MIXERG - An Equation of State and Opacity Computer Code

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R.R. Peterson and G.A. Moses

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

http://fti.neep.wisc.edu

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Robert R. Peterson and Gregory A. Moses
Department of Nuclear Engineering
University of Wisconsin, Madison, WI · U.S.A.

Program Summary

Title of program: MIXERG.

Catalogue number:

Program obtainable from: CPC Program Library, Queen's University of Belfast, Northern Ireland.

Computer: Univac 1110; Installation: Madison Academic Computing Center, University of Wisconsin, Madison, Wisconsin, U.S.A.

Operating system: Univac 1110 EXEC VIII.

Programming language: FORTRAN.

High speed storage required: 64,000 words.

No. of bits in a word: 36.

Overlay structure: None.

No. of magnetic tapes required: None.

Other peripherals used: Line printer, up to ten mass storage files or magnetic tapes.

No. of cards in combined program and test deck: 2485.

Card punching code: EBCDIC.

Key words: Semi-classical atomic physics, ionization, group opacities.

Nature of the physical problem: The calculation of group opacities and equations-of-state of gases is important to many areas of applied physics.

Specifically, to correctly predict the propagation of heat and shock waves through gases, one must have optical data, ionization states and internal energy densities for the gas.(1-4) MIXERG is a computer code which has been written to provide low cost data for mixtures of up to five gases. The optical data consists of Rosseland and Planck mean opacities or mean free paths, in single group and in multigroup form.

Method of solution: The ionization state of the mixture of gases is the first calculation done for each combination of plasma density and plasma temperature. This is done using the Saha model when the density is high and the temperature is low and is done using the Coronal model otherwise. Care is taken to insure that the transition between models is smooth. With the ionization state as a function of temperature, the plasma internal energy density, the heat capacity and the temperature derivative of the ionization state may be calculated. Once the state of the gas has been determined, MIXERG uses a semi-classical model to find the absorption coefficient of the plasma as a function of photon energy where photo-ionization, inverse Bremmstrahlung, Thomson scattering, absorption by plasma waves and atomic line absorption are considered as absorption mechanisms. This absorption coefficient is integrated with a specially designed method to give the opacities of the plasma. The output data is stored in a manner which is easily readable by hydrodynamic codes such as FIRE.(5)

Restrictions on the complexity of the problem: The ionization models used are only valid when the density is low enough that the electron wave functions are single atom wave functions. This means that the plasma density must be significantly less than the solid density. These models are also invalid if the plasma is not in local thermodynamic equilibrium. This sets a lower limit on the density. There are also limitations due to the absorption model. The most important inaccuracies occur at photon energies below 1 eV. This is particularly due to neglect of molecular states which may be dominant at these low energies but also comes from inaccuracies in the models used at these energies. This means that low energy group opacities and low radiation temperature single group opacities may be inaccurate.

Typical running time: On the UNIVAC 1110 at the Madison Academic Computer Center at the University of Wisconsin, MIXERG requires 0.4 seconds of CPU time for each combination of plasma density, plasma temperature and radiation temperature.

Unusual features of the program: The MIXERG code is written in standard FORTRAN except for the manner in which the COMMON blocks are used. The COMMON blocks are listed only at the beginning of the program, where they are equated to INCLUDE statements. Thereafter, the INCLUDE statements are used to represent the COMMON blocks. The use of INCLUDE statements abbreviates the listing of a program that uses the same COMMON blocks in many subroutines, because an INCLUDE statement occupies only one line, whereas a COMMON block might occupy many lines. INCLUDE statements only have meaning to a UNIVAC compiler, so the user may wish to replace them with the respective COMMON blocks.

References:

[1] M.A. Sweeney and D.L. Cook, "Blast-Wave Kinetics and Thermal Transport in a Particle-Beam Reactor Chamber", Bull. APS 24, 1072 (1979).

[2] L.A. Glenn, "The Influence of Radiation Transport on Lithium Motion in an ICF Reactor", Lawrence Livermore Laboratory Report UCID-18573, March 6, 1980.

[3] G.A. Moses and R.R. Peterson, "First Wall Protection in ICF Reactors by Inert Cavity Gases", University of Wisconsin Fusion Engineering Program Report UWFDM-323 (October 1979); "First Wall Protection in Particle Beam Fusion Reactors by Inert Cavity Gases", Nucl. Fus. 20, 859 (1980).

[4] R.R. Peterson, G.A. Moses, and G.W. Cooper, "Cavity Gas Analysis for Light Ion Beam Fusion Reactors", Nucl. Tech./Fusion 1, 377 (1981).

[5] T.J. McCarville, R.R. Peterson, and G.A. Moses,"Improvements in the FIRE Code for Simulating the Response of a Cavity Gas to Inertial Confinement Fusion Target Explosions", University of Wisconsin Fusion Engineering Program Report UWFDM-407 (June 1981, revised February 1982), submitted to Computer Physics Communications for publication.

I. Introduction

The calculation of opacities and equations of state of gases is important to many areas of applied physics. Specifically, in the design of inertial confinement fusion reactor target chambers, one must be able to predict the propagation of the target explosion generated fireball through the target chamber gas to the first wall.(1-5) To do this calculation correctly, one must have optical data, ionization states and internal energy densities for the target chamber gas.

MIXERG is a computer code which has been written to provide low cost data for mixtures of up to five gases. The optical data consists of Rosseland and Planck mean opacities or mean free paths, either in single group form or broken up into 20 or less frequency groups.

We have previously reported work done on the calculation of equations of state and optical data for single species monatomic gases.(6) However, we have subsequently found that a multiple species gas might better protect the first wall of a light ion beam fusion reactor from the fireball.(4) Also, target debris and matter evaporated from the reactor chamber(1) may be mixed with the cavity gas, making the single species gas an unrealistic approximation. Thus, it became necessary for us to modify our single species computer code MFP(6) into a multiple species code, MIXER.(7)

MIXERG has several improvements over MIXER and MFP. It computes group opacities and allows the option of opacities instead of mean free paths. It also leads to more accurate and less expensive results and is easier to use than its predecessors. The physical model for ionization has been improved to allow the code to choose between Saha ionization and Coronal ionization. Calculations of the absorption coefficient include better models of atomic line absorption and consider plasma wave absorption. A new method of integration is used which makes MIXERG more efficient than its predecessors.

Section II describes the improved ionization models used in MIXERG and provides examples of equations of state and average ionization states. These examples graphically show under what circumstances the inclusion of the Coronal model makes a difference.

In Section III, the calculation of the absorption coefficient is described. The new model for line absorption is presented in detail as is the analysis of absorption by the plasma. Representative results are shown for the improved calculations.

The improved integration method is described in Section IV and sample results for the opacities are presented. Conclusions are made in Section V.

A manual for operation of MIXERG is provided in Appendix A. Appendix B contains the input and output for a sample run of MIXERG.

II. Ionization Model

The ionization of the plasma is calculated with a model which is valid up to almost solid density and down to densities where the collision frequencies are just high enough to allow the approximation of local thermodynamic equilibrium (LTE). The Coronal model(8) is used when the dominant form of recombination is radiative recombination, which is the case when

$$n_e < 10^{16} \ (T_e)^{7/2} \ \mathrm{cm}^{-3} \ . \qquad (1)$$

Here n_e is the electron density and T_e is the electron temperature in eV. If this expression is not true, three body recombination will dominate over radiative recombination and the Saha model(9) is used. In the cases where $n_e \sim 10^{16} \ (T_e)^{7/2}$, we use the formula

$$\overline{m} = (1-f)\,\overline{m}_s + f\overline{m}_c \,, \qquad (2)$$

where f is a number between 0 and 1 and is a function of density. As the electron density grows, f approaches 0; as it decreases, f approaches 1 and at $n_e = 10^{16}\,T_e^{7/2}$, f = 1/2. In equation (2), $\overline{m}$ is the average ionization state, $\overline{m}_c$ is the value calculated in the Coronal model and $\overline{m}_s$ is the value in the Saha model. This smooth transition between models is used because it avoids sharp changes in the equation-of-state which could cause numerical difficulties when these data are used in a hydrodynamics code.

Since $n_e = \overline{m}\,n_i$ where n_i is the ion density, the choice of ionization model made by equation (1) is dependent upon the ionization state calculation so that this calculation is iterated until a stable solution is obtained for $\overline{m}$.

The Saha model for ionization has been discussed in the description of an earlier version of this code (MFP).(6) In the Saha model, the transcendental equation

$$I(\overline{m}_s + 1/2) = T_p \,\ln\left(\frac{AT_p^{3/2}}{n_e}\right) \qquad (3)$$

is solved for $\overline{m}_s$, where I(m) is a piecewise linear continuous extension of the ionization potential for the ionization of the mth electron from the atom. T_p is the plasma temperature and $A = 6.04 \times 10^{21}\ \mathrm{eV}^{-3/2}$. The densities of the six most populous ionization species follow a Gaussian distribution centered about $\overline{m}_s$. Since the solution of equation (3) is dependent upon the total electron density and since this code allows a mixture of up to five atomic species,(7) the average ionization state of each species is dependent upon ionization of the other species. Thus, equation (3) is solved iteratively until stable solutions, $\overline{m}_{sj}$, are obtained for all species j.

The average ionization state in the Coronal model is found from the reltionships(8)

$$n_{mj} = \left(\frac{S_{0,j}}{\alpha_{1,j}}\right) \left(\frac{S_{1,j}}{\alpha_{2,j}}\right) \cdots \left(\frac{S_{m-1,j}}{\alpha_{m,j}}\right) n_{oj} \tag{4}$$

$$n_{oj} = \left[1 + \sum_{m=1}^{Z_j} \left(\frac{S_{0,j}}{\alpha_{1,j}}\right) \left(\frac{S_{1,j}}{\alpha_{2,j}}\right) \cdots \left(\frac{S_{m-1,j}}{\alpha_{m,j}}\right)\right]^{-1} n_j \tag{5}$$

$$\frac{\alpha_{m+1,j}}{S_{m,j}} = 7.87 \times 10^{-9} \, \frac{I_j^2(m)}{\eta_{mj}} \left(\frac{I_j(m)}{T_p}\right)^{0.75} \exp\left(\frac{I_j(m)}{T_p}\right) . \tag{6}$$

Here, $S_{m,j}$ is the ionization rate of m-times ionized atoms of species j, $\alpha_{m,j}$, the recombination rate, η_{mj}, the number of outer shell electrons, n_{mj}, the population of atoms j which are m-times ionized and Z_j, the total number of electrons present in neutral atoms of species j. n_j is the number of atoms of species j. These equations are soluble in a straightforward manner and yield n_{mj} and the average ionization states of each atom species,

$$\overline{m}_{cj} = \frac{\sum\limits_{m=1}^{Z_j} n_{mj} \, m}{\sum\limits_{m=1}^{Z_j} n_{mj}} . \tag{7}$$

The main difference between the form of results obtained in the two models is that, in the Coronal model, the average ionization state is independent of ion density while it is a function of ion density in the Saha model. The physical reason for this is that both the collisional ionization and the radiative recombination rates are proportional to the density squared while the three body recombination rate is proportional to the density cubed. Thus, in the Coronal model, $S_{mj}/\alpha_{m-1,j}$ is independent of the ion density, while it is inversely porportional to the density in the Saha model. An example of the dependence of the ionization on the density is shown in Figure 1, where the average ionization state of argon, with a 0.2% impurity of sodium, is plotted against plasma temperature and total ion density. A curve where equation (1) is exactly satisfied is shown as the boundary between the regions in T_p-n_i space where the Coronal model and the Saha model are used. Points higher in density and lower in plasma temperature are seen to vary with density while those higher in temperature and lower in density are independent of density.

The energy density of the gas mixture is calculated from the ionization states. The energy of ionization, atomic excitation and particle kinetics are accounted for but the effects of degenerate particles and Madelung energies are neglected so that the results are not valid for solids. This is not an important limitation because the ionization calculations are not valid for solids either. Chemical energies, such as those of dissociation and molecular effects, are not included because the absorption model discussed in Section III does not address the problems of absorption during molecular transitions. The energy density versus total ion density and plasma temperature is shown in Figure 2 for argon with a 0.2% impurity of sodium.

III. Absorption Model

The absorption coefficient is found as a function of photon energy and ionization state using a semi-classical model.$^{(10)}$ This model was chosen because it is simple enough that the computing costs are reasonable while its accuracy is acceptable. The absorption mechanisms considered are photoionization, inverse Bremsstrahlung, bound state to bound state atomic line

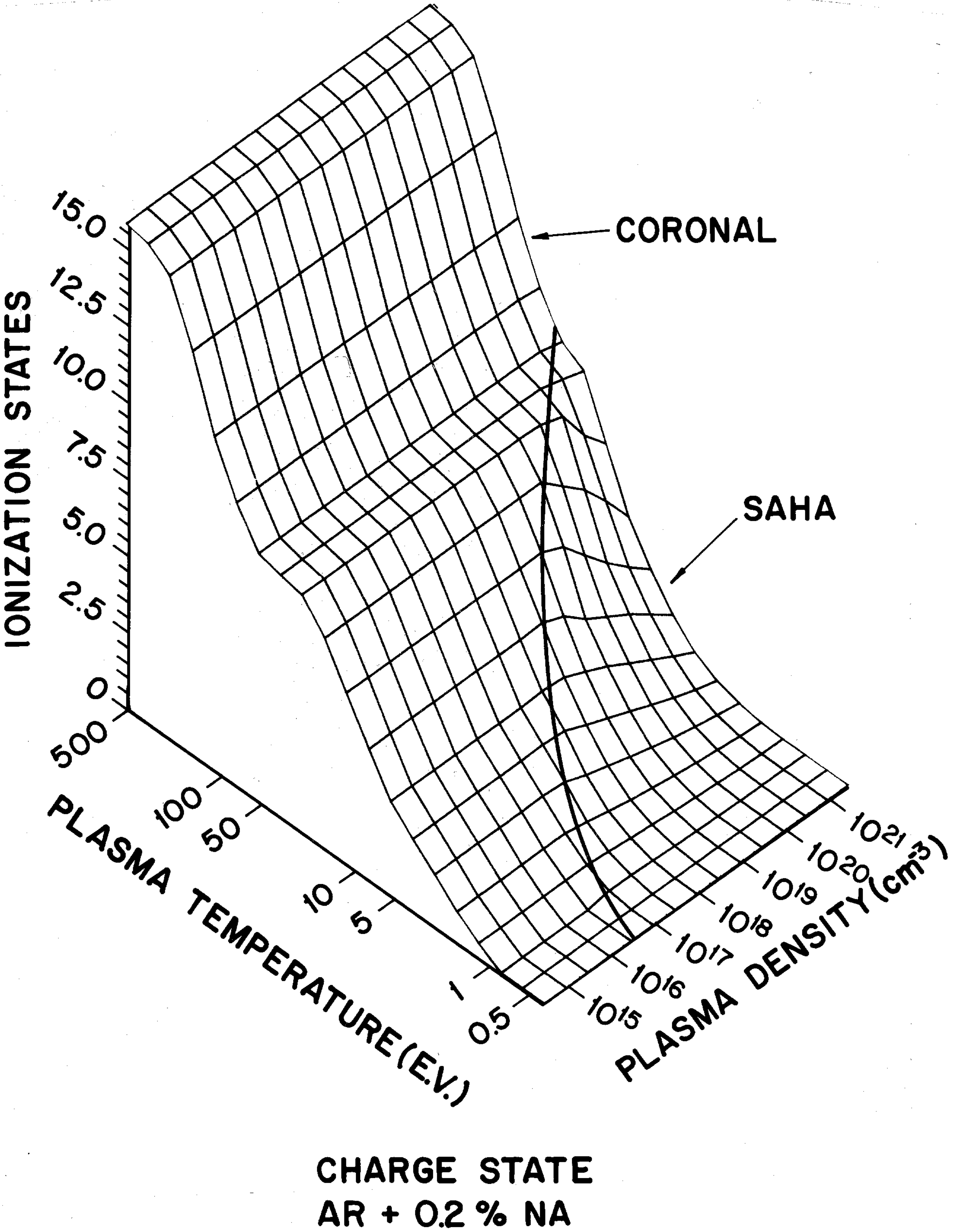
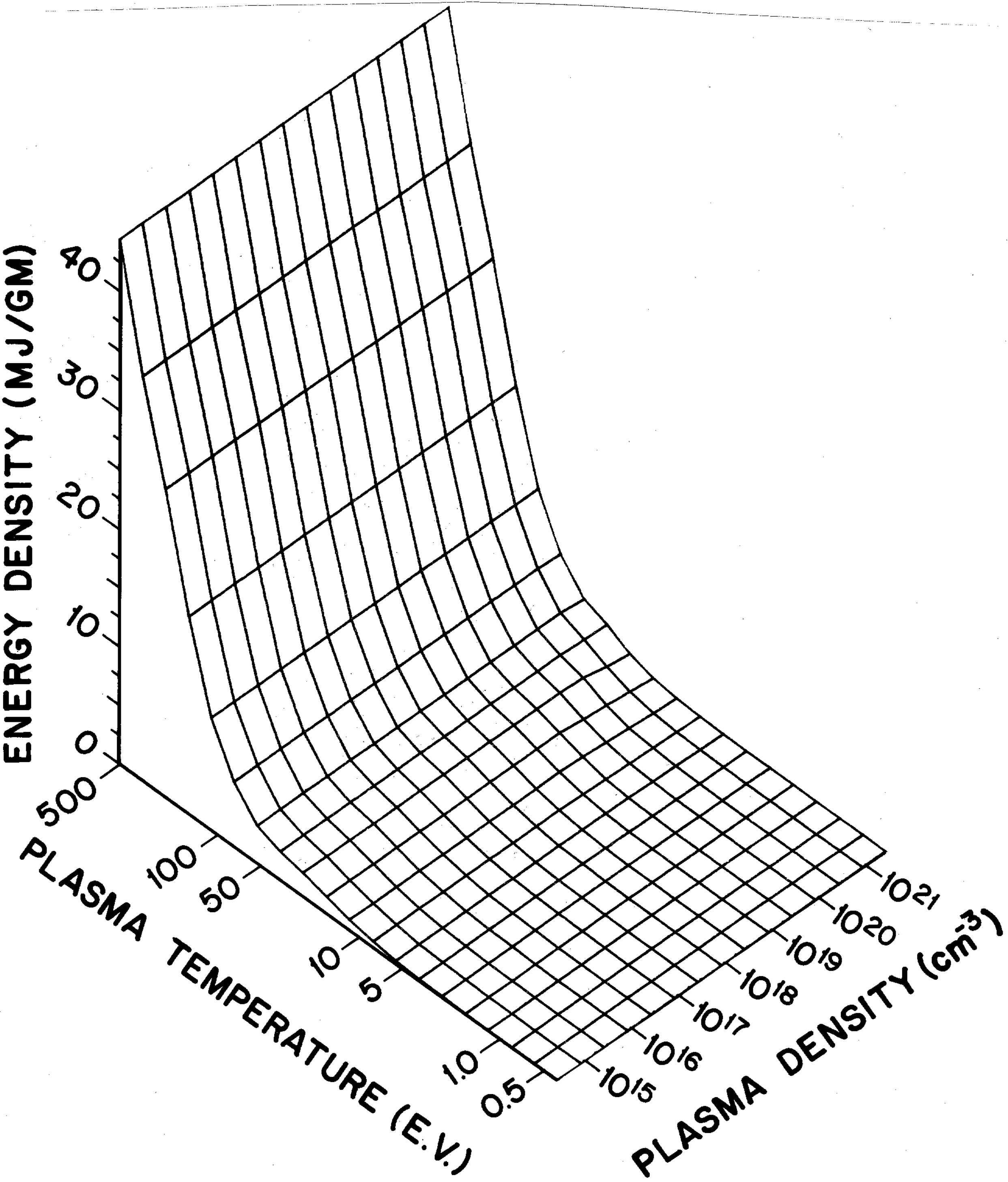


Figure 1 Ionization state of argon with a 0.2% impurity of sodium versus density and plasma temperature.



TOTAL INTERNAL ENERGY DENSITY
ARGON + 0.2 % SODIUM

Figure 2 Plasma internal energy density of argon with a 0.2% impurity of sodium versus density and plasma temperature.

absorption and absorption by plasma waves. Additionally, Thomson scattering is considered. Scattering is not considered in the absorption coefficient used to calculate the Planck opacities and mean free paths, but is used as a contribution to the Rosseland opacities and mean free paths. This is because the Rosseland opacity is traditionally used for radiation transport coefficients while the Planck is used for determination of emission and absorption rates.

The models for photo-ionization, inverse Bremsstrahlung and Thomson scattering are the same as in the earlier versions of the code.(6,7) The coefficients for these three types of absorption are taken as

$$\kappa_I(h\nu) = \sum_m \sum_{n=n^*(m)}^{\infty} \frac{64\pi^2}{3\sqrt{3}} \frac{e^{10} m_e (m)^4}{h^6 c \nu^3 n^5} n_i(m,n) \tag{8}$$

for photo-ionization,

$$\kappa_B(h\nu) = \sum_m \sum_{n=1}^{\infty} 2.4 \times 10^{-37} \frac{n_e g\, m^2 n_i(m,n)\, T_p^{1/2}}{(h\nu)^3} \tag{9}$$

for inverse Bremsstrahlung, and

$$\kappa_T(h\nu) = \left(\frac{e^2}{m_e c^2}\right)^2 \frac{8\pi}{3} n_e \tag{10}$$

for Thomson scattering. Here, m_e is the electron mass, h is Planck's constant and $n_i(m,n)$ is the density of atoms of type i, ionization state m and principal quantum number n, g is the Gaunt factor, e is the electronic charge and c is the speed of light. These processes are discussed in detail in discussions of the earlier codes and will not be dealt with here.

The treatment of atomic line absorption is much different in MIXERG from that in previous versions of the code. The model used for line absorption is somewhat different in the calculations of the Rosseland opacities from that used in the Planck opacities. The physical models are the same but, for numerical reasons, the actual expressions used are different.

The Rosseland opacities are most generally defined by the integral,(11)

$$\frac{1}{\sigma_R^n} \equiv \rho \frac{\int_{h\nu_n}^{h\nu_{n+1}} \frac{1}{\kappa(h\nu)} \frac{dB(h\nu)}{dT_R} \, dh\nu}{\int_{h\nu_n}^{h\nu_{n+1}} \frac{\partial B(h\nu)}{\partial T_R} \, dh\nu} , \tag{11}$$

where σ_R is the Rosseland opacity, $\kappa(h\nu)$ is the total absorption coefficient, $B(h\nu)$ is the Planck spectrum, T_R is the radiation temperature, ρ is the plasma mass density, and $h\nu_n$ is the nth frequency group boundary. If there is a single group for the whole frequency spectrum the limits to the integrations are 0 and ∞. The Planck opacities are defined as

$$\sigma_p^n \equiv \frac{1}{\rho} \frac{\int_{h\nu_n}^{h\nu_{n+1}} \kappa(h\nu) \, B(h\nu) \, dh\nu}{\int_{h\nu_n}^{h\nu_{n+1}} B(h\nu) \, dh\nu} . \tag{12}$$

There are numerical differences between equations (11) and (12) which require close attention. The inverse of the absorption coefficient used in equation (11) makes the integration over an absorption line difficult because the "wings" of the lines are more important than the line center.(12) The calculation of line absorption away from the center of the line must include Doppler broadening, the natural widths of the atomic energy levels and Stark broadening. The calculation of the absorption in the wings is straightforward as long as only Doppler and natural broadening are important because then, the well-known Voight profile may be used. If the material has a density much greater than the solid density, Stark broadening makes the calculation much more difficult. In MIXERG the density is kept below the solid density but many lines are considered so that, to avoid unacceptably large computing costs, the absorption coefficient cannot be calculated at many photon energies for each line. This would be necessary in equation (11) if the Voight profile(13) is used for the line shape. The method used in MIXERG is to reduce the integral in equation (11) to a function of parameters of the plasma and radiation field. The integration to obtain this function, which is done beforehand, may be done with many integration points for each line to properly obtain the contribution of absorption in the "wings". The line shape of the absorption coefficient near the line center is then taken to be a rectangular shape whose maximum value is adjusted to give the proper value for the Rosseland opacity. The advantage of this method is that the integration now only needs a few points. The line shape of the absorption coefficient for the Planck opacity is also taken to be a rectangular profile but the maximum is now that which provides the correct value for equation (12). Thus, two different absorption coefficients are used for the line contributions to the Planck and Rosseland mean opacities. Additionally, the Planck opacity contains no contributions from scattering.

The method prescribed in the preceding paragraph has been followed for absorption coefficients calculated in the semi-classical model. The atomic line absorption coefficient in this model is

$$\kappa_L\ (h\nu) = \sum_m \sum_{n=1}^{\infty} \sum_{n'=n+1}^{\infty} \left(\frac{h\pi^{1/2} e^2 f_{nn'} n_i(m,n)}{m_e c\ \Delta h\nu_D}\right) H(a,v) \qquad (13)$$

where $f_{nn'}$ is the oscillator strength for the transition from principal quantum number n to n'. The oscillator strength is obtained from tabulated values(14) for low n and n' transitions and in the semi-classical model(6) otherwise.

The Voight function(13) is defined as

$$H(a,v) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} dy \frac{e^{-y^2}}{(v-y)^2+a^2} \qquad (14)$$

and

$$a \equiv \frac{h\Gamma}{4\pi\Delta h\nu_D} \qquad (15)$$

and

$$v \equiv \frac{h\nu-h\nu_o(m,n,n')}{\Delta h\nu_D} \, . \qquad (16)$$

The spontaneous emission rate is

$$\Gamma = \frac{4\pi e^2 \, [h\nu_o(m,n,n')]^2}{3m_e c^3 h^2} \, , \qquad (17)$$

the Doppler width is

$$\Delta h\nu_D = (\frac{2T_p}{m_e})^{1/2} \frac{h\nu_o \, (m,n,n')}{c} \, , \qquad (18)$$

and the line center is

$$h\nu_o(m,n,n') = I_i(m) \, (\frac{1}{n^2} - \frac{1}{(n')^2}) \, . \qquad (19)$$

In calculating the Rosseland mean opacities, equation (11) is rewritten as

$$\frac{1}{\sigma_R^n} = \frac{1}{\rho\ \kappa_{cont}} \frac{\int_{h\nu_n}^{h\nu_{n+1}} \left(1 + \frac{\kappa_L}{\kappa_{cont}}\right)^{-1} \frac{\partial B}{\partial T_R}(h\nu)\ dh\nu}{\int_{h\nu_n}^{h\nu_{n+1}} \frac{\partial B}{\partial T_R}(h\nu)\ dh\nu} , \qquad (20)$$

where the continuous contributions to the absorption coefficient are designated by κ_{cont}.

Using equation (13),

$$\frac{\kappa_L}{\kappa_{cont}} = \sum_m \sum_{n=1}^{\infty} \sum_{n'=n+1}^{\infty} \left(\frac{h\pi^{1/2}e^2}{m_e c}\right) \left(\frac{f_{nn'} n_j(m,n)}{\kappa_{cont}}\right)$$

$$\left(\frac{1}{\Delta h\nu_D}\right) H\left(a(\Delta h\nu_D,\ h\nu_o),\ v(\Delta h\nu_D,\ h\nu_o,\ h\nu)\right)$$

$$\equiv f\left(\frac{f_{nn'} n_j(m,n)}{\kappa_{cont}},\ \Delta h\nu_D,\ h\nu_o\right) \qquad (21)$$

and the integral in the numerator of equation (20) becomes

$$\int \frac{1}{1+f} \frac{\partial B}{\partial T_R}(h\nu)\ dh\nu$$

$$\simeq \frac{dB}{\partial T_R}(h\nu_o) \int \frac{1}{1+f}\ dh\nu \qquad (22)$$

$$\equiv \frac{dB}{\partial T_R}(h\nu_o)\ g\left(\frac{f_{nn'}\ n_i(m,n)}{\kappa_{cont}},\ \Delta h\nu_D,\ h\nu_o\right)$$

where it has been assumed that $\frac{\partial B}{\partial T_R}$ (hν) is constant across the width of the line. Since g is a function of only three variables, a table of g can be made in three-dimensional $\frac{f_{nn'} n_i(m,n)}{\kappa_{cont}}$ - $\Delta h\nu_D$ - $h\nu_o$ space. This table is made either at the start of the MIXERG run or beforehand and read into MIXERG at the start of the run. When the line absorption coefficient is calculated, g is obtained through interpolation on the table of data. This interpolation is done on the three-dimensional mesh shown in Figure 3. The effective absorption coefficient for the Rosseland opacity becomes

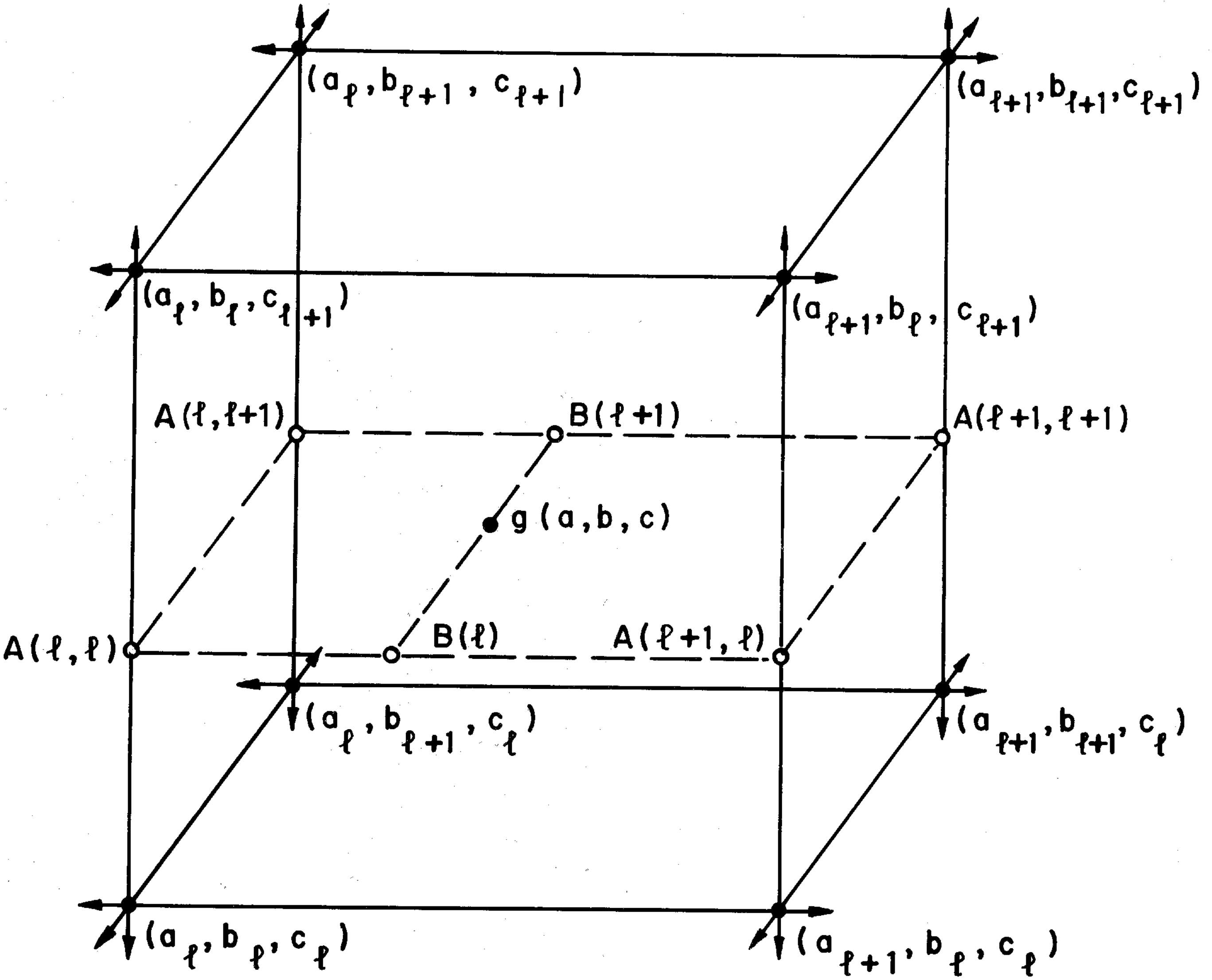
$$\kappa_{Ross} = \frac{2\kappa_{cont}\Delta h_\nu}{g} \qquad \text{if } |h\nu - h\nu_o| \leqslant \Delta h\nu_D$$

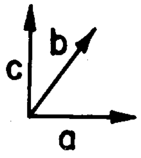
$$= \kappa_{cont} \qquad \text{if } |h\nu - h\nu_o| > \Delta h\nu_D \ . \tag{23}$$

The assumption is made here that individual lines are separated by more than $2\Delta h\nu_D$. This makes this method invalid in its present form when atomic lines are overlapping. As long as the densities are below the solid density, the line widths should be narrow enough that overlapping should not occur. The model is invalid for high density materials in any case because the ionization model neglects pressure ionization, because the equation-of-state neglects the Madelung energy and degeneracy effects and because Stark broadening has been neglected.

The calculation of the Planck mean opacities is much easier because the absorption coefficient is in the numerator of the integrand so that there is just an additive term in the opacity due to line absorption. That is,

$$\sigma_P^n = \frac{\int_{h\nu_n}^{h\nu_{n+1}} (\kappa_{cont} + \kappa_L)\, B(h\nu)\, dh\nu}{\rho \int_{h\nu_n}^{h\nu_{n+1}} B(h\nu)\, dh\nu} \ . \tag{24}$$





$$a_\ell = (h\nu_o)_\ell$$

$$b_\ell = (\Delta h\nu_{D_oP})_\ell$$

$$c_\ell = \left(\frac{fnn'\,N(n)}{K_{cont}}\right)_\ell$$

Figure 3 Interpolation mesh for g-integral.

If one assumes that $B(h\nu)$ is a constant over the width of the line, the κ_L term on the right hand side of equation (24) may be written, with the aid of equation (13), as

$$I = B(h\nu_o) \sum_m \sum_{n=1}^{\infty} \sum_{n'=n+1}^{\infty} \Big[\Big(\frac{h\pi^{1/2} e^2 f_{nn'} n_i(m,n)}{m_e c\ \Delta h\nu_D}\Big) \Delta h\nu_o \int_{\frac{h\nu_n - h\nu_o}{\Delta h\nu_D}}^{\frac{h\nu_{n+1} - h\nu_o}{\Delta h\nu_D}} H(a,v)\ dv\Big] . \tag{25}$$

It is well known that

$$\int_{-\infty}^{\infty} H(a,v)\ dv = \pi^{1/2} \tag{26}$$

so that, as long as $h\nu_{n+1} - h\nu_n$ is large compared to the line width and there is no line overlapping,

$$I = B(h\nu_o) \Big(\frac{h\pi e^2 f_{nn'} n_i(m,n)}{m_e c}\Big) . \tag{27}$$

This same contribution to the Planck opacity is obtained by using the effective absorption coefficient

$$\kappa_{Plan}(h\nu) = \frac{h\pi e^2 f_{nn'} n_i(m,n)}{2 m_e c \Delta h\nu_D} \qquad \text{if } |h\nu - h\nu_o| \leqslant \Delta h\nu_D$$

$$= 0 \qquad \text{if } |h\nu - h\nu_o| > \Delta h\nu_D . \tag{28}$$

In addition to line absorption, photo-ionization and inverse Bremmstrahlung, Thomson scattering and absorption by plasma waves are considered in the absorption coefficient for the Rosseland opacity. Thomson scattering is discussed in earlier publications$^{(6)}$ but plasma effects are a new feature in MIXERG. The model assumes that when the angular frequency of the photon is less than the plasma frequency of the material, the transmission probability of the photon is reduced by 1/e by travelling a distance of one skin depth through the plasma. Thus,

$$\kappa_{\text{Plas}}(h\nu) = \frac{(\omega_{pe}^2 - \omega^2)^{1/2}}{c} \qquad \text{if } h\nu < \hbar\omega_{pe}$$

$$= 0 \qquad \text{if } h\nu > \hbar\omega_{pe} , \tag{29}$$

where $\omega = 2\pi\nu$ and the electron plasma frequency is

$$\omega_{pe} = \left(\frac{4\pi e^2 n_e}{m_e}\right)^{1/2} . \tag{30}$$

Examples of the absorption coefficients for the Planck opacities are shown in Figures 4 and 5 for a plasma temperature of 0.4 eV and gas densities of 2.7 x 10^{14} cm^{-3} and 1 x 10^{19} cm^{-3}. The absorption coefficients for the Rosseland opacities are not shown but they are very similar to those for the Planck opacities, the only difference being that the atomic lines are not as pronounced. Comparison of Figures 4 and 5 shows that the shape of the absorption coefficient does not change much with density at this temperature and that it scales almost directly proportionally with the density.

The only lines important to Figures 4 and 5 are those corresponding to transitions where the electron is initially in an n = 1 state. This is

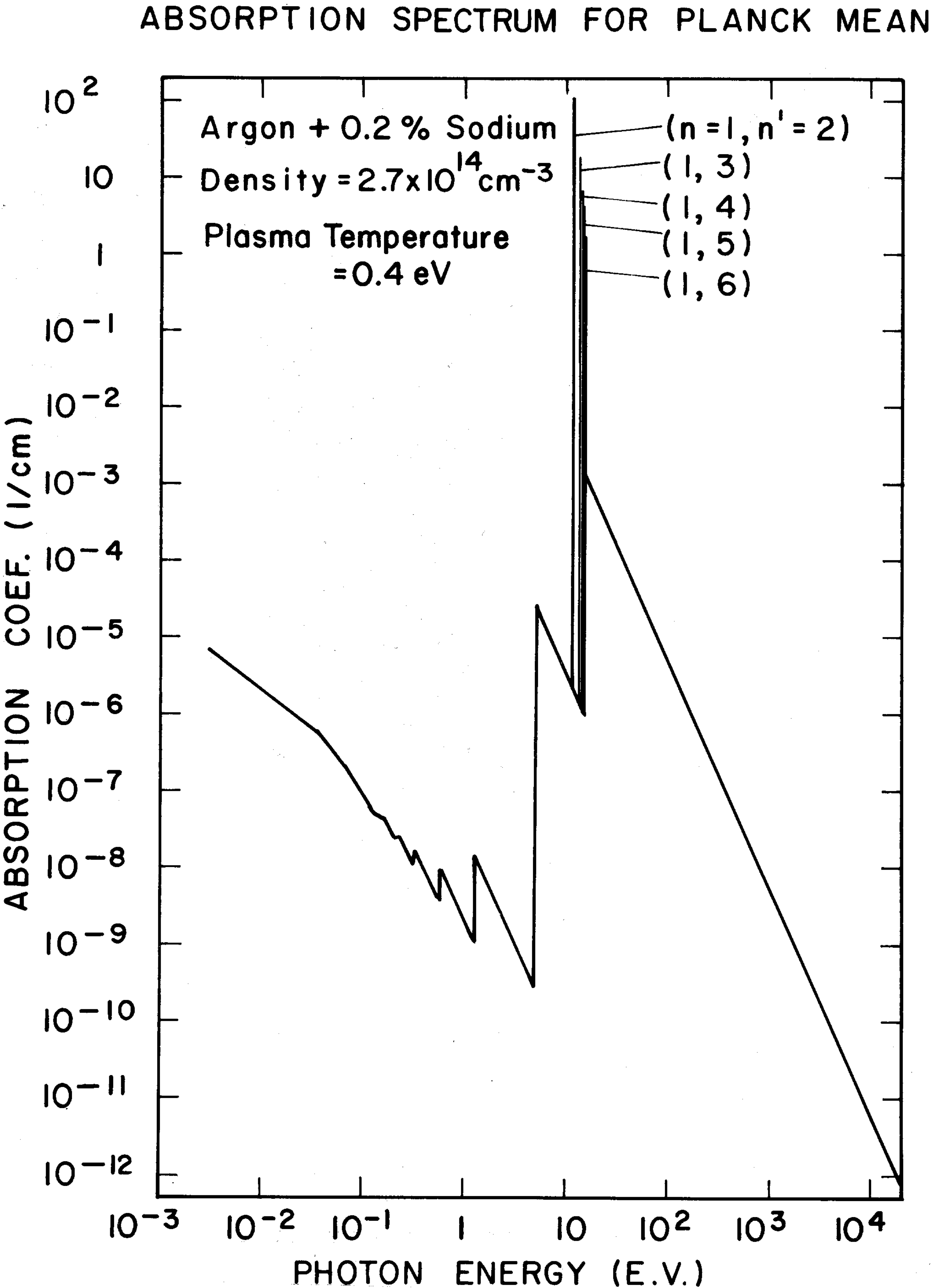


Figure 4 Absorption coefficient for the Planck opacities versus photon energy for 2.7×10^{14} cm^{-3} argon with 5.4×10^{12} cm^{-3} sodium at a plasma temperature of 0.4 eV.

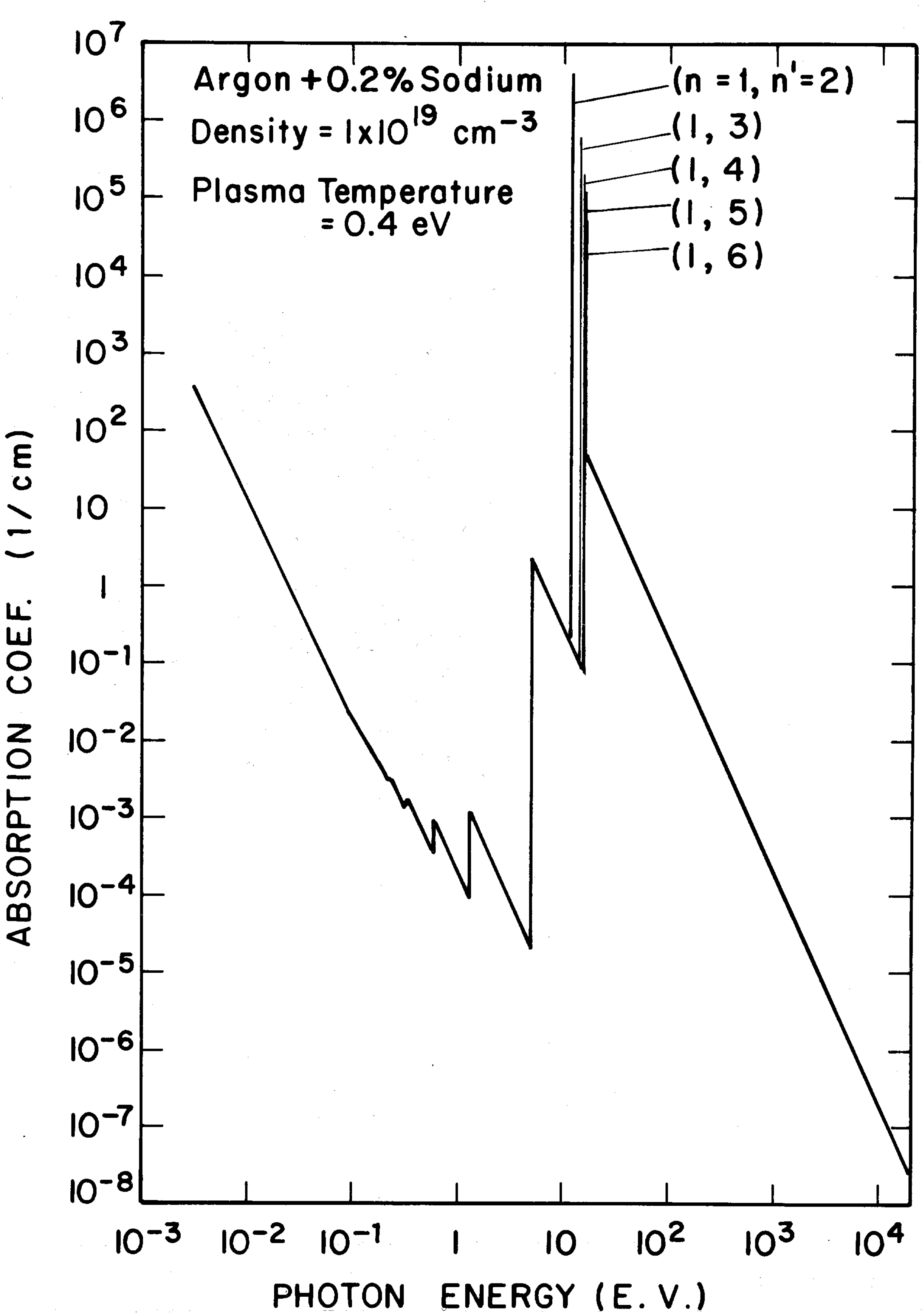


Figure 5 Absorption coefficient for the Planck opacities versus photon energy for 1×10^{19} cm^{-3} argon with 2×10^{16} cm^{-3} sodium at a plasma temperature of 0.4 eV.

because at this low temperature the atoms are almost entirely in the ground state and there are not significant numbers of outer shell electrons whose hydrogenic principal quantum numbers are greater than one. Figure 6 shows the absorption coefficient for the Planck opacities of argon with a 0.2% impurity of sodium at a plasma temperature of 10 eV and a plasma density of 1.0 x 10^{19} cm^{-3}. The populations of atoms with outer shell electrons with principal quantum numbers higher than one are much larger in this case and the lines corresponding to transitions starting in these states are much more important.

IV. Integration Method

A method of numerically integrating equations (11) and (12) which keeps the computing cost to a minimum but provides a maximum accuracy has been developed. The method lets MIXERG itself choose the integration points in hν so that computation time is not wasted by calculating the absorption coefficient many times in places where it either doesn't matter or doesn't change much.

MIXERG obtains the information needed to choose integration points in hν from its calculation of the populations of various ionization states. This tells the code at which photon energies the most important photoionizations will begin to occur. Since these "K-edges" provide sharp discontinuities in the absorption coefficient, one integration point is picked just below each such "K-edge" and one just above it. The interval between these edges is then filled with a fixed number of equally spaced integration points. Other discontinuities occur at the absorption lines, whose positions and widths are also determined by the populations of ionization states. The lines are taken to be rectangular in shape, as was discussed in Section III, and each requires four integration points. These points occur at $h\nu = h\nu_0 \pm \Delta h\nu_D \pm \varepsilon$, where ε is a small number.

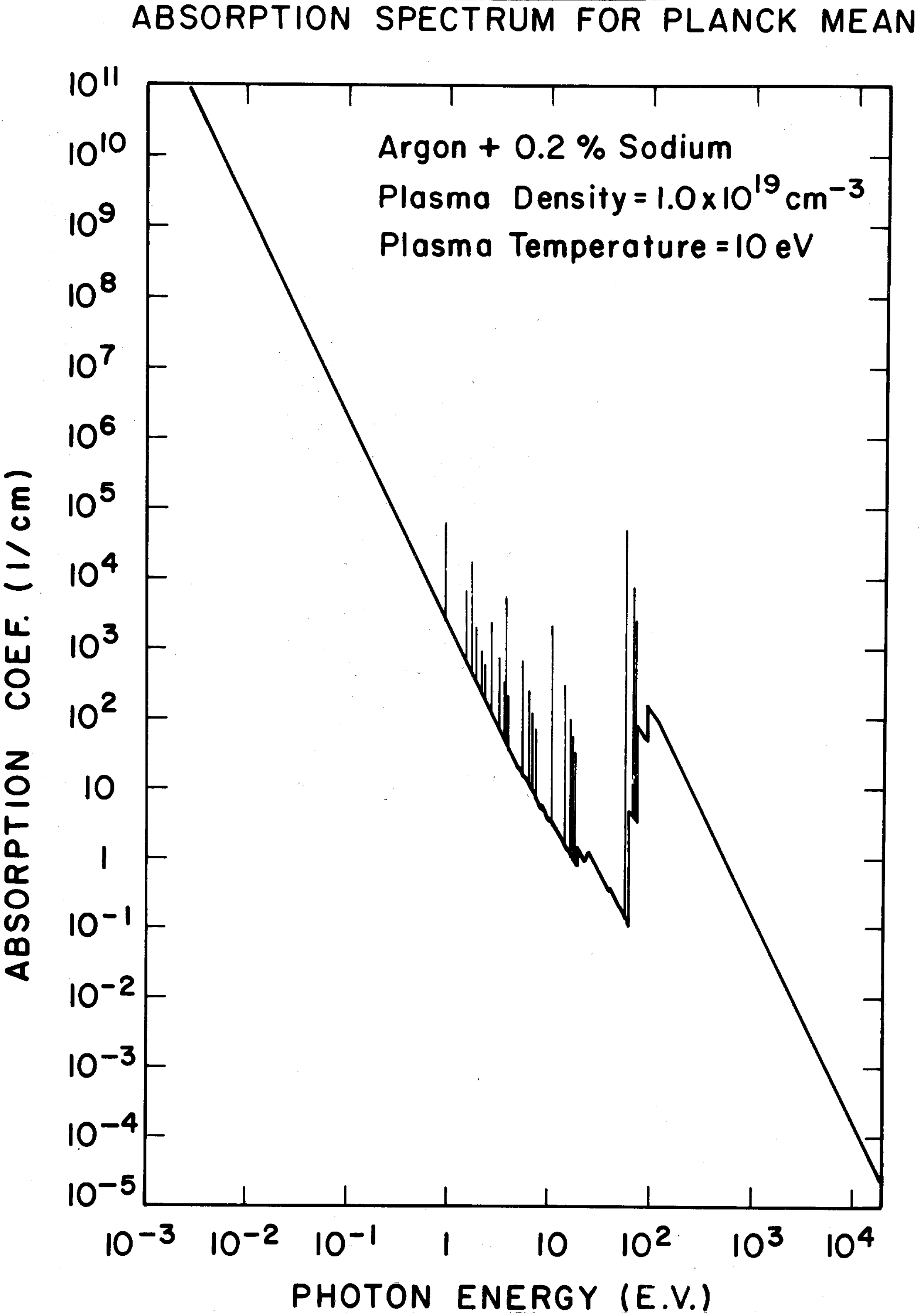


Figure 6 Absorption coefficient for the Planck opacities versus photon energy for 1 x 10^{19} cm^{-3} argon with 2 x 10^{16} cm^{-3} sodium at a plasma temperature of 10.0 eV.

There are also integration points which are not determined by the state of the material. These are the group boundaries $h\nu_n$ and the maximum and minimum values of the integration mesh. These points are input into the code at the start of the run. The interval between the most energetic important "K-edge" and the maximum $h\nu$ is filled with an arbitrary number of equally spaced integration points as is the interval between the minimum $h\nu$ and the lowest energy "K-edge".

The whole set of integration points, both those provided by the user and those determined by the code, are sorted into ascending order. Because of the variability of the mesh, a given group integral between $h\nu_n$ and $h\nu_{n+1}$ may have only two integration points for one set of T_p and density or many for another state of the gas. This is a desirable feature of MIXERG because a group having only two integration points should not be very important to the propagation, emission and absorption of radiation and it is not very important to have those group opacities calculated to high accuracy.

Sample results using this integration method are shown in Figures 7 and 8. In Figure 7, the whole-spectrum averaged Rosseland opacity is plotted against the radiation temperature T_R and the plasma temperature T_p for a gas of 2.7×10^{19} argon atoms per cm^3 and 5.4×10^{16} sodium atoms per cm^3. The Planck opacities for the same case are shown in Figure 8.

V. Conclusions

A computer code, MIXERG, has been developed which provides equation of state and opacity data for mixtures of gases. The methods used in the code should be valid from the limit of LTE at low density up to solid density. This data will be useful to the solution of many problems in engineering and applied physics. MIXERG is easy and inexpensive to use and should provide its users with flexibility in choosing gases in which they

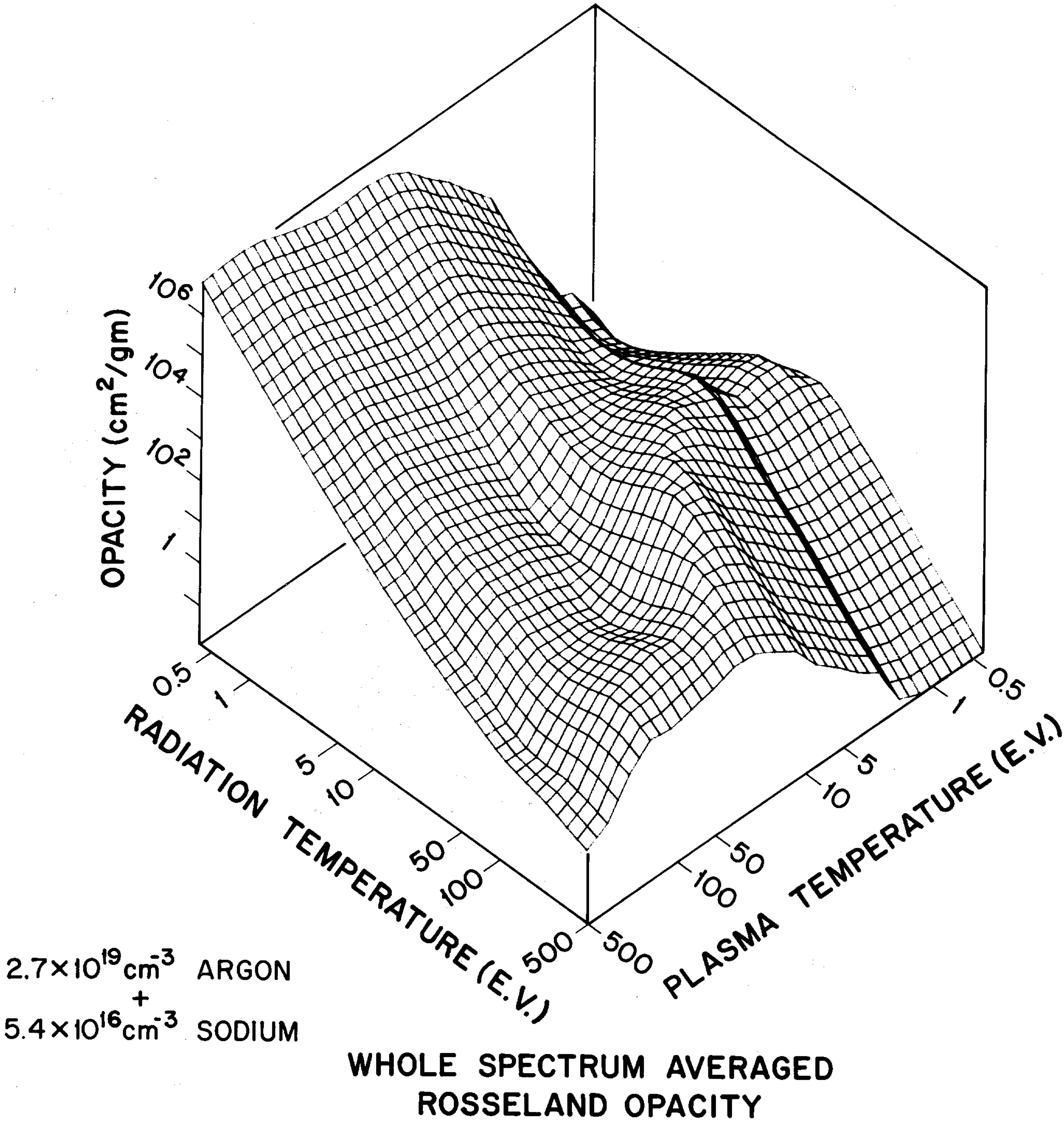


Figure 7 Whole spectrum averaged Rosseland opacity for 2.7 x 10^{19} cm^{-3} of argon and 5.4 x 10^{16} cm^{-3} of sodium versus plasma temperature T_p and radiation temperature T_R.

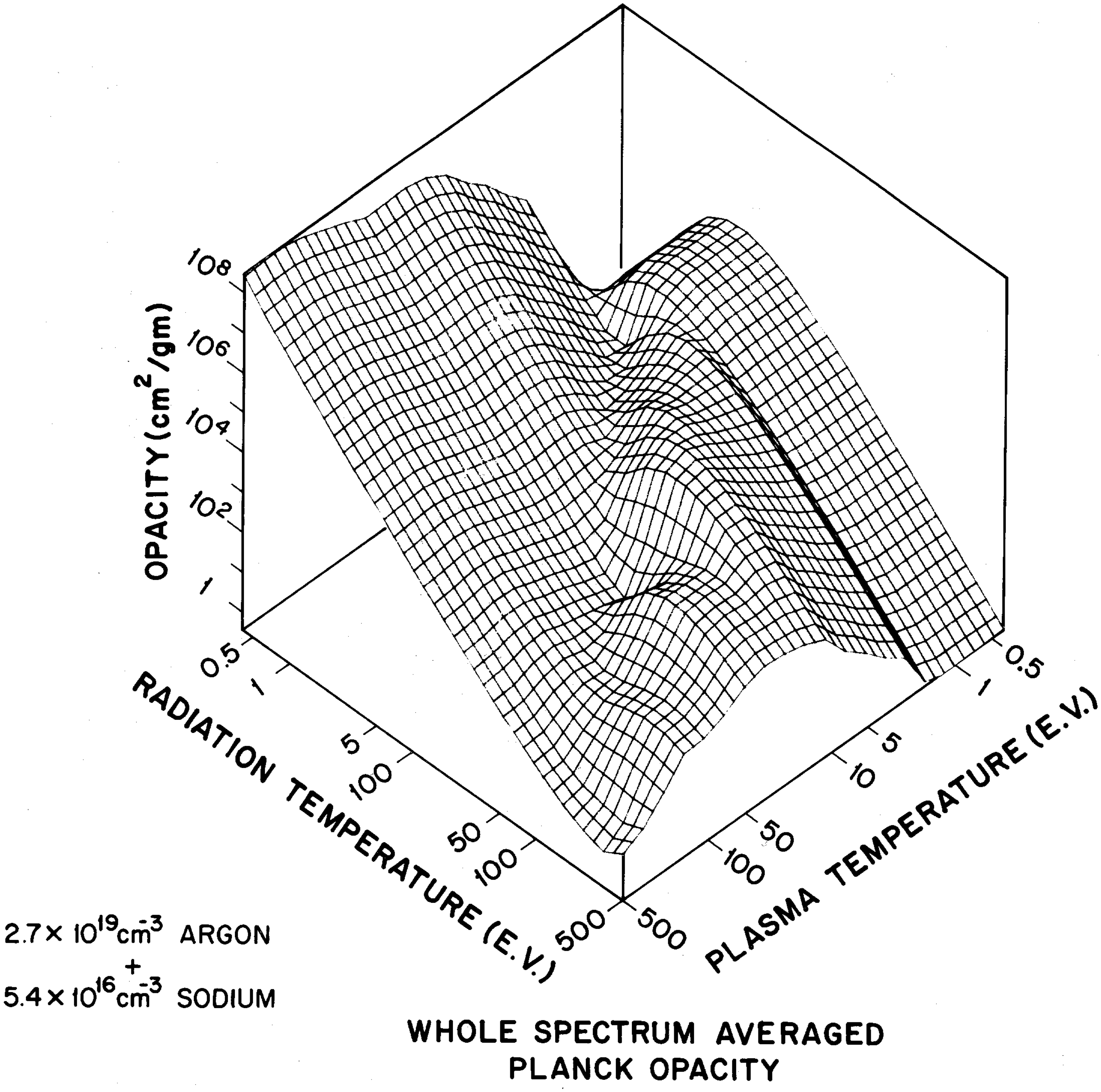


Figure 8 Whole spectrum averaged Planck opacity for 2.7×10^{19} cm^{-3} of argon and 5.4×10^{16} cm^{-3} of sodium versus plasma temperature, T_p, and radiation temperature, T_R.

study such things as radiation transport phenomena.

Acknowledgement

This work was supported by Sandia and Los Alamos National Laboratories under contract to the U.S. Department of Energy.

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Appendix A MIXERG User's Manual

A schematic flow diagram for MIXERG is shown in Figure 9. The code is written in standard FORTRAN with the exception that the UNIVAC FORTRAN V INCLUDE procedure has been used to insert common blocks into the source statements of the subroutines. On the UNIVAC at the Madison Academic Computer Center at the University of Wisconsin, MIXERG requires 0.4 seconds of CPU time for each combination of T_R, T_p and density and 64,000 36 bit words of fast memory.

In what follows, subroutines, common blocks, input and output are described for MIXERG.

Main Program

The main program in this code is MAIN. It does no calculations itself but leads the code from accepting input through the calculations to the printing and storing of results. The mesh in radiation temperature-gas temperature-gas density space over which the results are spread is determined by parameters passed from subroutine INPUT in common block CONTR. The results are passed in common block RITE to subroutine OUT, where they are printed and stored. Finally the results are collected, re-organized and written onto an output file in subroutine COLL.

COMMON BLOCKS: CONTR, POPU, OPCOM, RITE, TEMP

SUBROUTINES CALLED: INPUT, EOS, POPUL, MESH, ABSCON, INTEG, OUT, COLL

Subroutines

ABSCON: This subroutine calculates the absorption coefficient for values of the photon energy which are provided by subroutine MESH through common block ABSORP. The method of calculation of the absorption coefficient is described in Section III.

COMMON BLOCKS: SAHDT, POPU, CONTR, TEMP, ABSORP

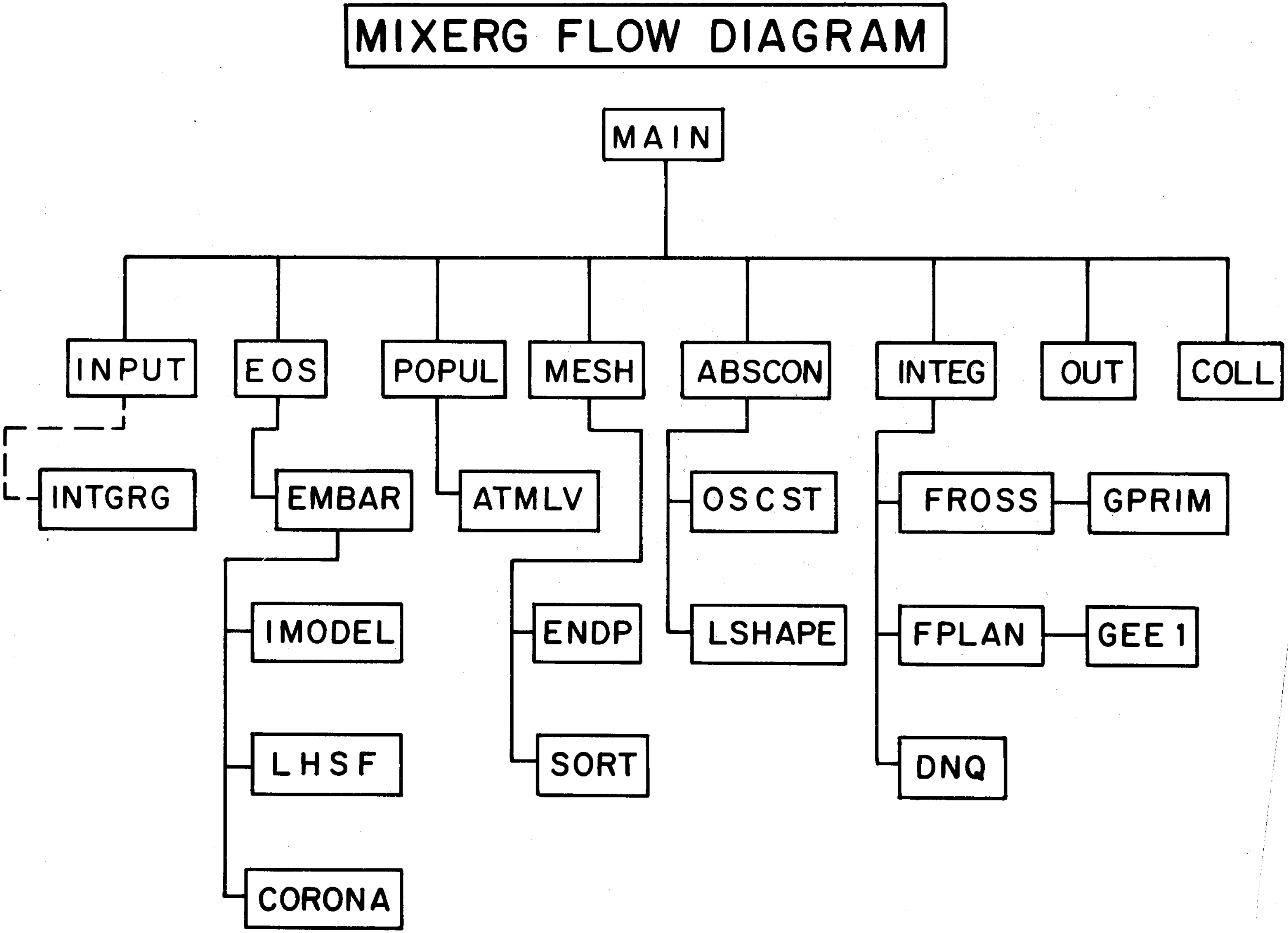
MIXERG FLOW DIAGRAM

Figure 9 Schematic flow diagram for MIXERG.

CALLED FROM: MAIN

SUBROUTINES CALLED: OSCST, LSHAPE

ATMLV: This subroutine calculates the densities of atoms in atomic levels of the outer shell electrons in the hydrogenic Bohr model. The atoms are assumed to be in equilibrium at temperature T_p and in ionization state KION-1. These densities are used in ABSCON.

COMMON BLOCKS: SAHDT, TEMP, POPU

CALLED FROM: POPUL

SUBROUTINES CALLED: None

COLL: This subroutine reads the results stored in file 20. These results are written into file 20 by subroutine OUT. COLL reorganizes the results into a form which is more convenient for storage and use in other programs. The reorganized results are written into file 11.

COMMON BLOCKS: None

CALLED FROM: MAIN

SUBROUTINES CALLED: None

CORONA: The ionization state is calculated in the Coronal model in this subroutine. The choice of ionization model is made in subroutine IMODEL and if the Coronal model is indicated CORONA is called by subroutine EMBAR. The method used here is described in Section IV of this paper.

COMMON BLOCKS: CONTR, POPU, SAHDT, TEMP

CALLED FROM: EMBAR

SUBROUTINES CALLED: None

DNQ(DNIP,DHOR,DOUT,INDMAX): This routine is a trapazoidal rule integrator. It is called by INTEG to do the integrations for the Rosseland and Planck whole-spectrum and multigroup mean opacities or mean free paths. INDMAX integrand values are passed to the routine as are the INDMAX photon energies in DHOR. The integral is passed back to INTEG as the scalar DOUT.

COMMON BLOCKS: None

CALLED FROM: INTEG

SUBROUTINES CALLED: None

EMBAR(TENER): This subroutine computes the average ionization states for each ion species by using an iterative solution to the transcendental continuous form of the Saha equation or by solving the Coronal model equations in a call to subroutine CORONA. If Eq. (1) is approximately an equality, both models are used and the averaging method described in Section II is used. The total energy density in the plasma is calculated and passed to subroutine EOS in the scalar TENER.

COMMON BLOCKS: CONTR, POPU, SAHDT, TEMP

CALLED FROM: EOS

SUBROUTINES CALLED: IMODEL, LHSF, CORONA

ENDP: To avoid discontinuities in κ_ν due to "K-edges," this routine is used to pick the end points of the integrations in photon energy used to calculate the opacities. The integrations are broken into smaller integrations where these shorter intervals have end points where the photon energies are equal to the first 5 atomic energy levels of the 2 most heavily populated ionization states.

COMMON BLOCKS: ABSORP, COMEND, CONTR, POPU, SAHDT

CALLED FROM: MESH

SUBROUTINES CALLED: None

EOS(TENER): This subroutine guides the calculation of the equation of state of the plasma. It calls subroutine EMBAR to obtain the internal energy density of the plasma at three slightly different plasma temperatures and calculates the heat capacity and the temperature derivative of the charge state of the plasma through differentiation. The internal energy density is passed to MAIN through the scalar TENER.

COMMON BLOCKS: CONTR, POPU, TEMP

CALLED FROM: MAIN

SUBROUTINES CALLED: EMBAR

FPLAN(ERAD,ABSCN,JMODE): This function is the integrand used in the integration over the photon energy in the computation of the Planck opacities. ERAD is the photon energy, ABSCN is the absorption coefficient at the photon energy, and JMODE is a flag telling FPLAN what normalization to use. To compute this integrand, this subroutine must call subroutine GEE1 to obtain the properly normalized weighting function g_1.

COMMON BLOCKS: TEMP

CALLED FROM: INTEG

SUBROUTINES CALLED: GEE1

FROSS(ERAD,ABSCN,JMODE): This function is the integrand used in the integration over photon energy for calculation of the Rosseland opacities or mean free paths. It is similar to FPLAN in that it has ERAD, ABSCN, and JMODE as arguments. FROSS calls the subroutine GPRIM to obtain g_1, the properly normalized weighting function for taking Rosseland means.

COMMON BLOCKS: TEMP

CALLED FROM: INTEG

SUBROUTINES CALLED: GPRIM

GEE1(ERAD,G1,JMODE): This subroutine calculates the weighting function used in the integration for the Planck means. The weighting function is unnormalized if JMODE=1, which corresponds to multigroup opacities and is normalized if JMODE=0, which corresponds to whole spectrum averaged opacities.

COMMON BLOCKS: TEMP

CALLED FROM: FPLAN

SUBROUTINES CALLED: None

GPRIM(ERAD,G,JMODE): This subroutine is very similar to GEE1 only it calculates the weighting function used in the Rosseland means.

COMMON BLOCKS: TEMP

CALLED FROM: FROSS

SUBROUTINES CALLED: None

IMODEL(FLINER): This subroutine uses Eq. (1) to determine which ionization model, Saha or Coronal, to use. When the system is near the boundary between the regions where the two different models should be used, an average is used as prescribed by Eq. (2). FLINER is the linear averaging parameter, f, in Eq. (2) and is passed back to EOS in the argument list.

COMMON BLOCKS: CONTR, POPU, TEMP

CALLED FROM: EOS

SUBROUTINES CALLED: None

INPUT: This subroutine reads input data, sets initial parameters, and prints a heading which lists the initial parameters used. The input data includes the integral g table which is read from unit 27, ionization potentials and numbers of electrons in outer atomic shells for each species from units 12, 13, 14, 15, and 16, and data controlling MIXERG which is read through namelist INIT from the normal input unit, 5.

COMMON BLOCKS: ABSORP, COMEND, CONTR, POPU, SAHDT

CALLED FROM: MAIN

SUBROUTINES CALLED: INTGLG

INTEG: This subroutine controls the integrations over photon energies to get the Rosseland and Planck means. It does both the whole spectrum averaged quantities and the multigroup values. It constructs the integrands through calls to FROSS and FPLAN and does the integrations with calls to DNQ. The mesh of photon energies is provided by an earilier call to MESH.

COMMON BLOCKS: ABSORP, CONTR, OPCOM, POPU, TEMP

CALLED FROM: MAIN

SUBROUTINES CALLED: FROSS, FPLAN, DNQ

INTGLG: This routine creates the data table containing the integral g for use in calculating the line absorption. This routine is only called by MAIN if ISW(10)=1. Otherwise, the data is read from a pre-existing table. In either case that data is read from input unit 27 in subroutine INPUT.

COMMON BLOCKS: None

CALLED FROM: INPUT

LHSF(EM,II,LHS,LGAS): This subroutine calculates one side of the continuous form of the Saha equation, LHS, which in EMBAR is compared with the calculation of the right hand side of the Saha equation. II is a parameter used in EMBAR, EM is the average ionization state and LGAS is the index labeling the atomic species.

COMMON BLOCKS: SAHDT

CALLED FROM: EMBAR

SUBROUTINES CALLED: None

LSHAPE(KION,NPRIN,NPP,ERAD,H1,H2,LGAS,KCONT,K): This routine calculates the shape function of the atomic line corresponding to atom number LGAS in ionization state KION-1 making a transition from a state with an outer shell electron with principal quantum number NPRIN to one with principal quantum number NPP. KCONT is the continuous part of the absorption coefficient and K is index of the particular ionization state. H1 and H2 are returned to ABSCON as the Rosseland and Planck shape functions at photon energy ERAD. This routine uses the methods discussed in Section III.

COMMON BLOCKS: ABSORP, CONTR, POPU, SAHDT, TEMP

CALLED FROM: ABSCON

SUBROUTINES CALLED: None

MESH: This routine determines the mesh of photon energies over which the integrations are done. The photon energies are chosen so the most prominent "K-edges" are closely bracketted by two points. These points are found with a call to subroutine ENDP. ISW(1) equally spaced photon energies are spread out between each of these "K-edges." Four points are chosen around the rectangularly shaped absorption lines to insure that they are accurately integrated. Frequency group boundaries are also made points. All of these photon energies are sorted into ascending order with a call to subroutine SORT.

COMMON BLOCKS: ABSORP, COMEND, CONTR, SAHDT, TEMP

CALLED FROM: MAIN

SUBROUTINES CALLED: ENDP, SORT

OSCST: This subroutine creates the oscillator strength needed for calculation of the line absorption. For cases where the initial and final principal quantum numbers are less than or equal to five, tabulated values are used. For other cases, a Bohr model estimate is used.

COMMON BLOCKS: ABSORP, CONTR

CALLED FROM: ABSCON

SUBROUTINES CALLED: None

OUT: This subroutine prints and stores the results of this code. The results are passed in common block RITE from the main program. Even though the calculations have been done with double precision variables, the results are stored as single precision. Parameters controlling the printing and storing of results are contained in common block CONTR. A complete description of the form of the output is given in the INPUT/OUTPUT part of this appendix. A sample of the printed output is given in Appendix B.

COMMON BLOCKS: ABSORP, CONTR, POPU, RITE

CALLED FROM: MAIN

SUBROUTINES CALLED: None

POPUL: This subroutine manages the calculation of the densities of atoms in various ionization states with electrons in various atomic states. Each of the atoms are assumed to be in one of the six ionization states which this subroutine chooses. With calls to ATMLV, this subroutine obtains and normalizes the atomic densities and then calculates the free electron densities and the electron plasma frequency.

COMMON BLOCKS: CONTR, POPU, SAHDT, TEMP

CALLED FROM: MAIN

SUBROUTINES CALLED: ATMLV

SORT: This routine puts the photon energy mesh points into ascending order.

COMMON BLOCKS: ABSORP, CONTR

CALLED FROM: MESH

SUBROUTINES CALLED: None

COMMON BLOCKS

ABSORP

KAPPA(500)	double prec.	Planck absorption coef. (cm^{-1})
PHOT(500)	double prec.	photon energies (eV)
FNN(20,20)	double prec.	oscillator strength
ERADO(20,20)	double prec.	line center (eV)

DNPI	double prec.	1/NPRIN
DNPPI	double prec.	1/NPP
GAMMA	double prec.	natural transition rate (sec^{-1})
DHNUD	single prec.	Doppler line width (eV)
NUMLIN	integer	number of lines considered per ionization state
KLINE	integer	number of ionization states with lines
KMESH(2)	integer	indices of the ionization states used in ENDP
KAPPA2(500)	double prec.	Rosseland absorption coef. (cm^{-1})
GINT(40,10,5)	single prec.	g-integral
GSCALE(20)	single prec.	scalar parameters needed to use g-integral table
GRPBD(21)	double prec.	photon energy group boundaries (eV)
INDGRP(21)	integer	index numbers of group boundaries in PHOT(500)
NGRP	integer	number of groups
NGRPP1	integer	NGRP+1

COMEND

END(10)	double prec.	important "K-edges" (eV)
HIPT	double prec.	largest photon energy in integration (eV)

CONTR

IPRT(20)	integer	vector controlling optional printing (see input descriptions)
ISW(20)	integer	vector of optional switches (see input description)
ICNTMX	integer	maximum number of inner iterations in Saha ionization solution
ITERMX	integer	maximum number of outer iterations in Saha ionization solution
ITR2MX	integer	maximum number of iterations of whole ioni-

		zation calculation
EPSL	double prec.	spacing between photon energies bracketting "K-edges" (eV)
IMAX	integer	number of total ion densities considered
JPMAX	integer	number of plasma temperatures considered
JRMAX	integer	number of radiation temperatures considered
DLOW	double prec.	$\log_{10}$ of lowest total ion density log (cm^{-3})
TLOW	double prec.	$\log_{10}$ of lowest temperatures log (eV)
DELTR	double prec.	$\log_{10}$ of the ratio of succeeding radiation temperatures log (eV)
DELTP	double prec.	$\log_{10}$ of the ratio of succeeding plasma temperatures log (eV)
DELD	double prec.	$\log_{10}$ of the ratio of succeeding total ion densities log (cm^{-3})
UNFAC	double prec.	the output energies are written on the disk file in units of MJ times UNFAC
IDEN(5)	integer	if IDEN(LGAS)=1, the density of ions of species # LGAS is DEN(LGAS*D(1). Otherwise, density is DEN(LGAS)
DEN(5)	double prec.	see above
BZFACT	double prec.	width of boundary zone between regions of Saha and Coronal model: (eV) if ISW(7)≠0, (cm^{-3}) otherwise
INDMAX	integer	number of photon energies in mesh

OPCOM

LROSS	double prec.	whole spectrum Rosseland mean free path (cm) if ISW(8)=0, opacity (cm^2/gm) otherwise
LPLAN	double prec.	whole spectrum Planck mean free path (cm) if ISW(8)=0, opacity (cm^2/gm) otherwise
ROPAC(21)	double prec.	Rosseland group opacities (cm^2/gm)
POPAC(21)	double prec.	Planck group opacities (cm^2/gm)

POPU

IMA(5)	integer	average ionization state of each atomic

		species (e)
NSUBN(5,6,20)	double prec.	density of atoms of a given species in a given ionization state and a particular excitation state (cm^{-3})
N(5,6)	double prec.	density of atoms of a given species in a given ionization state (cm^{-3})
MINM(5)	integer	minimum of the 6 ionization states considered for each species
ELDEN(5)	double prec.	free electron density due to ionization of a particular species (cm^{-3})
D(5)	double prec.	ion density of each species (cm^{-3})
MBAR	double prec.	total average ionization state (e)
NGAST	integer	number of species
EMA(5)	double prec.	average ionization for a particular species for latest iteration in Saha model (e)
EMB(5)	double prec.	average ionization state for a particular species on previous iteration in Saha model (e)
TIOND	double prec.	total ion density (cm^{-3})
TIONI	double prec.	inverse of total ion density (cm^{3})
DETOT	double prec.	total electron density (cm^{-3})
EPLAFR	double prec.	electron plasma frequency (Hz)
ICOR	integer	if ICOR=1, Coronal model is used. If ICOR=0, it is not used
ISAHA	integer	if ISAHA=0, Saha model is to be used. If ISAHA=1, it is not used
NCOR(5,6)	double prec.	density of ions of a particular species in a particular state as predicted by the Coronal model (cm^{-3})
MBARS	double prec.	the average total ionization state as predicted by the Saha model (e)
MBARC	double prec.	the average total ionization state as predicted by the Coronal model (e)
CORIST(5)	double prec.	the average ionization state of a particular species as predicted by Coronal model (e)

AVIST(5)	double prec.	average ionization state of a particular species (e)
TELDC	double prec.	total electron density predicted by Coronal model (cm^{-3})
MINL(5)	integer	lowest ionization state for a given species for which a population is predicted by the Coronal model
NSAHA(5,6)	double prec.	density of ions of a particular species in a particular ionization state as predicted in Saha model (cm^{-3})
NATOM(20)	double prec.	densities of excited states (cm^{-3})
TOTMS	double prec.	total mass density (gm/cm^3)

RITE

GROSS(20,20)	single prec.	Rosseland mean free path (cm) if ISW(8)=0; Rosseland opacity (cm^2/gm) if ISW(8)≠0 whole spectrum averaged versus T_R and T_P
GL1(30,20)	single prec.	Planck mean free path or opacity (see GROSS(20,20))
DENS(5)	single prec.	density of each atomic species (cm^{-3})
TMPR(20)	single prec.	radiation temperatures (eV)
TMPP(20)	single prec.	plasma temperature (eV)
EEM(20)	single prec.	ionization states versus T_P (e)
EEN(20)	single prec.	plasma internal energy versus T_P (J/gm)
CP(20)	single prec.	heat capacity versus T_P (J/gm eV)
ZDIR(20)	single prec.	temperature derivative of charge state versus T_P (e/eV)
RGRP(21,20)	single prec.	Rosseland group opacities versus group number and T_P (cm^2/gm)
PGRP(21,20)	single prec.	Planck group opacities versus group number and T_P (cm^2/gm)
OUTSCA(30)	single prec.	additional output scalars (not used in present version)
ICRPB(21,20)	integer	indices in photon energy mesh of group boundaries

SAHDT

POT(5,55)	double prec.	ionization potentials versus species and ionization state (eV)
STATE(55)	double prec.	ionization states. This is a vector running between 0 and the number of electrons in the neutral atom
IZGAS(5)	integer	number of electrons in neutral atom ($\leq$ 54) versus species
ATMAS(5)	double prec.	mass of atom versus species (gm)
IOCC(5,55)	integer	number of electrons in outer shell versus species and ionization state

TEMP

TR	double prec.	radiation temperature (eV)
TP	double prec.	plasma temperature (eV)
TRINV	double prec.	inverse of radiation temperature (eV^{-1})
TPINV	double prec.	inverse of plasma temperature (eV^{-1})
TINC	double prec.	change in T_P for differentiation (eV) used in EOS
HTCAP	double prec.	heat capacity (J/gm eV)
DTEMP	double prec.	|TINC| (eV)
DZDT	double prec.	temperature derivative of charge state (e/eV)

INPUT/OUTPUT

Input is taken by MIXERG from three general sources: ionization states and electron shell occupation numbers for each species through formatted reads from external files 12 through 16, g-integral values from external file 27 through a formatted read, and control and initialization parameters through a NAMELIST input from unit 5, the normal input channel. A sample of the input of ionization potentials and occupation numbers for argon is shown in Table I. The data in the file must be in the same form so that it may be read with a

Table I. Ionization Potential and Occupation # Input Files

Argon	
0	0
15.8	4
27.6	3
40.7	2
59.8	1
75.	2
91.	1
124	2
143	1
422	4
478	3
539	2
618	1
686	2
756	1
855	2
918	1
4120	2
4430	1

(D12.6,I2) formatted read. The data must have IZGAS(LGAS)+1 lines unless IZGAS(LGAS) > 54 and then it must have 55 lines. Data for species number 1 is read in from unit 12, number 2 from unit 13, etc. The data from unit 27 should have been generated by INTGLG at some point and will automatically be in the correct form. The NAMELIST input is described in Table II, where the optional input variables are listed along with their default values. If no default is shown, some input must be made for that variable through this NAMELIST.

The output of this code is in two forms, printed and data stored in an output file. An example of the printed output is shown in Appendix B. The output data is collected into a suitable form in subroutine COLL and output to unit 11. The first line in unit 11 contains IMAX, JPMAX, JRMAX, and NGRP, written in the 4I4 format. If NGRP > 1, the next lines contain GRPBD(IGRP), ICRP=1 to NGRP+1 written in the 4E12.6 format. The charge state of the plasma is then written with the same 4E12.5 format, where values for all JPMAX values of the plasma temperature are written before the density is changed. Data for all of the IMAX densities are stored in the file. Similarly, data for the internal energy of the plasma, the heat capacity and the temperature derivative of the charge state are written into file 11 in that order. The whole spectrum averaged Rosseland and Planck mean free paths or opacities are then written with the same format. In these two blocks of data, the radiation temperature most rapidly progresses through its JRMAX values while changes in the JPMAX values of the plasma temperature are next most rapidly varying. The density is most slowly varying. If NGRP=1, this is the end of file 11. Otherwise, the Rosseland and Planck multigroup opacities follow, written with the same format. The most rapidly varying index in these two blocks is the group number IGRP, which varies from 1 to NGRP. The next most frequent

Table II. NAMELIST Parameters and Default Values

Name	Default Value	Comment
IPRT(1)	0	if $\neq 0$, print absorption coefficient
IPRT(2)	0	not used
IPRT(3)	0	if $\neq 0$, print end points of subintegrations after they are sorted into numerical order
IRPT(4)	0	if $\neq 0$, print end points before they are sorted
IPRT(5)	0	if $\neq 0$, print out details of EMBAR calculations
IPRT(6)	0	if $\neq 0$, print details of POPUL calculations
IPRT(7)	0	if $\neq 0$, print details of CORONA calculations
IPRT(8)	0	if $\neq 0$, print ionization potentials
IPRT(9)	0	if $\neq 0$, print photon frequency and plasma frequency
IPRT(10)	0	if $\neq 0$, print oscillator strengths
IPRT(11)	0	if $\neq 0$, print details of LSHAPE calculations
IPRT(12)	0	if $\neq 0$, print details of MESH calculations
ISW(1)	20	number of mesh points between "K-edges"
ISW(2)	0	if $\neq 0$, skip opacity calculations
ISW(3)	0	if $\neq 0$, $T_R = T_P$
ISW(4)	0	if $\neq 0$, skip heat capacity calculation
ISW(5)	0	if $\neq 0$, don't use tabulated oscillator strengths
ISW(6)	3	if = 1, use only Saha model if = 2, use only Coronal model if = 3, let MIXERG choose models

ISW(7)	0	if = 0, cross boundary between Saha and Coronal with changes in the density if ≠ 0, cross boundary in temperature
ISW(8)	1	if ≠ 0, calculate opacities instead of mean free paths
ISW(9)	0	if ≠ 0, calculate group opacities; if ISW(9)≠0, ISW(8)≠0 automatically
ISW(10)	0	if ≠ 0, call INTGLG
EPSL	1.D-8	
DELD	.5D0	
DELTR	.162995D0	
DELTP	.162995D0	
DLOW	14.4314D0	
TLOW	-.39794D0	
IMAX	17	
JRMAX	20	
JPMAX	20	
HIPT	2.D4	
HIPOT	1.D10	Value of POT(I) when IZEE+1 < I < 55
ITERMX	15	
ICNTMX	25	
POT(5,55)		This is only needed if the values of POT(5,55) need to be changed from those read in from units 12 through 16
STATE(55)		same as POT(5,55)
ATMAS(5,55)		mandatory input
NGAST	1	
IDEN(5)	0	
DEN(5)	0.D0	
DTEMP	.01D0	

ITR2MX	3	
BZFACT	10.D0	
NUMLIN	5	
KLINE	2	
GRPBD(21)		mandatory if ISW(9)≠0
NGRP	20	

changes occur in the plasma temperature and the least frequent changes are in the plasma density. In summary, the blocks of data appear in unit 11 in the following order: IMAX, JPMAX, JRMAX, NGRP; GRPBD; the charge state; the internal energy of the plasma; the heat capacity; the temperature derivative of the charge state; the whole spectrum averaged Rosseland mean free path or opacity; the whole spectrum averaged Planck mean free path or opacity; the Rosseland group opacity; and the Planck group opacity.

Appendix B Sample Computer Run

A sample computer run has been made and its input and output are presented here. The run is for a mixture of 9.98 x 10^{18} cm^{-3} of argon and 1.99 x 10^{16} cm^{-3} of sodium at a plasma temperature of 10 eV. The radiation temperature varies from 10 eV to 30.8 eV. The NAMELIST input element, MIXERG INIT, is

```
&INIT IZGAS=18,11,
  NGAST=2,
  ATMAS=6.666D-23,3.8176D-23,
  DLOW=19.D0,
  TLOW=1.D0,
  IDEN(2)=1,
  DEN(2)=2.D-3,
  JPMAX=1,
  JRMAX=4,
  IMAX=1,
  DTEMP=1.D-3,
  KLINE=5,
  NGRP=20,
  GRPBD=0.D0,1.D0,3.D0,5.D0,7.5D0,
  10.D0,13.D0,1.57D1,25.D0,3.23D1,4.87D1,
  75.D0,1.D2,1.25D2,1.5D2,2.D2,
  3.D2,4.D2,5.D2,1.D3,
  ISW(9)=1,
  DENAV=1.D16,
&END
```

The printed output is shown on the next three pages. The first two pages are a heading giving initial parameters while the third page is the printed output.

```
      **************************************
      *                                    *
      *   MIXER4 - A CODE TO CALCULATE THE *
      *   EQUATIONS OF STATE AND OPACITIES *
      *    OF MIXTURES OF MONATOMIC GASES  *
      *                                    *
      *     WRITTEN BY ROBERT R. PETERSON  *
      *                                    *
      **************************************

           IPRT(I)

IPRT(1)=   0        PRINT ABSORPTION COEF?
IPRT(2)=   0
IPRT(3)=   0        PRINT ENDPOINTS AFTER SORT?
IPRT(4)=   0        PRINT ENDPOINTS BEFORE SORT?
IPRT(5)=   0        PRINT OUT IONIZATION CALC?
IPRT(6)=   0        PRINT POPUL VALUES
IPRT(7)=   0        PRINT CORONA VALUES
IPRT(8)=   0        PRINT IONIZATION POTENTIALS ?
IPRT(9)=   0        PRINT RAD FREQ. AND PLASMA FREQ.?
IPRT(10)=   0       PRINT OSC STRENGTHS?
IPRT(11)=   0       PRINT LSHAPE CALC?
IPRT(12)=   0       PRINT MESH CLAC?


           ISW(I)

ISW(1)=  20        # EQ. SPACED STEPS / SUBINTEGRAND
ISW(2)=   0        SKIP MFP CALCULATIONS ?
ISW(3)=   0        TR = TP ?
ISW(4)=   0        CALCULATE HEAT CAPACITY ?
ISW(5)=   0        USE TABULATED OSC. STRENGTHS ?
ISW(6)=   3        CHOOSE IONIZATION MODEL
ISW(7)=   0        CROSS BOUNDARY IN D OR TP?
ISW(8)=   1        MFP S OR OPACITIES
ISW(9)=   1        MULTI-GROUP VAULES
ISW(10)=   0       CREATE G-INTEGRAL?


           CONSTANTS USED

EPSL= .100000-007          SPACE BETWEEN INTERGRALS
HIPT= .200000+005          HIGHEST PHOTON ENERGY
HIPOT= .100000+011         DEFAULT IONIZATION POT
IZGAS(1)= 18               ATOMIC # OF GAS # 1
IZGAS(2)= 11               ATOMIC # OF GAS # 2
IZGAS(3)=  0               ATOMIC # OF GAS # 3
IZGAS(4)=  0               ATOMIC # OF GAS # 4
IZGAS(5)=  0               ATOMIC # OF GAS # 5
ATMAS(1)= .666600-022      MASS OF ATOM # 1
ATMAS(2)= .381760-022      MASS OF ATOM # 2
ATMAS(3)= .000000+000      MASS OF ATOM # 3
ATMAS(4)= .000000+000      MASS OF ATOM # 4
ATMAS(5)= .000000+000      MASS OF ATOM # 5
IDEN(2)=  1                DENSITY SWITCH OF GAS # 2
```

```
 IDEN(3)=  0                   DENSITY SWITCH OF GAS # 3
 IDEN(4)=  0                   DENSITY SWITCH OF GAS # 4
 IDEN(5)=  0                   DENSITY SWITCH OF GAS # 5
 DEN(2)= .200000-002           DENSITY FACTOR OF GAS # 2
 DEN(3)= .000000+000           DENSITY FACTOR OF GAS # 3
 DEN(4)= .000000+000           DENSITY FACTOR OF GAS # 4
 DEN(5)= .000000+000           DENSITY FACTOR OF GAS # 5
 UNFAC= .100000+001            JOULES PER ENERGY UNIT
 ITERMX= 15                    MAX # OF OUTER ITERATIONS IN EMBAR
 ICNTMX= 25                    MAX # OF INNER ITERATIONS IN EMBAR
 ITR2MX=  3                    MAX # OF BOUNDARY ITERATIONS
 DTEMP= .100000-002            TEMP DIFF FOR DERIVATIVES
 BZFACT= .100000+002           BOUNDARY WIDTH
 NUMLIN=  5                    # OF ATOMIC LINES / K-EDGE
 KLINE=  5                     # OF K-EDGES WITH ATOMIC LINES
 NGRP= 20                      # OF FREQUENCY GROUPS

             CONSTANTS FOR RESULT MESH

 IMAX=    1                    # OF DENSITIES
 JRMAX=    4                   # OF RAD TEMPS
 JPMAX=    1                   # OF GAS TEMPS
 DLOW= .190000+002             LOG OF LOWEST DENSITY
 TLOW= .100000+001             LOG OF LOWEST TEMPS
 DELTR= .162995+000            LOG OF RATIO OF SUCCEEDING RAD TEMPS
 DELTP= .162995+000            LOG OF RATIO OF SUCCEEDING GAS TEMPS
 DELD= .500000+000             LOG OF RATIO OF SUCCEEDING DENSITIES

             FREQUENCY GROUP BOUNDARIES

0.000000-001  1.000000+000  3.000000+000  5.000000+000  7.500000+000
1.000000+001  1.300000+001  1.570000+001  2.500000+001  3.230000+001
4.870000+001  7.500000+001  1.000000+002  1.250000+002  1.500000+002
2.000000+002  3.000000+002  4.000000+002  5.000000+002  1.000000+003
```

```
DENSITY OF FIRST GAS =  .996004+19  / CM **3

DENSITY OF SECOND GAS=  .199202+17  / CM **3

 GAS TEMP =   10.0000     E.V.

 RAD TEMP     ROSS OPAC    PLAN OPAC    CHARGE       ENERGY DENS HEAT CAP     DZ/DT
 E.V.         CM**2/GM     CM**2/GM     E            J/GM        J/GM.EV      E/EV

 .100000+02   .650659+03   .133046+05   .502046+01   .751193+06  .132135+06   .432009+00
 .145544+02   .866402+03   .400171+05   .502046+01   .751193+06  .132135+06   .432009+00
 .211831+02   .156256+04   .706162+05   .502046+01   .751193+06  .132135+06   .432009+00
 .308308+02   .315118+04   .779732+05   .502046+01   .751193+06  .132135+06   .432009+00

 MESH INDICIES OF GROUP BOUNDARIES

   1     12     49    113    158
 183    197    208    249    253
 260    290    313    314    315
 316    317    318    319    321
 359

 FREQUENCY GROUPS (E.V.)

 .300000-02   .100000+01   .300000+01   .500000+01   .750000+01
 .100000+02   .130000+02   .157000+02   .250000+02   .323000+02
 .487000+02   .750000+02   .100000+03   .125000+03   .150000+03
 .200000+03   .300000+03   .400000+03   .500000+03   .100000+04
 .200000+05

 ROSSELAND OPACITIES (CM**2/GM) FOR 20 GROUPS

 .722694+07   .262592+06   .491232+05   .152876+05   .677510+04
 .382251+04   .213026+04   .154687+04   .122532+04   .501436+03
 .426185+03   .111355+06   .176500+06   .111584+06   .695578+05
 .301668+05   .894146+04   .377255+04   .193120+04   .210099+00

 PLANCK OPACITIES (CM**2/GM) FOR 20 GROUPS

 .119273+08   .330675+06   .537694+05   .163529+05   .692190+04
 .460862+04   .231700+04   .163412+04   .131078+04   .553576+03
 .206299+05   .128069+06   .183536+06   .116899+06   .708951+05
 .301799+05   .894261+04   .377273+04   .193145+04   .686167+01
```