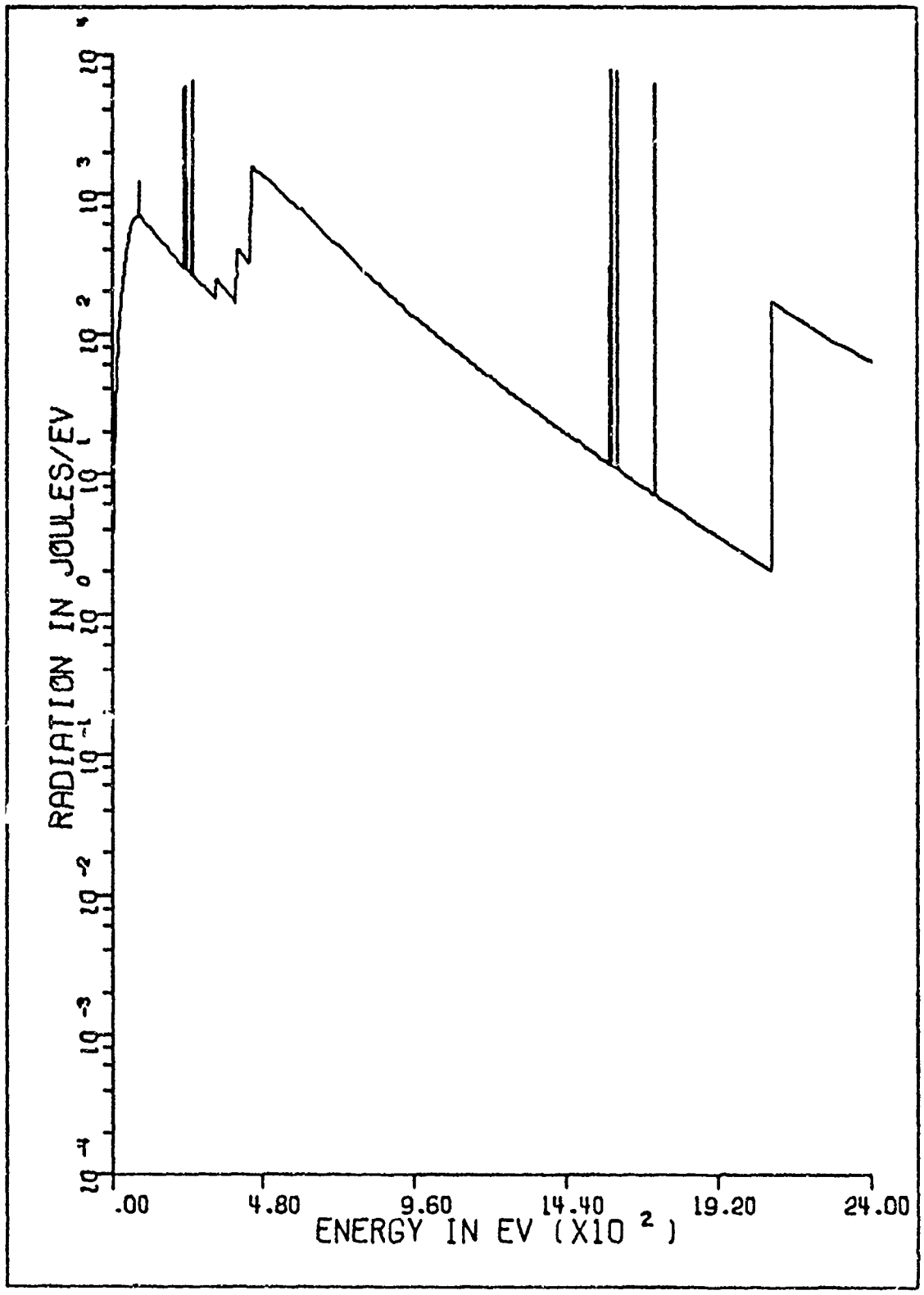
(a) Time-resolved spectrum at t = 1.98 nsec.
T_e = 183.5 eV T_i = 185 eV $\bar{z} \approx 11$

Fig. 3. Results of SHIVA project calculations.



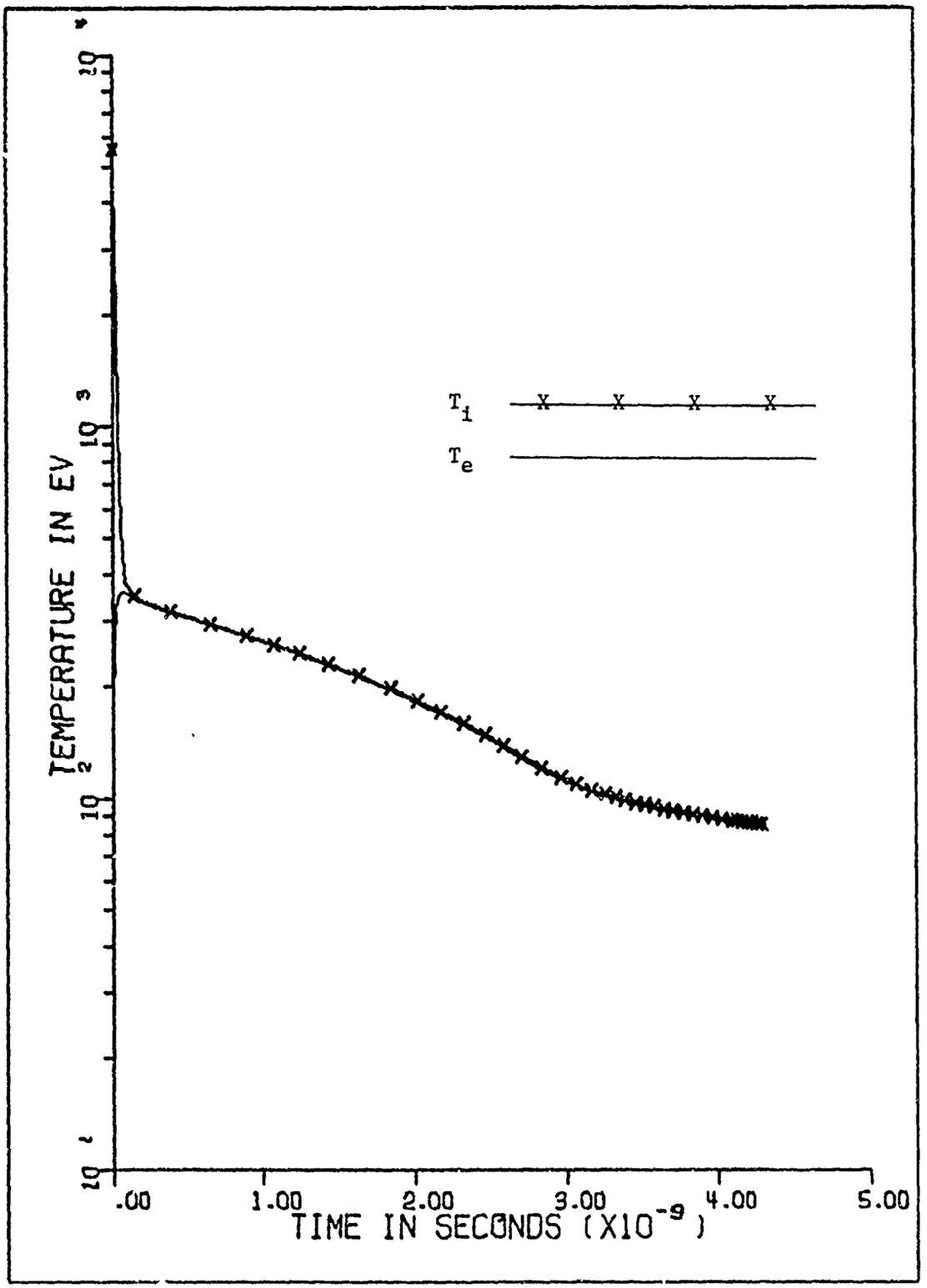
(b) Time-resolved spectrum at t = 4.29 nsec.
T_e = 84.4 eV T_i = 85.2 eV $\bar{z} \approx 10$

Fig. 3. (continued)



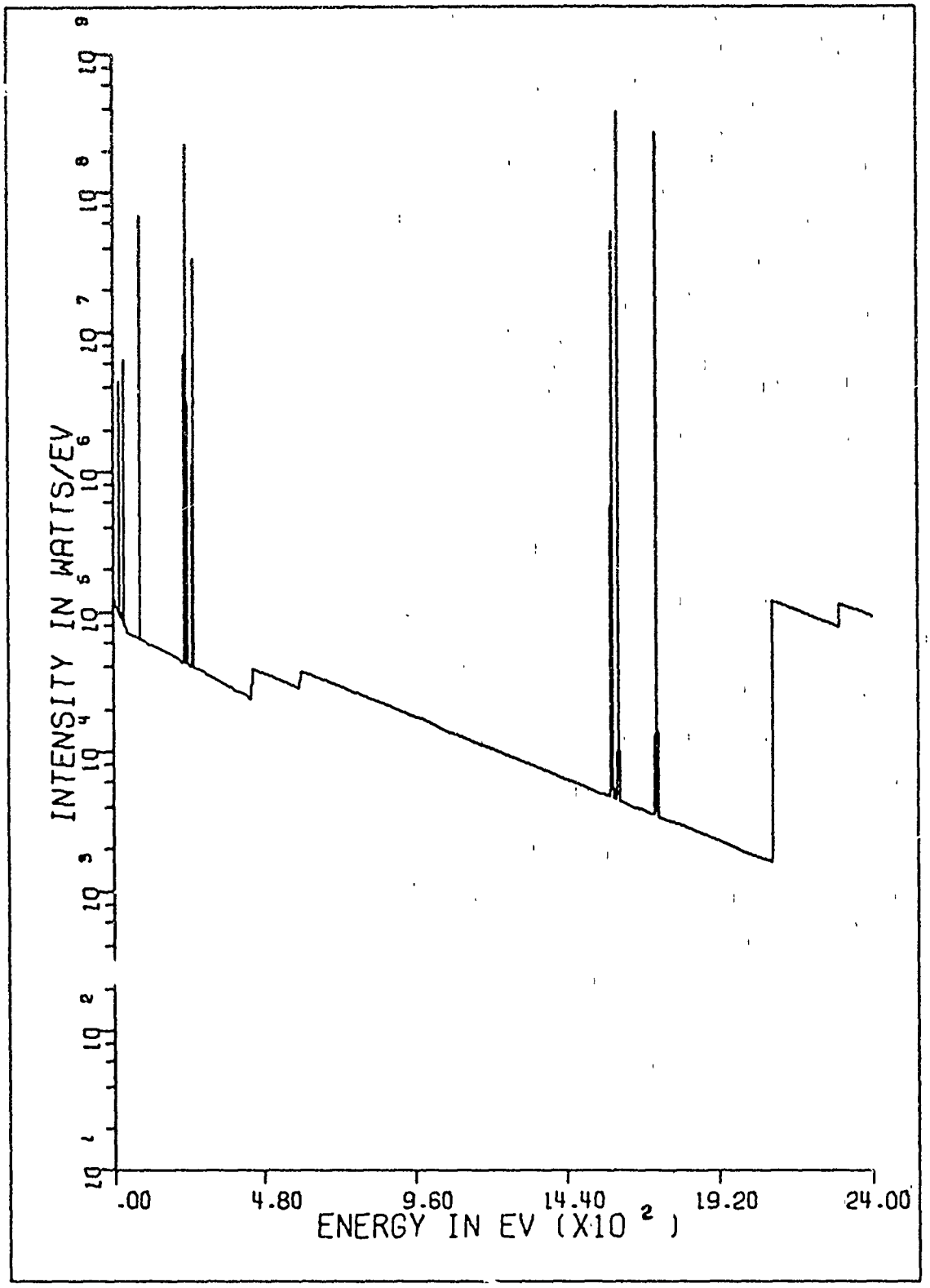
(c) Time-integrated spectrum at t = 4.29 nsec.

Fig. 3. (continued)



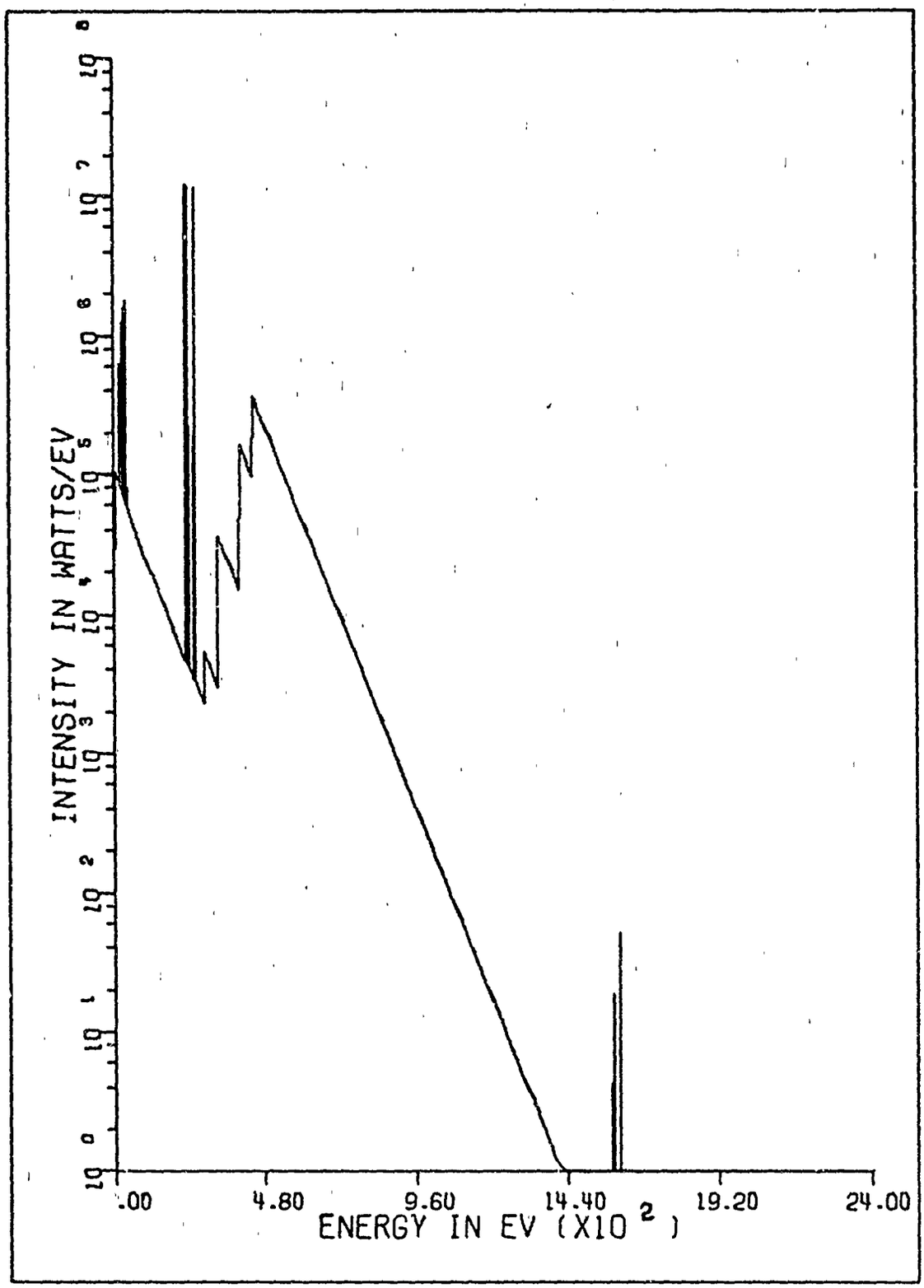
(d) Electron and ion temperatures vs. time.
$T_e\big|_{t=0} = 30$ eV $\quad T_i\big|_{t=0} = 5.53$ KeV

Fig. 3. (continued)



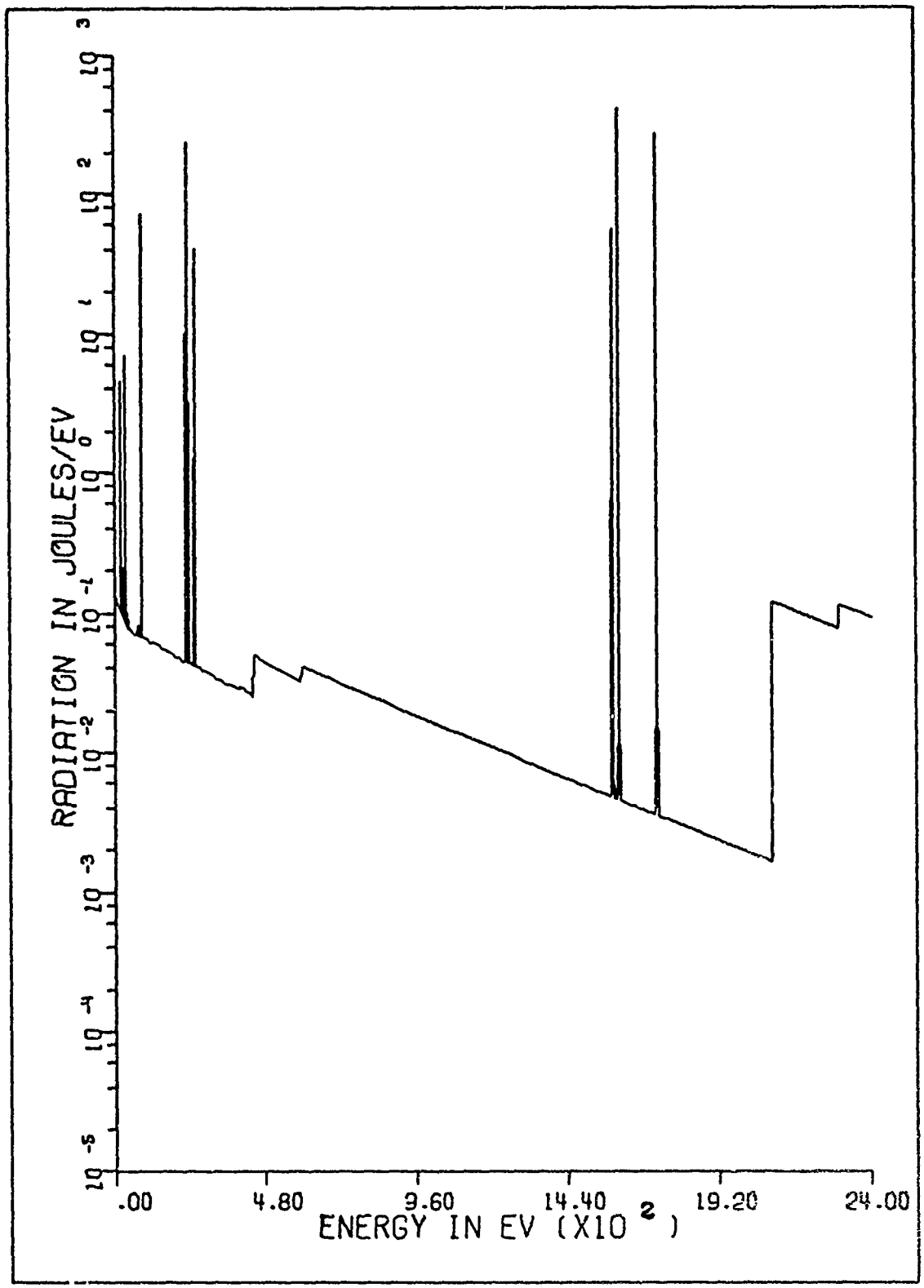
(a) Time-resolved spectrum at t = 7.46 nsec.
T_e = 480 eV T_i = 477 eV $\bar{z} \approx 12$

Fig. 4. Results of laser-heating calculations.



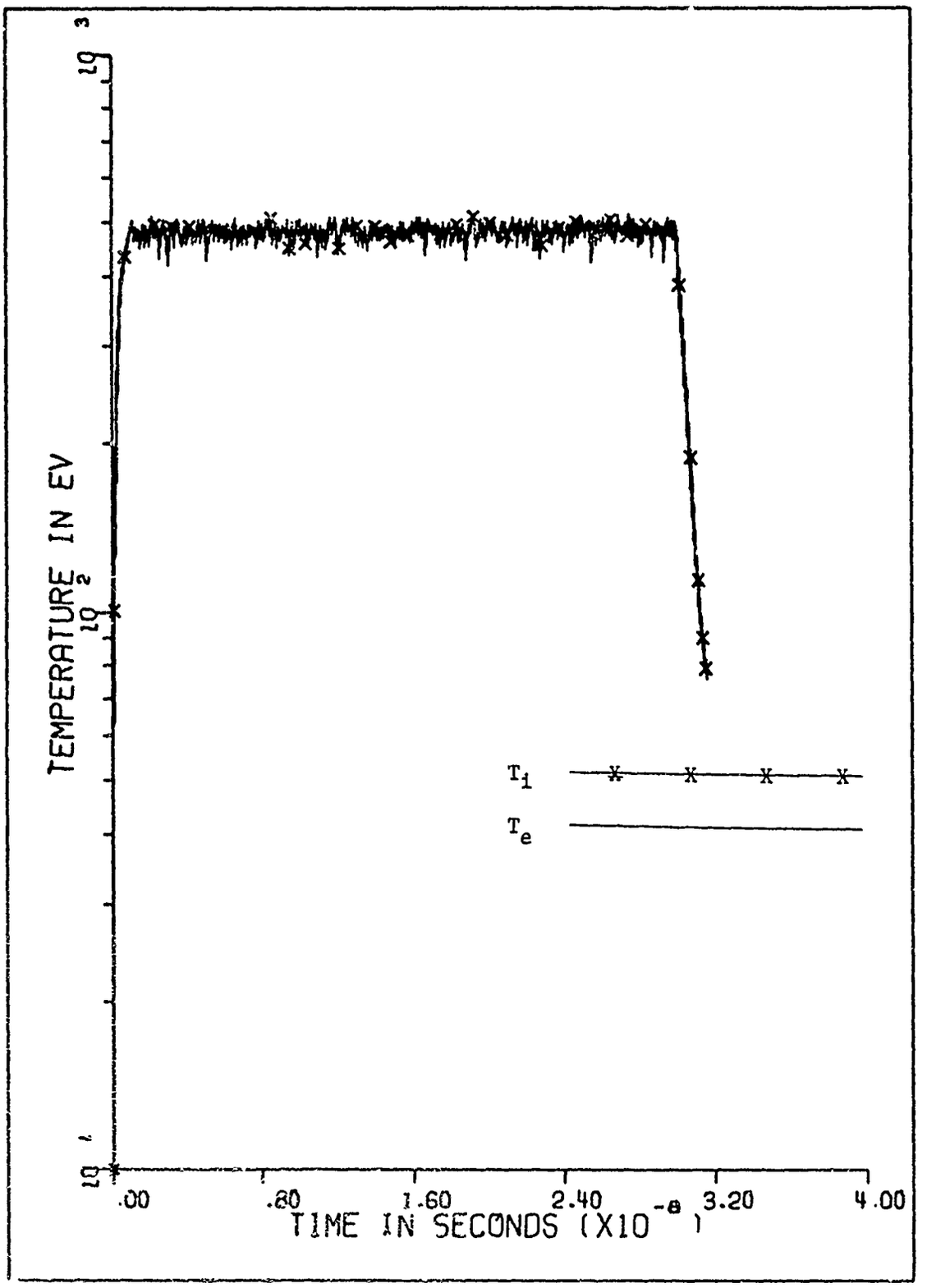
(b) Time-resolved spectrum at t = 31.58 nsec.
T_e = 75.5 eV T_i = 77 eV $\bar{z} \approx 10$

Fig. 4. (continued)



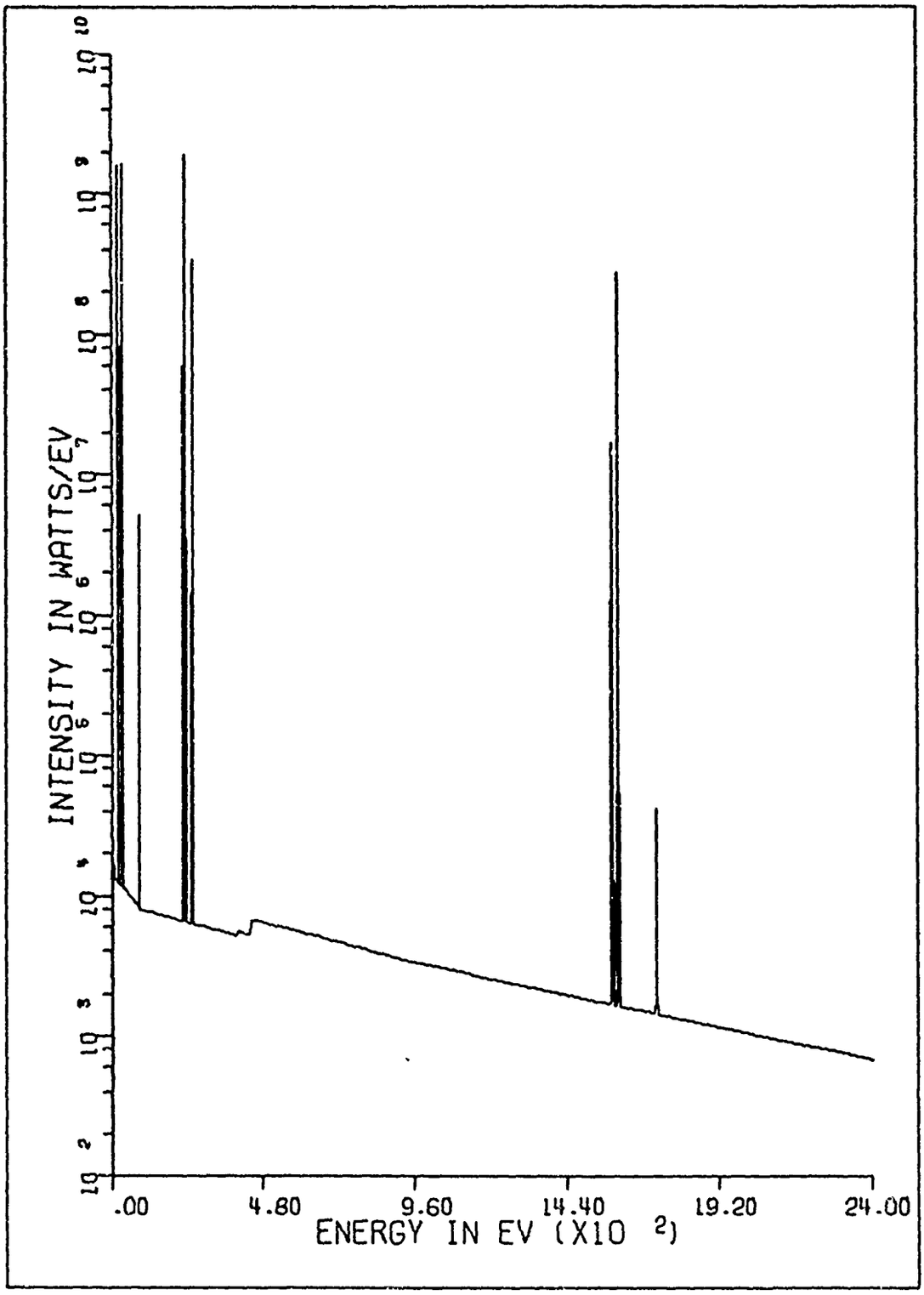
(c) Time-integrated spectrum at t = 31.58 nsec.

Fig. 4. (continued)



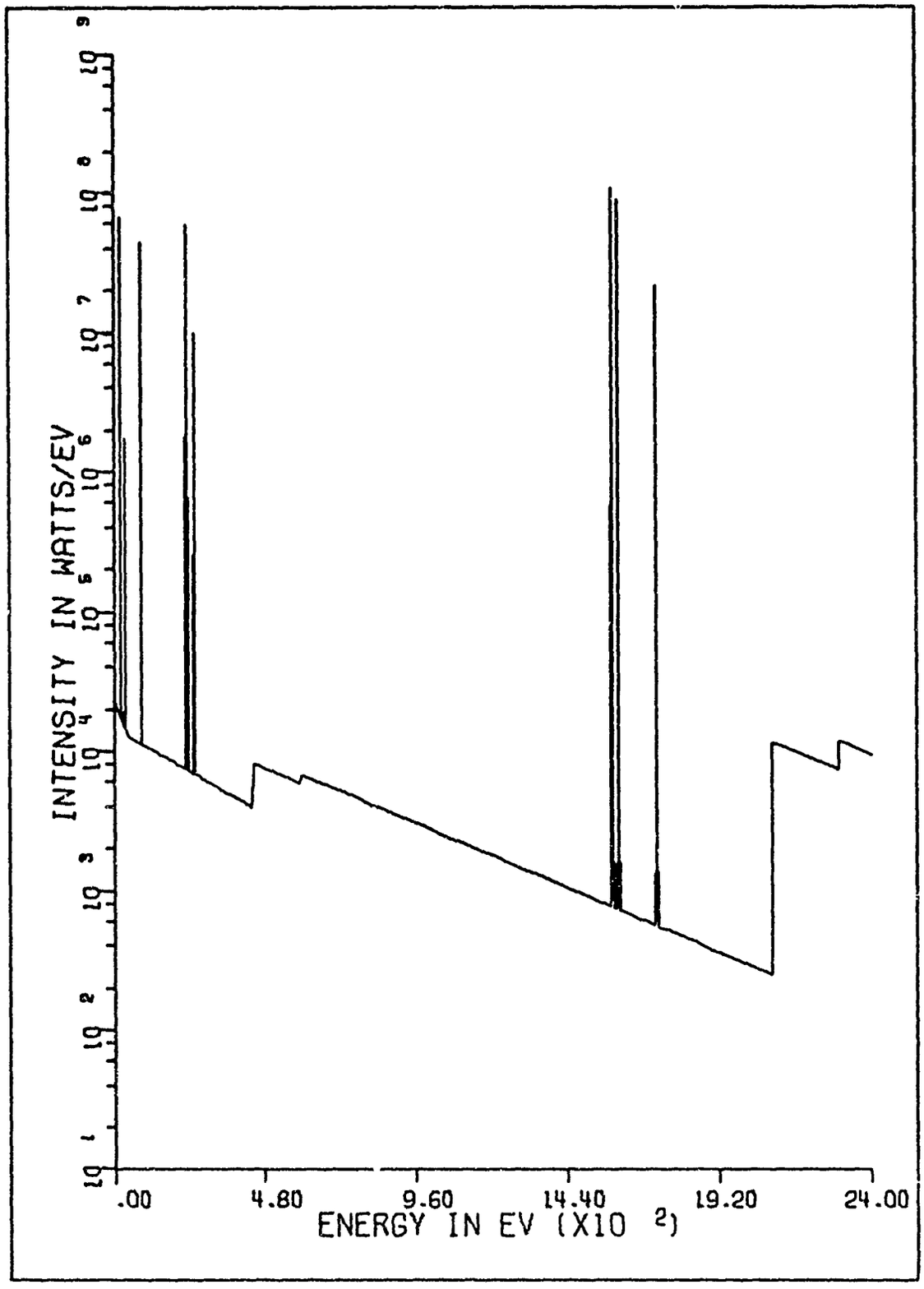
(d) Electron and ion temperatures vs. time.
$T_e|_{t=0} = 10$ eV $\quad T_i|_{t=0} = 10$ eV

Fig. 4. (continued)



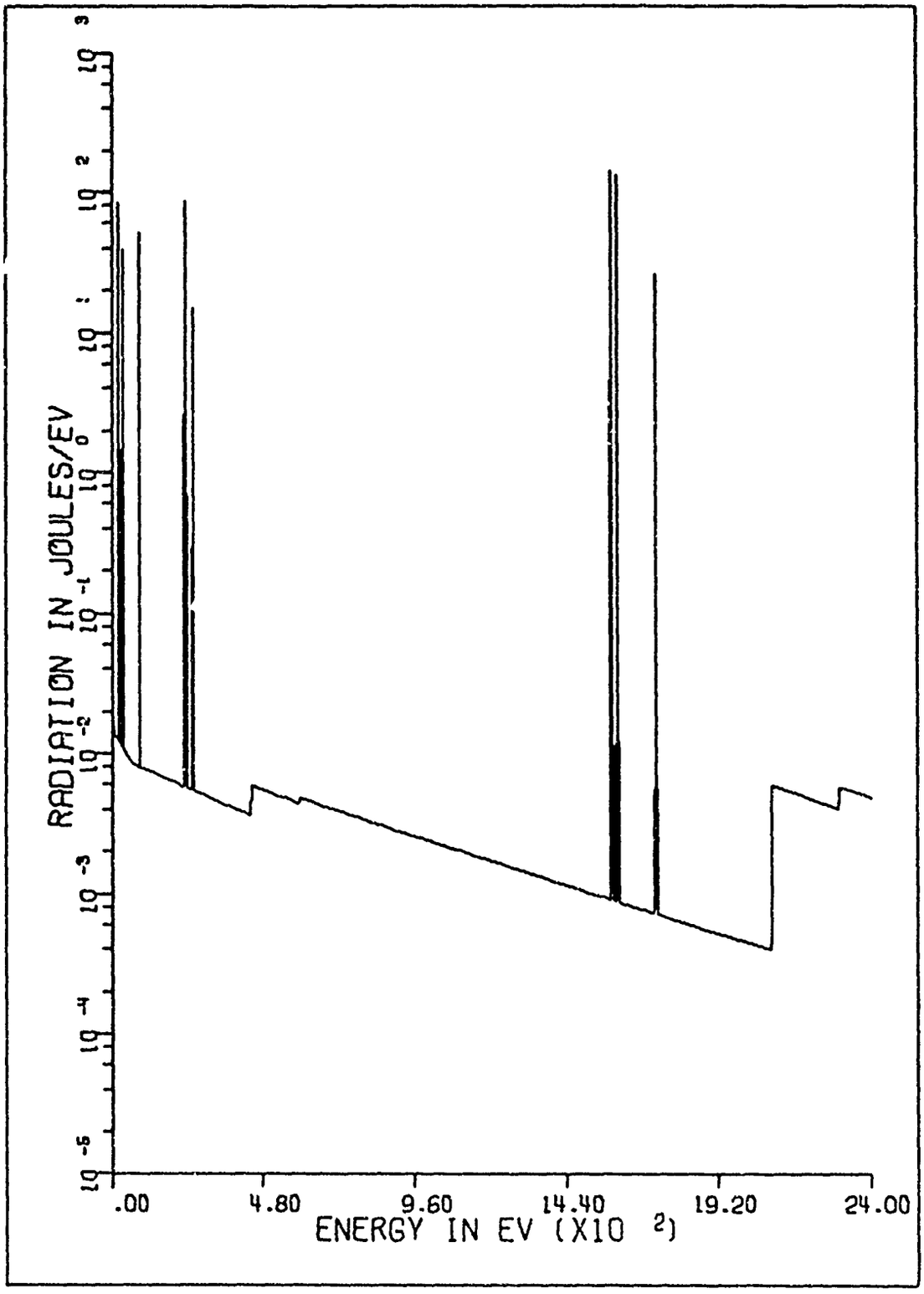
(a) Time-resolved spectrum at t = 5.99 psec.
T_e = 937.5 eV T_i = 938 eV $\bar{z} \approx 9.6$

Fig. 5. Results of impurity radiation calculations.



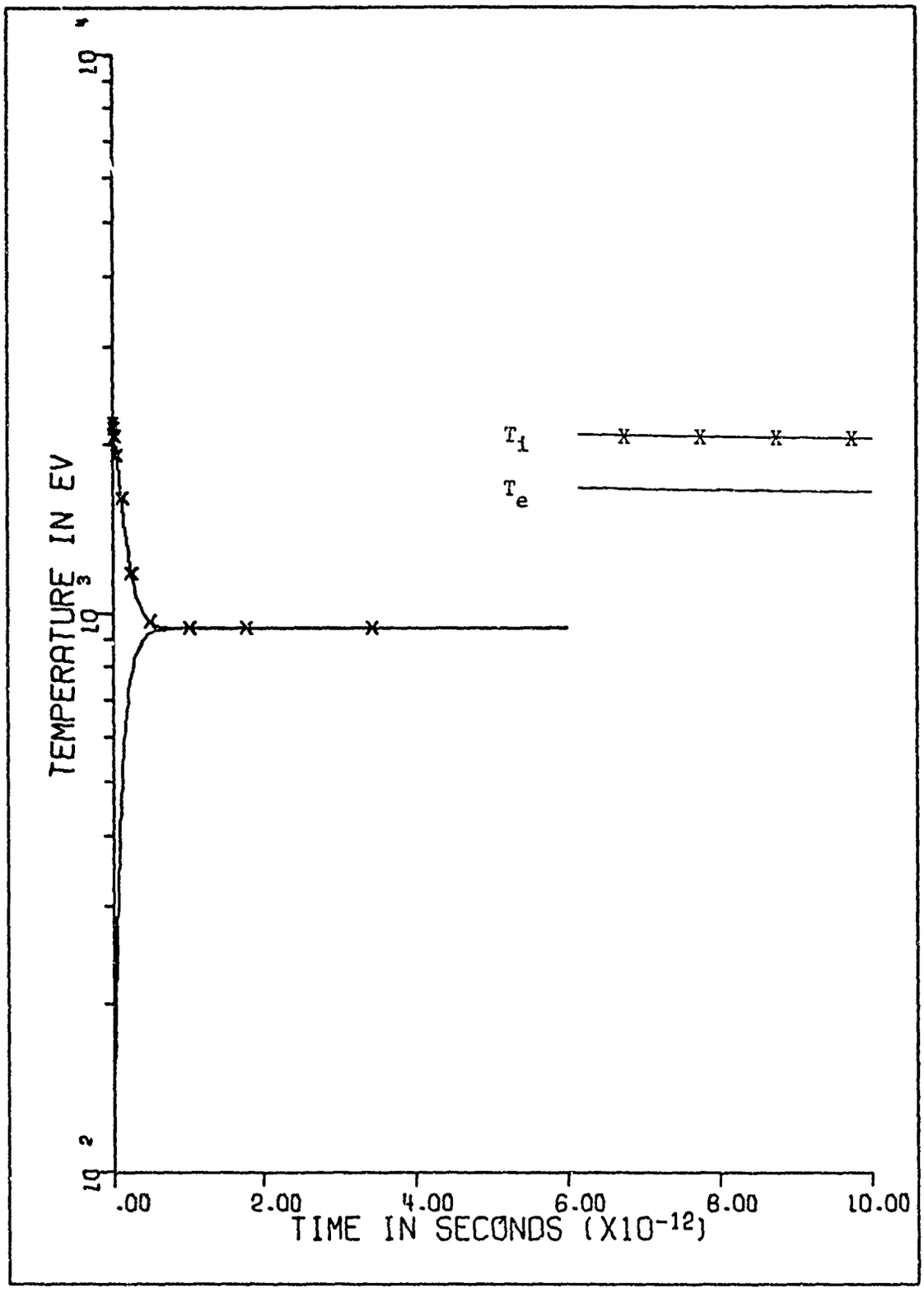
(b) Time-resolved spectrum at t = 31.33 nsec.
T_e = 456.3 eV T_i = 456.9 eV $\bar{z} \approx 10.4$

Fig. 5. (continued)



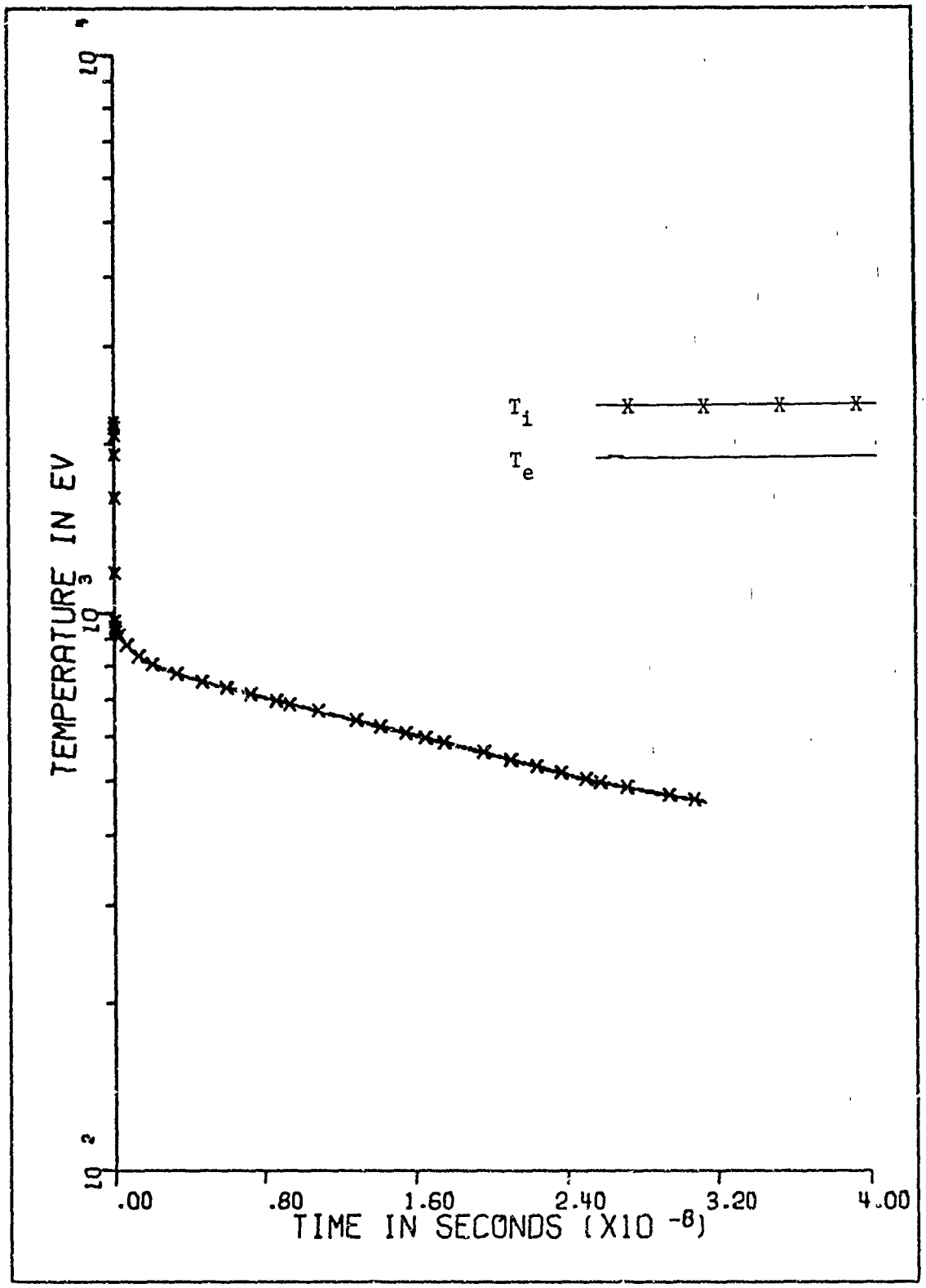
(c) Time-integrated spectrum at t = 31.33 nsec.

Fig. 5. (continued)



(d) Electron and ion temperatures vs. time at early time.
$T_e|_{t=0}$ = 100 eV $T_i|_{t=0}$ = 2.18 KeV

Fig. 5. (continued)



(e) Later plot of electron and ion temperatures vs. time.
$T_e|_{t=0}$ = 10^ [illegible] $T_i|_{t=0}$ = 2.18 KeV

Fig. 5. (continued)

VII. Conclusions and Recommendations

Their are very few definite conclusions which can be made at this time. An obvious need exists for a code such as TORCH which can be used to guide the experimentalist toward the optimum parameters to use in the laboratory. Hopefully, closer ties between the theorist and the experimentalist can lead to significant advances in the field of X ray production.

While there do not appear to be any major discrepancies in the results of the corona model, in general, and TORCH, in particular, there is certainly a great deal of work which remains to be completed. There are two main directions which can be taken. One is to stop building on TORCH and attempt a detailed comparison of experimental and theoretical data. The other is to continue modifying the code to eliminate some of the less justifiable assumptions. The latter is probably preferable in the long run, but will definitely require the coupling of TORCH to a new or existing hydrodynamics code in order to provide flexibility of application.

One of the first changes should be the replacement of the blackbody radiation limit with a more realistic, albeit more complex, method of accounting for optical thickness in the plasma. Also, improvement could very well result from the addition of more excited states in the highly charged ions as they are usually the most populated species. Stark broadening may also be an interesting effect to include - particularly since a significant amount of the radiated energy often results from the bound-bound transitions that occur.

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Appendix A

Atomic Data

The transitions used are due to Allen and are the transitions from the configuration that includes the ground level to the nearest configuration of opposite parity that leads to single electron jump transitions without change of multiplicity (Ref 1:50). The values for A_{ki} and f_{ik} are from Weise, et al. (Ref 17).

Table IV

Ion	Transition	X_i	X_k	A_{ki} ($\times 10^8 sec^{-1}$)	f_{ik}
I	3p - 4s	5.984	2.984	1.47	.115
II	$3s^2$-3s3p	18.82	11.82	14.6	1.84
III	3s - 3p	28.44	21.44	5.64	.875
IV	$2p^6$-$2p^5$3s	119.96	42.96	170.	.2
V	$2p^5$-$2s2p^6$	153.77	109.77	320.	.12
VI	$2p^4$-$2s2p^5$	190.42	150.42	140.	.21
VII	$2p^3$-$2s2p^4$	241.93	206.93	41.	.24
VIII	$2p^2$-$2s2p^3$	285.13	253.13	350.	.11
IX	2p -$2s2p^2$	330.1	298.1	160.	.2
X	$2s^2$-2s2p	398.5	361.5	57.	.287
XI	2s - 2p	441.9	419.9	8.35	.116
	2s - 3p	441.9	186.9	3140.	.330
	2p - 3s	419.9	189.9	[illegible]	.02
	2p - 3d	419.9	184.9	9800.	.672
XII	1^1S-2^1P	2085.5	485.5	2.78×10^5	.752
	1^1S-2^3P	2085.5	505.5	96.	10^{-5}
	2^3S-2^3P	595.5	505.5	910.	.1
XIII	1s - 2p	2299.	579.	2.1×10^6	.55

Appendix B

Listing of TORCH

A listing of the computer code TORCH follows. The program is set up to execute on the Air Force Weapons Laboratory CDC 6600 computer. The only difficulties which might be encountered in running on another machine should be the references to some of the library plot routines.

```
      PROGRAM TCFCH(INPUT,OUTPUT,PUNCH,FILMFL,TAPE10)
*****************************************************************************
*
*   THIS PROGRAM CALCULATES THE FOLLOWING IN TIME...                        *
*     1. THE NUMBER OF IONS PRESENT IN EACH STAGE OF IONIZATION AND THE TOTAL *
*        NUMBER OF ELECTRONS                                                *
*     2. THE RADIATION GIVEN OFF FROM SUCH A CONFIGURATION OF IONIC SPECIES  *
*     3. THE ELECTRON AND ION TEMPERATURES                                   *
*                                                                            *
*   THE INPUTS ARE...                                                        *
*     VOL=VOLUME OF PLASMA -- IN CM**3                                       *
*     AREA=SURFACE OF PLASMA -- IN M**2                                      *
*     PART=TOTAL NUMBER OF IONS AND ATOMS                                    *
*     ALFRAC=FRACTION OF IONS WHICH ARE ALUMINUM                             *
*     AND=NUMBER OF ALUMINUM IONS AND ATOMS                                  *
*  NOTE -- AND=ALFRAC*PART                                                   *
*   NOTE -- THE NON-ALUMINUM IONS ARE CONSIDERED TO BE DEUTERIUM             *
*                                                                            *
*   INITIAL CONDITIONS...                                                    *
*     TIN=INITIAL TEMPERATURE USED TO CALCULATE INITIAL SPECIES POPULATIONS  *
*         -- IN EV                                                           *
*     ENERGI=ENERGY TO BE ADDED TO IONS -- IN JOULES                         *
*     ENERGE=ENERGY TO BE ADDED TO ELECTRONS -- IN JOULES                    *
*   NOTE -- ENERGI AND ENERGE ARE ADDED AT TIME=0 BUT AFTER CALCULATING THE  *
*       INITIAL SPECIES POPULATIONS                                          *
*                                                                            *
*   CONTROL VARIABLES...                                                     *
*     KPRNT=NUMBER OF STEPS BETWEEN PRINTING POINTS                          *
*     NOFTEN=NUMBER OF CALLS TO SUBROUTINE F BETWEEN RADIATION CALCULATIONS. *
*        F IS CALLED ABOUT TWICE PER STEP.                                   *
*     NPT=NUMBER OF POINTS TO BE PRINTED                                     *
*  NOTE -- (2*KPRNT*NPT)/NOFTEN  IS THE NUMBER OF RADIATION CALCULATIONS     *
*        PERFORMED. THE RATE IS ABOUT 23 RADIATION CALCULATIONS PER CPU MINUTE.*
*     NN= 0 MEANS READ IN INITIAL SPECIES POPULATIONS                        *
*         1 MEANS STOP                                                       *
*         2 MEANS CALCULATE INITIAL SPECIES POPULATIONS                      *
*                                                                            *
*****************************************************************************
      COMMON/BLK1/T[illegible],TI,XI(14,5)
      COMMON /BLK4/CCSF(15,15),EN
      COMMON /BLK5/PCT(14),[illegible],AN,TOTPCT
      COMMON/BLK6/CU(32),[illegible],RSC1,CLNLAM
      COMMON/BLK7/RINT(1[illegible]),CNLIN(13,4),Y112P,Y11G
      COMMON/BLK8/NOSP
      COMMON/BLK9 [illegible](13,5,2)
      COMMON/BLK1[illegible]/NFFLO(210),PE(208),SPEC(210,2),VOL,AREA
      COMMON/BL[illegible]/NCCUNT,NOFTEN
      COMM[illegible] 13/DX,ALFRAC
      DIM[illegible] Y(22)
      DIM[illegible] FL1(210),FL2(21 ),PT(420)
      DIMENSION FL3(210)
      DIMENSION TFL(4[illegible]),TIFL(4[illegible]),XFL(4[illegible])
      DIMENSION TIP2(4[illegible]),TIP2(4[illegible])
      EQUIVALENCE (PL1(1),PT(1),SPEC(1,1))
      LOGICAL MODE,NOSP
      EXTERNAL F
      VOL=
      AREA=
      PART=
      ALFRAC=
      AND=ALFRAC*PART
      TIN=
      ENERGE=
      ENERGI=
      KPRNT=
      NOFTEN=
      NPT=
      NPLT=21[illegible]
      ND=[illegible]
```

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```
      NPIC=4
      NPIC=NPT/NPTC
CCC NOSP=.TRUE. CAUSES BYPASS OF ALL RADIATION CALCULATIONS
      NOSP=.FALSE.
      NCOUNT=NCRTRN
      IF(NOSP) GO TO 60
      CALL PLOTC(0.,0.,0,0,7)
      CALL PLOT(10.,10,56)                                          CALCOMP
   60 CONTINUE
      ENERLC(1)=0.
      DO 5000 I=1,200
 5000 ENERLC(I+1)=ENERLC(I)+DELT
      ENMX=ENERLC(NPLT)
      PRINT 9
      PRINT 12,ENERLC
   50 DO 1000 I=1,16
      IF(I.LE.13) ENLTN(I,1)=ABS(XI(I,1)-XI(I,2))
 1000 Y(I)=0
      ENLIN(11,2)=ABS(XI(11,1)-XI(11,4))
      ENLIN(11,3)=ABS(XI(11,2)-XI(11,3))
      ENLIN(11,4)=ABS(XI(11,2)-XI(11,5))
      ENLIN(12,2)=ABS(XI(12,1)-XI(12,3))
      ENLIN(12,3)=ABS(XI(12,1)-XI(12,4))
      ENLIN(12,4)=ABS(XI(12,2)-XI(12,3))
      ENERG=0.
      READ 1,NN
    1 FORMAT(I3)
      IF(NN.LE.0) GO TO 100
      IF(NN.EQ.1) GO TO 7777
      TE=TIN
      Y(15)=S(13,1)/ALPH(14,1)
      Y(14)=S(12,1)/ALPH(13,1)
      RAT=1.+Y(14)*(1.+Y(15))
      Y(13)=0
      DO 69 I=2,12
      J=14-I
      Y(J)=S(J-1,1)/ALPH(J,1)
   69 RAT=1.+Y(J)*RAT
      Y(1)=AN/RAT
      DO 96 I=2,12
   96 Y(I)=Y(I)*Y(I-1)
      Y(14)=Y(14)*Y(12)
      Y(15)=Y(15)*Y(14)
      X=0
      GO TO 110
  100 CONTINUE
      READ 7,X,TE,TI,Y
  110 CONTINUE
      N=22
      FOT(1)=XI(1,1)
      TOTFOT=0
      AN=0
      DO 4000 J=2,15
      AN=AN+Y(J)
      IF(J.LT.11) FOT(J)=FOT(J-1)+XI(J,1)
      IF(J.EQ. 12) FOT(13)=FOT(11)+XI(12,1)
      IF(J.EQ.13) FOT(12)=FOT(13)-XI(12,2)
      IF(J.EQ.14) FOT(14)=FOT(13)+XI(13,1)
      TOTFOT=TOTFOT+Y(J)*FOT(J-1)
 4000 CONTINUE
      AN=AN+Y(1)
      AN=AN/ALFAO
      CALL ELECON(X,Y,15)
      IF(NN.LE.0) GO TO 360
CCC CALCULATE ENERGY/ION IN EV.....MASS IN KG
      ENERI=1.5*TIN
      TI=2./3.*ENERI
CCC NOW GET ENERGY OF IONS IN EV
      ENERI=1.5*AN*TI+ENERGI/1.6025E-19
```

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```
      Y(22)=ENERI
CCC NEXT ... ELECTRON ENERGY
      ENERE=1.5*EN*TE+ENERGE/1.602E-19
      Y(19)=ENERE
CCC NOW TOTAL ENERGY
      ENERC=ENERI+ENERE+TOTPOT
      FIRSTEN=ENERC
      Y(16)=ENERC
      TE=2./3.*ENERE/EN
      TI=2./3.*ENERI/AN
  999 CONTINUE
      XC=X
      PRINT 8,PCT
    8 FORMAT(* PCT...*,/,2(7F15.8/))
      PRINT 12,PALIN
   12 FORMAT(*J*,4(13F10.2/))
      PRINT 9
      DIS=1.E-7
      MODE=.FALSE.
      DX=1.E-15
      DXMAX=1.E-9
      DXMIN=0.
      ENERC=Y(16)
      TEMAX=TE
      TIMAX=TI
      TMIN=AMIN1(TE,TI)
      TEPL(1)=TE
      TIPL(1)=TI
      XPL(1)=X
      PRINT 2,X,EN,DX,TE,AN,(Y(I),I=1,16),TI
      PRINT 7,Y(18),TOTPOT
    3 FORMAT(* ENERG=*,E15.5,* TOTPOT=*,E15.5)
      CALL SET (N,X,Y,DX,F,DIS,MODE,DXMAX,DXMIN)
      DIFF=Y(16)-(Y(19)+Y(22)+TOTPOT)
      PRINT 2,X,EN,DX,TE,DIFF,(DD(I),I=1,16),TI
      KK=1
  200 CONTINUE
      DO 201 I=1,KPRNT
      DXTEMP=DX
      CALL STEP(N,X,Y,DX,F,DIS,MODE,DXMAX,DXMIN)
      ENERG=Y(16)
      ENERE=Y(19)
      ENERI=Y(22)
      IF(X.LT.DXTEMP)KK=1
  201 CONTINUE
      DIFF=Y(16)-(Y(19)+Y(22)+TOTPOT)
      IF(MOD(KK,8).NE.1) GO TO 300
      IF(NOSP) GO TO 301
      PRINT 11,Y(11),Y110,Y112P
   11 FORMAT(*1LI-LIKE.. *E15.5*   GROUND STATE.. *E15.5*   2P.. *E15.5)
      YTJ=(FIRSTEN-Y(16))*1.602E-19
      PRINT 13,Y(17),YTJ,(Y(I),I=19,31)
   13 FORMAT(*0 0.0 - 0.5 KEV...*E10.3* JOULES.   ENERGY LOST ... *E10.3
     1* JOULES.   0.5 - 1.0 KEV...*E10.3* JOULES.*/*31.-1.4 KEV ..*E10.3
     2* JOULES.   1.4 -1.8 KEV ... *E10.3* JOULES.*)
      PRINT 12,PINT
      PRINT 12,(PT(I),I=211,420)
      F1=1.602E-19
      E1=ENERE*F1
      E2=ENERI*F1
      FREC1=FREC1/AN
      FREC=FREC/AN
      C1=CC(22)*F1
      PRINT 14,E1,E2,CLNLAM,FREC1,FREC,C1
   14 FORMAT(*0ENERE= *E11.4* JOULES ... ENERI= *E11.4* JOULES*
     1 /* LN(LAMBDA)= *E10.3*   FREQ(E-I)= *E10.3*  + FREQ(ES)= *E10.3*
     2    C(ENERI)/CI= *E10.3)
  301 CONTINUE
      KPAGE=KK/8+2
```

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```
      PRINT 6,KPAGE
    6 FORMAT(*1*,50X,*PAGE*,I3)
  300 CONTINUE
      PRINT 2,X,EN,DX,TE,DIFF,(Y(I),I=1,16),TI
      KK=KK+1
      TEPL(KK)=TE
      TIPL(KK)=TI
      XPL(KK)=X
      IF(TE.GT.TEMAX) TEMAX=TE
      IF(TI.GT.TIMAX) TIMAX=TI
      IF(TE.LT.TMIN.OR.TI.LT.TMIN) TMIN=AMIN1(TE,TI)
  799 CONTINUE
      IF(KK.GE.NST) GO TO 400
  798 IF(MOD(KK,NPIC).EQ.0) GO TO 400
      GO TO 200
    2 FORMAT(*,TIME=*,E15.8,* SEC....EN=*,E15.9,* ... DX=*,E15.9,* ... T
     1E=*,E15.9,* .. DIFF= *,E15.9,/3(/5E15.5),*      ENERG= *,E15.8,
     2*  TI= *E15.9/)
  400 CONTINUE
      IF(NOSP) GO TO 445
CCC PLOT TIME INTEGRATED SPECTRUM
      XLB=10HENERGY IN       OXL2=10HEV
      ALB=7HTIME =
      BLB=10HENERGY  =
      CLB=10HTEMPERATURE     OCL2=10HE =
      YLB=10HRADIATION
      YL2=10HIN JOULES/
      YL3=10HEV
      ENERG=Y(16)*1.6025E-19
      YMIN=0.
      YMAX=0.
      DO 304 I=1,NPLT
      IF(PL1(I).GT.YMAX) YMAX=PL1(I)
  304 CONTINUE
      YMIN=YMAX*1.E-7
      CALL GRIDC(ENMX,0.,YMAX,YMIN,XT,XB,YT,YB,ND, 0, 1,3,XLB,12,YLB,21,
     1   ALB,7,X,BLB,10,ENERG,CLB,14,TE)
      YMAX=ALOG10(ABS(YT))
      YMIN=ALOG10(ABS(YB))
      DO 305 I=1,NPLT
      PL3(I)=PL1(I)
      IF(PL3(I).LT.YB) PL3(I)=YB
  305 PL3(I)=ALOG10(ABS(PL3(I)))
      CALL LINPLT(ENEPLC,PL3,NPLT,ENMX,0.,YMAX,YMIN)
      T1=ENEPLC(NPLT+1)                                                 CALCOMP
      T2=ENEPLC(NPLT+2)                                                 CALCOMP
      XAX=5.                                                            CALCOMP
      ENEPLC(NPLT+1)=0.                                                 CALCOMP
      ENEPLC(NPLT+2)=ENMX/XAX                                           CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL AXIS(0.,0.,XLB,-12,XAX,0.,ENEPLC(NPLT+1),ENEPLC(NPLT+2),0)   CALCOMP
      YAX=7.                                                            CALCOMP
      YD=8./YAX                                                         CALCOMP
      PL3(NPLT+1)=YMIN                                                  CALCOMP
      PL3(NPLT+2)=YD                                                    CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL FIXFRM(XAX,YAX)                                              CALCOMP
      CALL LAXIS(0.,0.,YLB,22,YAX,90.,YMIN,YD,DUM)                      CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL LINE(ENEPLC,PL3,NPLT,1,0,DUM)                                CALCOMP
      ENEPLC(NPLT+1)=T1                                                 CALCOMP
      ENEPLC(NPLT+2)=T2                                                 CALCOMP
      CALL PLOT(XAX+5.,0.,-3)                                           CALCOMP
      CALL PLOTC(0.,0.,0,0,12)
CCC PLOT TIME RESOLVED SPECTRUM
      YMAX=0
      DO 302 I=1,NPLT
      IF(SPEC(I,2).GT.YMAX) YMAX=SPEC(I,2)
  302 CONTINUE
```

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```
      YMIN=YMAX*1.E-7
      ENERG=Y(16)*1.6 2E-19
      YLB=1HMINTENSITY      YL2=1HMIN WATTS/S     YL3=10HV
      CALL GRIDC(EMAX,0.,YMAX,YMIN,XT,XB,YT,YB,NB, 0, 1,3,XLB,12,YL3,21,
     1   ALB,7,XTL ,10,ENERG,CLB,14,TE)
      YMAX=ALOG10(ABS(YT))
      YMIN=ALOG10(ABS(YB))
      DO 303 I=1,NPLT
      PL2(I)=SPEC(I,2)
      IF(PL2(I).LT.YB) PL2(I)=YB
  303 PL2(I)=ALOG10(ABS(PL2(I)))
      CALL LINPLT(ENEPLC,PL2,NPLT,EMAX,0.,YMAX,YMIN)
      T1=ENEPLC(NPLT+1)
      T2=ENEPLC(NPLT+2)                                                  CALCOMP
      XAX=5.                                                             CALCOMP
      ENEPLC(NPLT+1)=0.                                                  CALCOMP
      ENEPLC(NPLT+2)=EMAX/XAX                                            CALCOMP
      CALL AXIS(0.,0.,XLB,-12,XAX,0.,ENEPLC(NPLT+1),ENEPLC(NPLT+2),0)    CALCOMP
      YAX=7.                                                             CALCOMP
      YD=8./YAX                                                          CALCOMP
      PL2(NPLT+1)=YMIN                                                   CALCOMP
      PL2(NPLT+2)=YD                                                     CALCOMP
      CALL PLOT(0.,0.,0)                                                 CALCOMP
      CALL PIXFRAM(XAX,YAX)                                              CALCOMP
      CALL LAXIS(0.,0.,YLB,28,YAX,90.,YMIN,YD,CUM)                       CALCOMP
      CALL PLOT(0.,0.,0)                                                 CALCOMP
      CALL LINE(ENEPLC,PL2,NPLT,1,0,CUM)                                 CALCOMP
      ENEPLC(NPLT+1)=T1                                                  CALCOMP
      ENEPLC(NPLT+2)=T2                                                  CALCOMP
      CALL PLOT(XAX+5.,0.,-3)                                            CALCOMP
      CALL PLOTC(0.,0.,0,0,12)                                           CALCOMP
      XMIN=0
      YMIN=0
      XMAX=XPL(KK)/10.
      ITEMP=ALOG10 (XMAX)
      IF(ITEMP.LT.0) ITEMP=ITEMP-1
      NXDIV=INT(XPL(KK)*10.**(-ITEMP))+1
      NFACT=5
      IF(NXDIV.LE.80) NFACT=4
      IF(NXDIV.LE.40) NFACT=2
      IF(NXDIV.LE.20) NFACT=1
      NXDIV=(NXDIV+NFACT-1)/NFACT
      XMAX=NFACT*NXDIV*10.**ITEMP
      XLB=10HTIME IN SE     XL2=10HCONDS
      ALB=10HINITIAL TE
      BLB=10HINITIAL TI
CCC PLOT TE VS TIME -- LINEAR-LINEAR
      YLB=10HELECTRON T     YL2=10HEMPERATURE     YL3=10H IN EV
      ITEMP=ALOG10(TEMAX)
      NYDIV=INT(TEMAX*10.**(-ITEMP))+1
      YMAX=NYDIV*10.**ITEMP
      NYDIV=2*NYDIV
      CALL GRIDC(XMAX,XMIN,YMAX,YMIN,YT,XB,YT,YB,NXDIV,NYDIV,1,2,XLB,10,
     1 YLB,26,ALB,10,TEPL(1),BLB,10,TIPL(1),CUM,CUM,CUM)
      CALL LINPLT(XPL,TEPL,KK,XMAX,YMIN,YMAX,YMIN)
      XAX=5.
      YAX=7.                                                             CALCOMP
      CALL SCALE(XPL,XAX,KK,1)                                           CALCOMP
      CALL SCALE(TEPL,YAX,KK,1)                                          CALCOMP
      CALL PIXFRAM(XAX,YAX)                                              CALCOMP
      CALL AXIS(0.,0.,YLB,-10,XAX,0.,XPL(KK+1),XPL(KK+2),0)              CALCOMP
      CALL PLOT(0.,0.,3)                                                 CALCOMP
      CALL AXIS(0.,0.,YLB,26,YAX,90.,TEPL(KK+1),TEPL(KK+2),0)            CALCOMP
      CALL PLOT(0.,0.,3)                                                 CALCOMP
      CALL LINE(XPL,TEPL,KK,1,0,CUM)                                     CALCOMP
      CALL PLOT(XAX+5.,0.,-3)                                            CALCOMP
      CALL PLOTC(0.,0.,0,0,12)                                           CALCOMP
CCC PLOT TI VS TIME -- LINEAR-LINEAR
      YLB=10H    ION T
```

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```
      ITEMP=ALOG10(TIMAX)
      NYDIV=INT(TIMAX*10.**(-ITEMP))+1
      YMAX=NYDIV*10.**ITEMP
      NYDIV=2*NYDIV
      CALL GRIDC(XMAX,XMIN,YMAX,YMIN,XT,XB,YT,YB,NXDIV,NYDIV,1,2,XLB,15,
     1 YLB,26,ALB,10,TEPL(1),PLB,10,TIPL(1),DUM,DUM,DUM)
      CALL LINFLT(XPL,TIPL,KK,XMAX,XMIN,YMAX,YMIN)
      CALL SCALE(TIPL,YAX,KK,1)                                         CALCOMP
      CALL PIXFRAM(XAX,YAX)                                             CALCOMP
      CALL AXIS(0.,0.,XLB,-15,XAX,0.,XPL(KK+1),XPL(KK+2),0)             CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL AXIS(0.,0.,YLB,26,YAX,90.,TIPL(KK+1),TIPL(KK+2),0)           CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL LINE(XPL,TIPL,KK,1,1,DUM)                                    CALCOMP
      CALL PLOT(XAX+5.,0.,-3)                                           CALCOMP
      CALL PLOTC(0.,0.,0,12)                                            CALCOMP
CCC PLOT TE AND TI VS TIME -- LOG-LINEAR
      YLB=10HTEMPERATUR   YYL2=10HE IN EV
      YMIN=TMIN
      YMAX=AMAX1(TEMAX,TIMAX)
      CALL GRIDC(XMAX,XMIN,YMAX,YMIN,XT,XB,YT,YB,NXDIV,0,1,2,XLB,15,
     1 YLB,17,ALB,10,TEPL(1),PLB,10,TIPL(1),DUM,DUM,DUM)
      YMAX=ALOG10(ABS(YT))
      YMIN=ALOG10(ABS(YB))
      DO 444 I=1,KK
      TEP2(I)=ALOG10(TEPL(I))
  444 TIP2(I)=ALOG10(TIPL(I))
      CALL LINFLT(XPL,TEP2,KK,XMAX,XMIN,YMAX,YMIN)
      CALL LINFLT(XPL,TEP2,KK,XMAX,XMIN,YMAX,YMIN)
      CALL LINFLT(XPL,TIP2,KK,XMAX,XMIN,YMAX,YMIN)
      TEP2(KK+1)=YMIN
      TEP2(KK+2)=(YMAX-YMIN)/YAX                                        CALCOMP
      TIP2(KK+1)=TEP2(KK+1)                                             CALCOMP
      TIP2(KK+2)=TEP2(KK+2)                                             CALCOMP
      CALL PIXFRAM(XAX,YAX)                                             CALCOMP
      CALL AXIS(0.,0.,XLB,-15,XAX,0.,XPL(KK+1),XPL(KK+2),0)             CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL LAXIS(0.,0.,YLB,17,YAX,90.,TEP2(KK+1),TEP2(KK+2),DUM)        CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL LINE(XPL,TEP2,KK,1,0,3)                                      CALCOMP
      CALL PLOT(0.,0.,3)                                                CALCOMP
      CALL LINE(XPL,TIP2,KK,1,10,4)                                     CALCOMP
      CALL PLOT(XAX+5.,0.,-3)                                           CALCOMP
      CALL PLOTC(0.,0.,0,12)                                            CALCOMP
      PRINT 7,X,TE,TI
  445 CONTINUE
      IF(KK.LT.NFT) GO TO 250
      PRINT 9,NFT,KK
    5 FORMAT(*1*,*NFT=*,I4,*  KK=*,I9)
      PRINT 2,X,SN,DY,TE,AM,(DD(I),I=1,16),TI
    7 FORMAT(5X,3E15.9,5(/1X,5E15.9))
      PRINT 8
    9 FORMAT(*1*)
      PRINT 7,X,TE,TI,V
      GO TO 50
 7777 IF(NDSP) STOP
      CALL EXIT
      STOP
      END
```

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```
      SUBROUTINE F(N,X,Y,DY)
*************************************************************************
*                                                                       *
*   THIS SUBROUTINE EVALUATES THE DERIVATIVES OF THE IONIC SPECIES (AFTER *
*     CALLING NDENS) AS WELL AS THE DERIVATIVES OF THE ION ENERGY AND THE *
*     ELECTRON ENERGY. THE RADIATION LOSS IS HELD CONSTANT BETWEEN TIMES RAD IS*
*     CALLED.                                                           *
*                                                                       *
*************************************************************************
      COMMON/BLK1/TE,TI,XI(14,5)
      COMMON /BLK4/COEF(15,15),EN
      COMMON /BLK5/RC(14),ENERO,AN,TOTRCT
      COMMON/BLK6/CO(30),FREQ,FREQ1,DLNLAM
      COMMON/BLK10/ENERLO(210),DE(209),SPEC(210,2),VOL,AREA
      COMMON/BLK11/NCOUNT,NORTEN
      COMMON/BLK13/DX,ALFAAC
      DIMENSION Y(22),DY(22)
      CALL ELECTR(X,Y,15)
      ENERO=Y(16)
      ENERE=Y(18)
      ENERI=Y(22)
      TE=2./3.*ENERE/EN
      TI=2./3.*ENERI/AN
      IF(TE.LE...) GO TO 3000
      CALL NDENS
      DO 1000 I=1,15
       DY(I)=
      DO 4000 J=1,15
 4000 DY(I)=DY(I)+COEF(I,J)*Y(J)/VOL
      CO(I)=DY(I)
 1000 CONTINUE
CCC POWERE AND POWERI ARE POWER INPUTS TO THE ELECTRONS AND IONS
      POWERE=0
      POWERI=0
      IF(NCOUNT.LT.NORTEN) GO TO 50
      CALL RAD(X,Y,DY(16))
      NCOUNT=0
      RADLOS=DY(16)
   50 NCOUNT=NCOUNT+1
      DY(16)=RADLOS+(POWERE+POWERI)/1.6022E-19
CCC INTEGRATE THE TIME INTEGRATED SPECTRUM ONE MORE STEP
      DO 55 NF=1,210
   55 SPEC(NF,1)=SPEC(NF,1)+SPEC(NF,2)*DX
      TOTRCT=0
      DRCT=0.
      DNE=0.
      K=1
      DO 2000 J=2,15
      TOTRCT=TOTRCT+Y(J)*RCT(J-1)
      DRCT=DRCT+DY(J)*RCT(J-1)
      IF(J.GE.13) K=2
      Z=J-K
      DNE=DNE+DY(J)*Z
 2000 CONTINUE
      IF(POWERE.NE.0..OR.POWERI.NE.0.) GO TO 6000
      IF(ABS(TE-TI).GT.AMIN1(TE,TI,100.)*.01) GO TO 6000
CCC  DO THIS INSTEAD OF LATER CALCULATION OF D(ENERI)/DT IF TEMPS ARE CLOSE
      DNE2=AN*Y(18)/(EN*TE)*DNE
      DY(18)=EN/(AN+EN)*(DY(16)+DNE2-DRCT)
      DY(22)=AN/EN*(DY(18)-DNE2
      DLNLAM=0
      FREQ1=0
      FREQ=0
      GO TO 7000
 6000 CONTINUE
CCC NOW CALCULATE DERIVATIVE OF ENERI IN EV/SEC
      K=1
      SUM=0.
      CHECK=SQRT(36.2/TE)
```

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```
      CHECK=AMIN1(1.,CHECK)
      DLAM1= 1.54E1*SQRT(TE**3/EN/VOL)*CHECK
      DO 5000 I=2,15
      IF(I.GT.1) K=2
      Z=I-K
      DLAM=DLAM1/Z
      DLNLAM=ALOG(DLAM)
      SUM=SUM+Y(I)*Z**2*DLNLAM*Y(I)
 5000 CONTINUE
      DLNLAM=ALOG(DLAM1)
      FREQ1=SUM/1.3E5/(TE*1836.+TI/36.99)**1.5
      FREQ1=FREQ1/VOL
CCC NOW ADD HARD SPHERE CONTRIBUTION
      A1=ALFRAC*AN                                                      IMPURITY
      FREQ=FREQ1+1.3E1E-11*A1*SQRT(TE)*A1/VOL
      A2=(1.-ALFRAC)*AN                                                 IMPURITY
      DLAMD=ALOG(DLAM1)                                                 IMPURITY
      FREQ=FREQ+(1.26E-4*DLAMD/(TE*1836.+TI/2.)**1.5+2.65E-8*SQRT(TE))  IMPURITY
     1   *A2*A2/VOL                                                     IMPURITY
      DY(22)=3./2.*(TE-TI)*FREQ+POWERI/1.602E-19
      DY(18)=DY(18)-DY(22)-DEOT
 7000 CONTINUE
      DD(16)=DY(16)
      DD(18)=DY(18)
      DD(22)=DY(22)
       RETURN
 8000 CONTINUE
      PRINT 1,(Y(I),I=16,20),TI
    1 FORMAT(*1*1PE13.4)
      PRINT 2,X,EN,TE,AN,(Y(I),I=1,15)
    2 FORMAT(*,TIME=*,E15.8,* SEC....EN=*,E15.8,                  * ... T
     1E= *,E15.5,* ... AN= *,E15.8,//3(5E15.5/))
      PRINT 3,ENERG,TOTEOT
    3 FORMAT(* ENERG=*,E15.5,* TOTEOT=*,E15.5)
      STOP 777
       END
```

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```
      SUBROUTINE ELECON(T,DN,N)
*****************************************************************
*                                                               *
*   THIS SUBROUTINE CALCULATES THE TOTAL NUMBER OF ELECTRONS IN A *
*        SELF-CONSISTENT MANNER.                                *
*                                                               *
*****************************************************************
      COMMON /BLK4/COEF(15,15),EN
      COMMON/BLK5/EOT(14),ENERG,AN,TOTEOT
      COMMON/BLK1/DX,ALFRAC
      DIMENSION DN(20)
      EN=0
      KK=1
      DO 500 I=1,N
      IF(I.GE.N-2) KK=2
500    EN=EN+DN(I)*(I-KK)
      EN=EN+(1.-ALFRAC)*AN
      RETURN
      END
```

```
      SUBROUTINE MOENS
*****************************************************************************
*                                                                           *
*   THIS SUBROUTINE CALCULATES THE COEFFICIENTS FOR PRODUCTION (OR LOSS) OF *
*     EACH IONIC SPECIES.  THE COEFFICIENTS ARE IN UNITS OF CM**3/SEC SO THAT *
*                                                                           *
*         SUM OVER J(COEFF(I,J)*Y(J)/VOL)                                   *
*                                                                           *
*     GIVES THE DERIVATIVE OF Y(I).                                         *
*                                                                           *
*****************************************************************************
      COMMON/BLK1/TE,TI,YI(14,5)
      COMMON/BLK2/F(13,2,5)/BLK3/M(14,5)
      COMMON /BLK4/COEF(15,15),EN
      COMMON/BLK5/ A(13,5,2)
      COMMON/BLK1?/FNEFLO(210),DF(209),SPEC(210,2),VOL,AREA
      DO 500 I=1,15
      DO 500 J=1,15
  500 COEF(I,J)=0
      COEF(1,1)=-EN*(S(1,1)+ALPH(1,1))
      COEF(1,2)=EN*ALPH(2,1)
      DO 1000 N=2,12
      COEF(N,N-1)=EN*S(N-1,1)
      COEF(N,N)=-EN*(S(N,1)+ALPH(N,1))
 1000 COEF(N,N+1)=EN*ALPH(N+1,1)
      N=12
      COEF(N,12)=COEF(N,12)-EN*XX(12,1,2)
      COEF(N,14)=COEF(N,12)
      COEF(N,13)=VOL*A(12,3,1)+EN*YY(12,2,1)
      N=13
      COEF(N,12)=EN*XX(12,1,2)
      COEF(N,13)=-EN*(YY(12,2,1)+S(12,2))-VOL*A(12,3,1)
      COEF(N,14)=EN*ALPH(13,2)
      N=14
      COEF(N,12)= EN*S(12,1)
      COEF(N,13)= EN*S(12,2)
      COEF(N,14)=-EN*(S(13,1)+ALPH(13,1)+ALPH(13,2))
      COEF(N,15)=EN*ALPH(14,1)
      N=15
      COEF(N,14)=EN*S(13,1)
      COEF(N,15)=-EN*ALPH(14,1)
CCC ADJUST THE COEFFICIENT CONTRIBUTING TO THE LOSS OF EACH SPECIES SO THAT
CCC     IONS ARE CONSERVED
      DO 2000 K=1,15
      K2=K-2
      K3=K+2
      KK=MAX (K2,1)
      JJ=MIN (K3,15)
      COEF(K,K)=0
      DO 2000 J=KK,JJ
      IF(K.NE.J) COEF(K,K)=COEF(K,K)-COEF(J,K)
 2000 CONTINUE
      RETURN
      END
```

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```
      SUBROUTINE PAC(X,Y,DOD)
*****************************************************************************
*                                                                           *
*   THIS SUBROUTINE CALCULATES THE POWER RADIATED BY EACH LINE, AND, AFTER  *
*     CALLING SPECTRM, RETURNS THE FOLLOWING...                             *
*        DOD(1)=TOTAL LOSS DUE TO RADIATION                                 *
*        DOD(2)=LOSS FROM .  TO  .5 KEV                                     *
*        DOD(4)=LOSS FROM .5  TO  1. KEV                                    *
*        DOD(5)=LOSS FROM 1.  TO 1.4 KEV                                    *
*        DOD(6)=LOSS FROM 1.4 TO 1.8 KEV                                    *
*                                                                           *
*****************************************************************************
      COMMON/BLK1/TE,TT,YI(14,5)
      COMMON/BLK4/COEF(15,15),EN
      COMMON/BLK7/RINT(13,4),ENLIN(13,4),Y112P,Y11G
      COMMON/BLK8/ NOSP
      COMMON/BLK9/ A(13,5,2)
      COMMON/BLK11/ENERGY(210),DE(209),SPEC(210,2),VOL,AREA
      LOGICAL NOSP
      DIMENSION Y(22)
      DIMENSION DOD(7)
      IF(NOSP) GO TO 3000
      DO 1000 I=1,10
 1000 RINT(I,1)=EN*Y(I)*ENLIN(I,1)*XX(I,1,2)
      RINT(13,1)=EN*Y(14)*ENLIN(13,1)*XX(13,1,2)
      ATEMP=A(11,2,1)*VOL
      Y112P=Y(11)*(1./((ATEMP+EN*YY(11,2,1))/(EN*XX(11,1,2))+1.))
      Y11G=Y(11)-Y112P
      RINT(11,1)=Y11G *EN*ENLIN(11,1)*XX(11,1,2)
      RINT(11,2)=Y11G *EN*ENLIN(11,2)*XX(11,1,4)
      RINT(11,3)=Y112P*EN*ENLIN(11,3)*XX(11,2,3)
      RINT(11,4)=Y112P*EN*ENLIN(11,4)*XX(11,2,5)
      RINT(12,1)= .0
      RINT(12,2)=Y(12)*A(12,2,1)*ENLIN(12,2)*VOL
      RINT(12,3)=Y(12)*EN*ENLIN(12,3)*XX(12,1,4)
      RINT(12,4)=Y(12)*EN*ENLIN(12,4)*XX(12,2,3)
CCC CONVERT EV*CC/SEC TO WATTS
      DO 302 I=1,13
      DO 302 J=1,4
      RINT(I,J)=RINT(I,J)*1.602E-19/VOL
  302 CONTINUE
      CALL SPCTRM(Y,NFLAST)
      LAST=NFLAST-1
      DOD(1)=0
      DO 4000 NF=1,LAST
 4000 DOD(1)=DOD(1)-(SPEC(NF,2)+SPEC(NF+1,2))*DE(NF)
      DOD(1)=DOD(1)-2.*SPEC(NFLAST,2)*TE
      DOD(1)=.5*DOD(1)/1.602E-19
      DOD(2)=0.
      DO 5000 L=1,113
 5000 DOD(2)=DOD(2)+(SPEC(L,2)+SPEC(L+1,2))*DE(L)
      DOD(2)=.5*DOD(2)
      DOD(4)=0.
      DO 6000 L=114,133
 6000 DOD(4)=DOD(4)+(SPEC(L,2)+SPEC(L+1,2))*DE(L)
      DOD(4)=.5*DOD(4)
      DOD(5)=0.
      DO 7000 L=134,149
 7000 DOD(5)=DOD(5)+(SPEC(L,2)+SPEC(L+1,2))*DE(L)
      DOD(5)=.5*DOD(5)
      DOD(6)=0.
      DO 8000 L=150,199
 8000 DOD(6)=DOD(6)+(SPEC(L,2)+SPEC(L+1,2))*DE(L)
      DOD(6)=.5*DOD(6)
      RETURN
 3000 CONTINUE
      DO 2000 J=1,6
 2000 DOD(J)=
      RETURN
      END
```

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```
      SUBROUTINE SPECTRM(Y,NPLAST)
*****************************************************************************
*                                                                           *
*   FROM THE POWER RADIATED BY EACH LINE SUPPLIED BY RAD, THIS SUBROUTINE   *
*     CALCULATES THE SPECTRUM DUE TO RECOMBINATION, BREMSSTRAHLUNG, AND THE *
*     LINES -- ALL LIMITED BY THE APPROPRIATE BLACKBODY SPECTRUM.           *
*                                                                           *
*****************************************************************************
      COMMON/BLK1/TE,TI,XI(14,5)
      COMMON/BLK2/RCOE(15,15),RN
      COMMON /BLK3/RCT(14),RFRO,RN,TOTRCT
      COMMON/BLK7/RTNT(13,4),RNLIN(13,4),Y112R,Y11C
      COMMON/BLK1 /ENERLO(210),DE(300),SPEC(210,2),VOL,AREA
      COMMON /BLK12/ NA(2),TABX(15),TABY(50)
      COMMON/BLK17/RX,RLFRAC
      DIMENSION X1(2)
      DIMENSION Y(22)
      HC=1.2454
      XH=13.595
      SPEC(1,1)=0.
      SPEC(1,2)=1.
      GRF=1.
      DO 1000 NP=1,210
      X=ENERLO(NP)
      IF(X.LE.0.) GO TO 1000
CCC     GET BR SPECTRUM IN W/EV GIVEN E IN EV
      FACT1=X/TE
      IF(FACT1.GT.100.) GO TO 5000
      BRSPEC=6.031E7*AREA*Y*X*X/(EXP(FACT1)-1.)*3.14159
      SPEC(NP,2)=0.
      XN=3.
CCC     GET RECOMB AND BREM IN W/EV GIVEN E IN EV
      DO 4000 K=1,13
      FACT2=(AINT(XI(K,1)+.5)-X)/TE
      IF(FACT2.GT.100.) GO TO 4000
      J=K+1
      DEL=K
      IF(K.LE.3) GO TO 4100
      DEL=K-3
      XN=2.
      IF(K.LE.11) GO TO 4100
      J=K+2
      DEL=K-11
      XN=1.
 4100 SPEC(NP,2)=SPEC(NP,2)+Y(J)*XI(K,1)*XI(K,1)*DEL*GRF*EXP(FACT2)/XN
 4000 CONTINUE
      FACT2=(AINT(XI(12,2)+.5)-X)/TE
      IF(FACT2.GT.100.) GO TO 4001
      SPEC(NP,2)=SPEC(NP,2)+Y(14)*XI(12,2)*XI(12,2)*GRF*EXP(FACT2)
 4001 CONTINUE
      SPEC(NP,2)=SPEC(NP,2)/TE
      K=1
      SUM=0.
      XA(1)=FACT1
      DO 100 I=2,15
      IF(I.GE.13) K=2
      Z=I-K
      XA(2)=Z*Z*XH/TE
      GRF=TPLKCC(1,2,TABY,TABX,NA,XA)
  100 SUM=SUM+Y(I)*Z*Z*GRF
      SPEC(NP,2)=SPEC(NP,2)+SUM*XH*EXP(-X/TE)
      SPEC(NP,2)=SPEC(NP,2)*4.112-33/VOL*RX/SQRT(XH*TE)
      XA(2)=XH/TE
      GRF=TPLKCC(1,2,TABY,TABX,NA,XA)                                   IMPURITY
      SPEC(NP,2)=SPEC(NP,2)+4.112-33*RX*GRF*AN*SQRT(XH/TE)              IMPURITY
     1   *EXP(-X/TE)/VOL*(1.-DLFRAC)                                    IMPURITY
      IF(SPEC(NP,2).LT.BRSPEC) GO TO 3000                               IMPURITY
CCC     GET BREMSSTRAHLUNG IN W/EV GIVEN BINT IN W
      DO 20 I=1,13
```

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```
      DO 200 L=1,4
      IF(RINT(I,L).LE. .) GO TO 3100
      IF(ENLIN(I,L).LE. .) GO TO 2000
      XLN=HC/ENLIN(I,L)
      DXC=9.07E-6*XLN*SQRT(TE)
      FACT=(ABS(XLN-HC/X)/DXC)**2
      IF(FACT.GT.100.) GO TO 2000
      TEMP=RINT(I,L)*6.326E3/X/X/DXC*EXP(-FACT)
      SPEC(NP,2)=SPEC(NP,2)+TEMP
      IF(SPEC(NP,2).GT.3*SPEC) GO TO 3000
 2000 CONTINUE
      GO TO 1000
 3000 SPEC(NP,2)=3*SPEC
 1000 CONTINUE
      RETURN
 5000 NPLAST=NP-1
      DO 6000 I=NP,210
 6000 SPEC(I,2)=0.
      RETURN
      END
```

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```
        BLOCK DATA
      COMMON/BLK1/TE,TI,XT(14,5)
      COMMON/BLK2/S(10,2,5)/BLK3/W(14,5)
      COMMON/BLK9/ A(13,5,2)
      COMMON/BLK10/ENERGY(210),DE(209),SPEC(210,2),VOL,AREA
      COMMON /BLK12/ TAX(0),TAX(16),TAXY(60)
      DATA NA/1 ,6/
      DATA TAGX/ .001, .01, .1, 1., 5., 10., 20., 30., 100., 200.,
     1   .01, .1, 1., 10., 1 .., 1.E3 /
      DATA TAGY/ 4.35, 4.1, 3.8, 3.25, 2.7, 2.05, 3.., 2.98, 2.7, 2.25,
     1   1.8, 1.5, 1.9, 1.05, 1.0, 1.0, 1.3, 1.2, .97, 1.18,
     2   1.20, 1.2, 1.11, 1.05, .935, .74, 1.18, 1.14, 1.078, 1.037,
     3   .79, .59, .87, 1.17, 1.09, 1.04, .29, .45, .94, 1.11,
     4   1.09, 1.45, .24, .78, .76, 1.09, 1. 95, 1.35, .13, .37,
     5   .63, .94, 1.15, 1. 8, .14, .02, .53, .8, 1.3, 1.12  /
      DATA XI/5.034,10.83,26.44,119.9,153.77,190.42,241.93,
     1 285.13,330.1,369.3,441.9,2.85,5,3344.,  ,2.994,11.83,21.44,42.99,
     2 109.77,15 .43,216.93,250.17,298.1,361.5,419.9,599.5,579.,11*0,
     3 189.9,515.5,12* .,156.9,445.5,10*0.,134.9,7*0./
      DATA F/28* ,.115,1.04,.775,.2,.13,.21,.74,.11,.5,.297,.116,.7,.55,
     124*0,1.5-5,11*0,.03,.1,11*0,.33,.790 37*0,.672,2*0./
      DATA W/0.,1.,2.,1.,6.,9.,4.,9.,5.,1., .,1.,2., ,2.,3.,8.,3.,2.,9.,
     112.,3.,8.,7.,6.,7.,6.,11*0.,9.,12*0,5.,3.,12*0.,11.,3*0/
      DATA A/13*0,1.475E8,1.469E9,5.847E8,1.751 .3.251E10,1.471E10,4.129E9,7.551E10
     1,1.651E10,5.759E9,3.759E9,2. 3514,2.113E14,11*0,9.655E9,11*0,3.145E11,
     22.785E13,5.*0,1.465E11,9.251 ,24*0,9.9E11,2*0/
      DATA DE/ 50*1., 2*1 ., 2*3., 2*1., 3., 2*4., 2*1., 4., 15., 9.,
     1  1., 5., 15., 17., 1., 16., 15., 4., 1., 1., 15., 10., ., 7*1.,
     2  5., 1., 8., 4., 2*1., 4., 15., 9., 1., 5., 2*15., 9., 1., 5.,
     3  3*15., 19., 1., 15., 15., 11., 1., 13., 2*15., 10., 2*25., 45.
     3 ,1., 29., 37*25., 75.,
     4  4., 2*1., 4., 4 ., 4*11., 4., 2*1., 4., 2*5., 4., 2*1., 4.,
     5  11*1., 4., 2*1., 4., 3*1 ., 45., 4*5., 85., 1., 212., 1.,
     6  101., 4.725E4, 8*5.,64/
      END
```

```
      FUNCTION S(L,M)
CCC IONIZATION COEFFICIENT IN CM**3/SEC FOR IONIZATION FROM ION L (L=1 MEANS
CCC       NEUTRAL,L=14 MEANS FULLY STRIPPED), LEVEL M
      COMMON/BLK1/TE,TI,XI(14,5)
      IF(L.LE.0)GO TO 50
      IF(XI(L,M).LE. )GO TO 50
      S=1.64E-6*EXP(-XI(L,M)/TE)/(XI(L,M)*SQRT(TE))
      RETURN
   50 S=0
      RETURN
      END


      FUNCTION ALPH(L,M)
CCC RECOMBINATION COEFFICIENT IN CM**3/SEC FOR RECOMBINATION TO ION L, LEVEL M
CCC       FROM THE GROUND LEVEL OF ION L+1
      COMMON/BLK1/TE,TI,XI(14,5)
      COMMON/BLK4/COEF(13,15),EN                                        LUBIN
      COMMON/BLK1/ ENFELC(21 ),DF(2,9),SEFC(216,2),VOL,AREA             LUBIN
      ITEST=0
      GO TO 10
      ENTRY ALPHFAC
      ITEST=1
   10 IF(L.LE.1) GO TO 50
      IF(XI(L-1,M).LE.0)GO TO 50
      Z=L-1
      IF(L.GE.13) Z=L-2
      XLAM=XI(L-1,M)/TE
      XLAM2=SQRT(XLAM)
      ALPH=5.2E-14*Z*XLAM2*(.429+.5*ALOG(XLAM)+.469/XLAM2)
      IF(ITEST.EQ.1) RETURN
CCC ADD 3-BODY RECOMBINATION                                            LUBIN
      PRIMEN=2.                                                         LUBIN
      ALPH=ALPH+1.4E-31*EXP(PRIMEN/Z)**6*(XI(L-1,M)/TE)**2              LUBIN
     1   *EXP(XI(L-1,M)/(PRIMEN+1.)**2/TE)/VOL                          LUBIN
      RETURN
   50 ALPH=0
      RETURN
      END
```

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```
      FUNCTION XX(L,M,N)
CCC EXCITATION COEFFICIENT IN CM**3/SEC FOR EXCITATION FROM LEVEL M TO N
CCC       IN ION L
      COMMON/BLK1/TE,TI,XI(14,5)
      COMMON/BLK2/F(13,2,5)/BLK3/W(14,5)
      XE=ABS(XI(L,M)-XI(L,N))
      IF(XE.LE.0)GO TO 50
      FACT1=XE/TE
      IF(FACT1.GT.2 (.) GO TO 50
      XX=6.E-6*F(L,M,N)*EXP(-FACT1)/(XE*SQRT(TE))
      RETURN
   50 XX=0
      RETURN
      END


      FUNCTION YY(L,N,M)
CCC DE-EXCITATION COEFFICIENT IN CM**3/SEC FOR DE-EXCITATION FROM LEVEL N TO M
      COMMON/BLK1/TE,TI,XI(14,5)
      COMMON/BLK2/F(13,2,5)/BLK3/W(14,5)
      IF(W(L,N).LE.0)GO TO 5
      XE=ABS(XI(L,M)-XI(L,N))
      IF(XE.LE.0)GO TO 50
      YY=6.E-6*W(L,M)*F(L,M,N)/(XE*SQRT(TE)*W(L,N))
      RETURN
   50 YY=0
      RETURN
      END
```

```
      SUBROUTINE SET(N,X,Y,DX,F,DIS,MCOF,DXMAX,DXMIN)
      COMMON /CLKS/ECT(14),DNEFC,AN,ICTECT
      DIMENSION Y(N)
      DIMENSION C(9,5), W(9,5)
      DIMENSION W13(20)
      EXTERNAL F
      LOGICAL MCOF,COFE
      DATA AMAX/5./
      DATA EPF/1 -7./
      DATA DXF/3./
      XSIG=1 .**(IFIX(ALOG10(AN)-12.))
      M=N
      IF (M.LT.1.OR.M.GT.NMAX) GO TO 20
      PA=DIS
      COOF=MCOF
      HMAX=DXMAX
      HMIN=DXMIN
      EP=EPF
      BETA=DXF
      K=0
      K2=0
      DO 10 I=1,M
      IF(Y(I).LE. .) Y(I)=0.
10    W(I,1)=Y(I)
      CALL F(M,X,Y,C(1,F))
      RETURN
20    PRINT 30
30    FORMAT(55H1SUBROUTINE SET HAS ARGUMENT OUT-OF-RANGE. SEE LISTING.)
      CALL SYSTEM(20,1L )
      RETURN
      ENTRY STEP
40    XC=X
      H=DX
      IF (K.NE.0) IF (K-2) 50,50,110
      XP=XC
      DO 45 I=1,M
45    W(I,5)=W(I,1)
50    K1=4-K
      DO 70 I=1,M
      DO 60 J=K1,4
60    C(I,J)=C(I,J+1)
      W(I,2)=H*C(I,4)
      W(I,1)=W(I,1)+.5*W(I,2)
      IF(W(I,1).LE.0.) W(I,1)=0.
70    Y(I)=W(I,1)
      X=XC+.5*H
      CALL F(M,X,Y,C(1,5))
      DO 80 I=1,M
      W(I,3)=H*C(I,5)
      W(I,1)=W(I,1)+.5*(W(I,3)-W(I,2))
      IF(W(I,1).LE.0.) W(I,1)=0.
80    Y(I)=W(I,1)
      CALL F(M,X,Y,C(1,5))
      DO 90 I=1,M
      W(I,4)=H*C(I,5)
      W(I,1)=W(I,1)+W(I,4)-.5*W(I,3)
      IF(W(I,1).LE.0.) W(I,1)=0.
90    Y(I)=W(I,1)
      X=XC+H
      CALL F(M,X,Y,C(1,5))
      DO 100 I=1,M
      W(I,1)=W(I,1)-W(I,4)+.1666666666666667*(W(I,2)+2.*(W(I,3)+W(I,4))+H
     1*C(I,5))
      IF(W(I,1).LE.0.) W(I,1)=0.
100   Y(I)=W(I,1)
      K=K+1
      K1=K
      CALL F(M,X,Y,C(1,5))
      RETURN
110   DO 120 I=1,M
      W(I,2)=W(I,1)
      DO 120 J=1,4
```

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```
120   D(I,J)=D(I,J+1)                                                  DFEQ.109
      W(I,3)=W(I,2)+.41666666666667E-1*H*(55.*D(I,4)-59.*D(I,3)+37.*D(IDFEQ.110
     1,2)-9.*D(I,1))                                                   DFEQ.111
      IF(W(I,3).LE. .) W(I,3)=0.
130   Y(I)=W(I,3)                                                      DFEQ.112
      X=X0+H                                                           DFEQ.113
      CALL F(M,X,Y,D(1,5))                                             DFEQ.114
      DO 140 I=1,M                                                     DFEQ.115
      W(I,1)=W(I,3)+.41666666666667E-1*H*(9.*D(I,5)+19.*D(I,4)         DFEQ.116
     1-5.*D(I,3)+D(I,2))                                               DFEQ.117
      IF(W(I,1).LE.0.) W(I,1)=0.
140   Y(I)=W(I,1)                                                      DFEQ.118
      CALL F(M,X,Y,D(1,5))                                             DFEQ.119
      IF (CODE) RETURN                                                 DFEQ.120
      EPR=0.                                                           DFEQ.121
      DO 150 I=1,M                                                     DFEQ.122
      EPR=AMAX1(EPR,ABS(W(I,1)-W(I,3))/(14.*AMAX1(ABS(W(I,1)),XSIG)))
150   CONTINUE
      IF (EPR.GE.RA) IF (HMIN-ABS(H)) 160,155,155                      DFEQ.124
      K1=0                                                             DFEQ.125
      IF (RB*EPR.LT.RA) IF (HMAX-ABS(H)) 155,155,210                   DFEQ.126
155   K2=0                                                             DFEQ.127
      RETURN                                                           DFEQ.128
160   IF (K1.NE.0) GO TO 180                                           DFEQ.129
      DO 170 I=1,M                                                     DFEQ.130
      W(I,1)=W(I,5)                                                    DFEQ.131
170   D(I,5)=D(I,4)                                                    DFEQ.132
      X=X0                                                             DFEQ.133
      GO TO 200                                                        DFEQ.134
180   DO 190 I=1,M                                                     DFEQ.135
      W(I,1)=W(I,2)                                                    DFEQ.136
190   D(I,5)=D(I,4)                                                    DFEQ.137
      X=X0                                                             DFEQ.138
200   K=0                                                              DFEQ.139
      K2=0                                                             DFEQ.140
      DX=SIGN(AMAX1(ABS(H)/BETA,HMIN),H)                               DFEQ.141
      GO TO 40                                                         DFEQ.142
210   K2=K2+1                                                          DFEQ.143
      IF (K2.LT.6) RETURN                                              DFEQ.144
      K=0                                                              DFEQ.145
      DX=SIGN(AMIN1(ABS(H)*BETA,HMAX),H)                               DFEQ.146
      K2=0                                                             DFEQ.147
      RETURN                                                           DFEQ.148
      END                                                              DFEQ.149
```

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```
      SUBROUTINE EXIT                                                  CALCOMP
      CALL PLOT(X,X,40)                                                CALCOMP
      END                                                              CALCOMP

      SUBROUTINE BIXBAM(XAX,YAY)                                       CALCOMP
      REAL MAR1,MAR2                                                   CALCOMP
      MAR1=.7                                                          CALCOMP
      MAR2=.3                                                          CALCOMP
      CALL PLOT(0.,0.,3)                                               CALCOMP
      CALL PLOT(-MAR1,-MAR1,2)                                         CALCOMP
      CALL PLOT(XAX+MAR2,-MAR1,2)                                      CALCOMP
      CALL PLOT(XAX+MAR2,YAY+MAR2,2)                                   CALCOMP
      CALL PLOT(-MAR1,YAY+MAR2,2)                                      CALCOMP
      CALL PLOT(-MAR1,-MAR1,2)                                         CALCOMP
      CALL PLOT(0.,0.,3)                                               CALCOMP
      RETURN                                                           CALCOMP
      END                                                              CALCOMP
```

Appendix C

Gaunt Factors

The free-free Gaunt factors have been extracted from the graphical presentation of Karzas and Latter (Ref 6:172-174).

Table V
Free-Free Gaunt Factors

	$\gamma^2 \equiv Z^2\chi_H/T_e$					
$U \equiv h\nu/T_e$	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}
.001	4.25	4.1	3.8	3.25	2.7	2.05
.01	3.0	2.98	2.7	2.25	1.8	1.5
.1	1.9	1.95	1.8	1.5	1.3	1.2
1.	.97	1.18	1.29	1.2	1.11	1.05
5.	.525	.74	1.08	1.14	1.078	1.037
10.	.39	.59	.97	1.13	1.08	1.04
20.	.29	.45	.84	1.11	1.09	1.045
30.	.24	.38	.76	1.09	1.095	1.05
100.	.18	.37	.63	.94	1.15	1.08
200.	.14	.22	.53	.8	1.2	1.12

The bound-free Gaunt factors have been integrated over a Maxwellian energy distribution to eliminate the dependence of g_{bf} on the electron energy. Karzas and Latter give a table for:

$$g_{bf} = g_{bf}[\, E_e/Z^2\chi_H \,,\, n \,] \tag{73}$$

for recombination into the nth shell of an ion.

Now,

$$dn_e = \frac{1}{T_e} \exp[\ -E_e/T_e\ ]\ dE_e \tag{74}$$

but one can define the following parameters:

$$\gamma^2 \equiv Z^2\chi_H/T_e \qquad \text{and} \qquad U \equiv E_e/Z^2\chi_H \tag{75}$$

such that:

$$dn_e = \frac{\gamma^2}{Z^2\chi_H} \exp[\ -U\gamma^2\ ]\ dE_e \tag{76}$$

From Eq. (75), it may be seen that:

$$dE_e = Z^2\chi_H\ dU \tag{77}$$

and consequently one finds:

$$dn_e = \gamma^2 \exp[\ -U\gamma^2\ ]\ dU \tag{78}$$

Finally, the bound-free Gaunt factor, averaged over a Maxwellian electron energy distribution is given by:

$$\langle g_{bf}(n,\gamma^2)\rangle = \int_0^\infty g_{bf}(n,U)\ \gamma^2 \exp[\ -U\gamma^2\ ]\ dU \tag{79}$$

Equation (79) was integrated numerically to give the results shown in Table VI on page 77.

Table VI

Bound-Free Gaunt Factors

	$\gamma^2 \equiv Z^2\chi_H/T_e$					
n	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}
1	.6703	.9624	.93121	.88476	.8872	.90033
2	.67896	1.0064	1.0359	.99364	.97936	.98985
3	.6809	1.0174	1.0703	1.0425	1.0189	1.0257
4	.6816	1.0216	1.0858	1.0704	1.0426	1.0457

VITA

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