



**EOSOPC – A Code for Computing the  
Equations of State and Opacities of High  
Temperature Plasmas with Detailed Atomic  
Models**

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**December 1993**

**UWFDM-933**

***FUSION TECHNOLOGY INSTITUTE  
UNIVERSITY OF WISCONSIN  
MADISON WISCONSIN***

**EOSOPC — A CODE FOR COMPUTING THE EQUATIONS  
OF STATE AND OPACITIES OF HIGH TEMPERATURE  
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Ping Wang

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

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## 1. Introduction

The equations of state and opacities of partially ionized plasmas are often required to study the physical properties of laboratory and astrophysical plasmas.

For a thermodynamic equilibrium ideal gas, the Saha-Boltzmann equations can be used to describe the ionization balance and the level occupation numbers, and the equations of state and opacities are readily obtained. However, for the physical conditions encountered in most laboratory plasmas, especially fusion plasmas, where plasma densities can vary from  $\sim 10^{10}$  to  $\sim 10^{22}$  ions/cm<sup>3</sup> and temperatures from  $\sim 1$  eV to 1 keV, the calculations of equations of state and opacities become quite difficult because the electrons and different ionic and atomic species cannot be always regarded as simple ideal gases. A number of physical effects, including electron degeneracy, coulomb interactions among free charges, bound-state level perturbation (destroy or/and shifts), and neutral atomic interactions, etc., must be taken into account. On the other hand, the approximation of thermodynamic equilibrium (or even local thermodynamic equilibrium) may not be adequate for such plasmas. Detailed solutions of rate equations with detailed atomic models are required in determining the ionization balance and level occupation numbers in such cases.

In this report, we describe the features of EOSOPC, a computer code we have developed for computing the equations of state and opacities of high temperature plasmas. The major features of EOSOPC include:

1. employing detailed atomic models;
2. accounting for important nonideal plasma effects;
3. solving rate equations for determining the ionization balance and atomic level occupation number of the plasma.

Detailed discussions of these features have been given elsewhere [Wang, 1991], and only a brief overview of the models will be presented here. This report is intended to be a “users’ guide”. Thus, the focus here will be on the structure of the code and how to use it. A users’ guide for the atomic physics package which sets up atomic data files for the EOSOPC code is described elsewhere [Wang, MacFarlane, 1993].

The EOSOPC code computes the steady-state ionization and excitation populations for a mixture of up to 5 different atomic species. The radiative absorption, emission, and scattering coefficients are calculated at a large number ( $\sim$  several thousand) of photon energies, and integrated over selected energy intervals to determine the multigroup Planck and Rosseland mean opacities. The code also calculates the thermodynamic properties of the plasma, such as the specific energy, average charge state, pressure, and heat capacity. The results are applicable to plasmas where: (1) the radiation energy field can be neglected in computing the ionization and excitation rates (i.e., optically thin plasmas), and (2) molecular effects are unimportant.

Sections 2 through 5 of this report provide brief descriptions of the statistical equilibrium, continuum lowering model, calculations of equations of state and opacities. Input and output files are described in Section 6, while the computational procedures are described in Section 7. The subroutines and common block descriptions are provided in Sections 8 and 9, respectively.

## **2. Statistical Equilibrium**

In this section we describe a collisional-radiative equilibrium model for calculating ionic charged-state abundance and the level occupation number in plasmas. The nonideal effects on the population distribution are considered by introducing a survival probability factor for each level included in the calculation.

A general rate equation for the population density in level  $j$  of ion  $z$ ,  $n_{z,j}$  can be written as

$$\begin{aligned}
\frac{dn_{z,j}}{dt} = & - \sum_k I(z, j; z+1, k) n_e n_{z,j} + \sum_k I(z-1, k; z, j) n_e n_{z-1,k} \\
& - \sum_k R(z, j; z-1, k) n_e n_{z,j} + \sum_k R(z+1, k; z, j) n_e n_{z+1,k} \\
& - \sum_{u>j} E(z, j; z, u) n_e n_{z,j} - \sum_{l<j} D(z, j; z, l) n_e n_{z,j} \\
& + \sum_{l<j} E(z, l; z, j) n_e n_{z,l} - \sum_{u>j} D(z, u; z, j) n_e n_{z,u}
\end{aligned} \tag{2.1}$$

where  $n_e$  is the density of electrons,  $I(z, j; z+1, k)$  is the ionization rate coefficient for the ionization of ion  $z$  in level  $j$  to ion  $z+1$  in level  $k$ ,  $R(z, j; z-1, k)$  is the recombination rate coefficient (radiative+collisional+dielectronic),  $E(z, j; z, u)$  is the electron collisional excitation rate coefficient, and  $D(z, j; z, l)$  is the deexcitation rate coefficient (spontaneous decay + collisional). For a steady-state plasma, we have  $\frac{dn_{z,j}}{dt} = 0$ .

There are two factors affecting the atomic level occupation numbers : (1) *does this level survive?* (2) *how is it occupied?* If we assume the level survival probability is  $w_{z,j}$  and the occupation probability is  $p_{z,j}$ , then the level occupation number density can be expressed as

$$N_{z,j} = w_{z,j} p_{z,j} A_z \tag{2.2}$$

with

$$N_z = \sum_j^{jmax} w_{z,j} p_{z,j} A_z + (A_{z-1} - N_{z-1}) \tag{2.3}$$

and

$$N_{z+1} = \sum_j^{jmax} w_{z+1,j} p_{z+1,j} A_{z+1} + (A_z - N_z) \tag{2.4}$$

where  $N_z$  is the ion abundance of ion  $z$ ,  $A_z$  is the corresponding ion abundance calculated with  $w_{z,j} = 1$ , and  $jmax$  is the maximum index of the atomic level in the atomic model.

In EOSOPC, the occupation probability  $p_{z,j}$  of each level and  $A_z$  are calculated by solving the steady-state rate equations of Eq. 2.1 with a large number of  $jmax$ , while the level survival probability  $w_{z,j}$  is calculated by using the model developed by Mihalas and Hummer [Mihalas and Hummer, 1988]. It should be noted that for a given temperature and ion density, the calculations of  $w_{z,j}$ ,  $p_{z,j}$ ,  $A_z$ ,  $n_{z,j}$ , and  $N_z$  are nonlinearly coupled. A self-consistent iterative scheme is used in EOSOPC for solving these quantities. The overall procedure for computing the level populations is as follows:

1. Make an initial guess for population distribution (e.g., LTE population).
2. Solve steady-state rate equations of Eq. 2.1 for  $n_{z,j}$ , then  $A_z = \sum_j^{jmax} n_{z,j}$ , and  $p_{z,j} = \frac{n_{z,j}}{A_z}$ .
3. Compute level survival probability  $w_{z,j}$  by using Mihalas' model for the population distribution obtained from (2).
4. Compute  $N_{z,j}$  and  $N_z$  with Eq. 2.2 and Eq. 2.3.
5. If new populations are consistent with previous iteration, calculation for population distribution is complete; otherwise go back to step (2).

The iteration parameter in this iteration calculation is electron density instead of level population vector. In another words, we check the consistency of electron density in two consecutive calculations. This interative procedure converges very fast. Typically after 5 iterations, the rate of convergence can reach  $10^{-2}$ .

### 3. Pressure Ionization Effect and Level Survival Probability

The great difference between atomic structure for isolated atoms and those in the plasma is the finite number of bound states in the latter case. As the plasma density rises and the number and intensity of interparticle interactions increase, less tightly bound states are strongly perturbed, broadened into distributions resembling conduction bands, and ultimately destroyed and shifted into the continuum. These phenomena

imply a ‘*pressure ionization*’ which leads at very high densities to a fully ionized plasma comprising, in the first approximation, an ideal gas of degenerate electrons that can move freely with respect to a “lattice” of bare ions. *Pressure ionization* is dominately a volume effect: When particles are jammed closely together, bound electron orbitals filling too large a volume fail to survive and the electrons migrate from atom to atom.

In EOSOPC, the pressure ionization effect is taken into account by using the model suggested by Hummer and Mihalas [Hummer and Mihalas, 1988], i.e., the “occupation probability formalism”. In this procedure, a factor,  $w_{ijk}$  ( $0 \leq w_{ijk} \leq 1$ ), is introduced for each atomic level. The physical significance of  $w_{ijk}$  is the probability of finding the ion  $j$  of species  $k$  in question in state  $i$  relative to that of finding it in a similar ensemble of non-interacting ions. Alternatively,  $w_{ijk}$  can be considered as a factor expressing the *survival probability* of the level due to the perturbation of surrounding particles, neutral and charged. The *survival probability* has to be calculated directly from a physical description of interparticle interactions. It is here that one makes contact with atomic physics and can attempt to introduce some level of realism into the model.

In the models suggested by Hummer et al., perturbations by neutral particles are based on an excluded volume treatment and perturbations by charges are calculated from a fit to a quantum mechanical Stark ionization theory. The level *survival probability* can then be expressed as

$$\begin{aligned} \ln(w_{ijk}) = & -\left(\frac{4\pi}{3}\right)\left\{\sum_{\nu'k'}[(r_{ijk} + r_{1\nu'k'})^3 + \beta(r_{ijk} + r_{1\nu'k'})^\gamma]\right. \\ & \left.+ 16\left[\frac{\sqrt{z_{jk} + 1}e^2}{\sqrt{K_{ijk}I_{ijk}}}\right]^3 \sum_{s \neq e} n_s z_s^{3/2}\right\} \end{aligned} \quad (3.1)$$

Here the index  $\nu'$  runs over neutral particles, the index  $s$  runs over charged ions,  $r_{ijk}$  is the radius assigned to a particle in state  $i$  of ion  $j$  of species  $k$ ,  $I_{ijk}$  is the ionization potential of such a level,  $z_{jk}$  is the net charge of a particle of ion  $j$  of species  $k$ ,  $\beta$  and  $\gamma$

are two empirical parameters, and

$$K_{ijk} = \begin{cases} 1 & p_i \leq 3 \\ \frac{16}{3} \left( \frac{p_i}{p_i+1} \right)^2 \frac{p_i+7/6}{p_i^2+p_i+1/2} & p_i > 3 \end{cases} \quad (3.2)$$

is a quantum mechanical correction and  $p_i$  is the effective quantum number of the state  $i$ .

The *occupation probability formalism* has several advantages. (1) The  $w_{ijk}$  decrease continuously and monotonically as the strength of the relevant interaction increases relative to the binding energy of a level. (2) The continuous state-by-state fadeout with decreasing  $w_{ijk}$  allows one to assure continuity of all material properties (pressure, internal energy, opacity, etc.). (3) The probabilistic interpretation of  $w_{ijk}$  allows us to combine survival probabilities from statistically independent interactions. It is thus straightforward to allow for the simultaneous action of different mechanisms, as well as of several different species of perturbers by any one mechanism. Hence the method provides a scheme for treating partially ionized plasmas, and it goes smoothly to the limits of completely neutral or completely ionized gas.

## 4. Calculations of Equations of State

For the physical conditions encountered in most laboratory plasmas, especially fusion plasmas, where plasma densities can vary from  $10^{10}$  to  $10^{22}$  ions/cm<sup>3</sup> and temperatures from 1 eV to 1 keV, the ideal gas model is not always appropriate. Non-ideal effects need to be taken into account in the computations of equations of state for these plasmas. In EOSOPC, the equations of state of plasmas come from four different contributions: (1) *the translation of ions and atoms*, (2) *the partially degenerate electrons*, (3) *configuration effects from coulomb interactions (Debye-Hückel correction)*, (4) *atomic internal contributions (excitations and ionizations)*.

### I. Translational Contribution of the Ions and Atoms

$$E_1 = \frac{3}{2}kT \sum_{s \neq e} N_s = 2.403 \times 10^{-12} T(eV) \sum_{s \neq e} N_s \text{ (erg/cm}^3\text{)} \quad (4.1)$$



$$P_1 = kT \sum_{s \neq e} N_s = 1.602 \times 10^{-12} T(\text{eV}) \sum_{s \neq e} N_s \text{ (dyn/cm}^2\text{)} \quad (4.2)$$

## II. Contribution of Partially Degenerate Electrons

$$E_2 = N_e kT \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)} = 1.602 \times 10^{-12} N_e T(\text{eV}) \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)} \text{ (erg/cm}^3\text{)} \quad (4.3)$$

$$P_2 = \frac{2}{3} N_e kT \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)} = 1.068 \times 10^{-12} N_e T(\text{eV}) \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)} \text{ (dyn/cm}^2\text{)} \quad (4.4)$$

where  $\eta$  is the degeneracy factor determined by

$$F_{1/2}(\eta) = \frac{\sqrt{\pi}}{4} \left( \frac{2\pi m_e k}{h^2} \right)^{-3/2} \frac{N_e}{T^{3/2}} = 1.468 \times 10^{-22} \frac{N_e}{T^{3/2}(\text{eV})} \quad (4.5)$$

## III. Debye-Hückel Correction Terms

In a partially ionized plasma, the major nonideality effect is known to be the coulombic interactions between the charged components. The coulomb perturbation enters the equations of state in two ways: through the interparticle interaction potential it modifies the configuration integral, and through the internal potential it perturbs the bound states (destroy or/and shifts). The latter effect partially contributes to the effects of ‘*pressure ionization*’. A modified Debye-Hückel model may be used for describing the configurational coulomb interaction. In this modified DH model, the electrons are treated as fermions, but the ions are treated as classical particles, and the energy and pressure contribution is given by

$$\begin{aligned} E_3 &= - \left( \frac{2\sqrt{\pi}e^3}{3\sqrt{kT}} \right) \left( \sum_s N_s z_s^2 \theta_s \right)^{3/2} \tau(x) \\ &\times \left( 1.5 - 1.5 \frac{TN_e \theta'_e}{\sum_s N_s z_s^2 \theta_s} \frac{\partial \eta}{\partial T} - \frac{\tau(x)'}{\tau(x)} T \frac{\partial x}{\partial T} \right) \\ &= -1.037 \times 10^{-22} \frac{1}{\sqrt{T(\text{eV})}} \left( \sum_s N_s z_s^2 \theta_s \right)^{3/2} \tau(x) \\ &\times \left( 1.5 - 1.5 \frac{TN_e \theta'_e}{\sum_s N_s z_s^2 \theta_s} \frac{\partial \eta}{\partial T} - \frac{\tau(x)'}{\tau(x)} T \frac{\partial x}{\partial T} \right) \text{ (erg/cm}^3\text{)} \end{aligned} \quad (4.6)$$

$$\begin{aligned}
P_3 &= - \left( \frac{2\sqrt{\pi}e^3}{3\sqrt{kT}} \right) \left( \sum_s N_s z_s^2 \theta_s \right)^{3/2} \tau(x) \\
&\times \left( 0.5 - 1.5 \frac{TN_e \theta'_e}{\sum_s N_s z_s^2 \theta_s} \frac{\partial \eta}{\partial V} - \frac{\tau(x)'}{\tau(x)} T \frac{\partial x}{\partial V} \right) \\
&= -1.037 \times 10^{-22} \frac{1}{\sqrt{T(eV)}} \left( \sum_s N_s z_s^2 \theta_s \right)^{3/2} \tau(x) \\
&\times \left( 0.5 - 1.5 \frac{TN_e \theta'_e}{\sum_s N_s z_s^2 \theta_s} \frac{\partial \eta}{\partial V} - \frac{\tau(x)'}{\tau(x)} T \frac{\partial x}{\partial V} \right) \text{ (dyn/cm}^2\text{)} \quad (4.7)
\end{aligned}$$

where

$$\begin{aligned}
\theta_e &= \frac{F_{-1/2}(\eta)}{F_{1/2}(\eta)} & \theta'_e &= \theta_e \left( \frac{F'_{1/2}(\eta)}{F_{-1/2}(\eta)} - \theta_e \right) \\
\theta_s &= 1 & \theta'_s &= 0 \quad (s \neq e)
\end{aligned} \quad (4.8)$$

$$\begin{aligned}
\tau(x) &= 3x^{-3} \left[ \ln(1+x) - x + \frac{x^2}{2} \right] \simeq 1 - 0.75x \quad (x \ll 1) \\
\tau'(x) &= -\frac{3}{x} \left( \tau - \frac{1}{1+x} \right) \quad (4.9)
\end{aligned}$$

$$\begin{aligned}
x &= \left( \frac{2\sqrt{\pi}e^3}{k^{3/2}} \frac{1}{T^{3/2}} \right) \frac{F_{1/2}(\eta)}{F_{3/2}(\eta)} \left( \frac{\sum_{s \neq e} N_s z_s}{\sum_{s \neq e} N_s} \right) \left( \sum_s N_s z_s^2 \theta_s \right)^{1/2} \\
&= 1.9377 \times 10^{-10} \frac{1}{T^{3/2}(eV)} \frac{F_{1/2}(\eta)}{F_{3/2}(\eta)} \left( \frac{\sum_{s \neq e} N_s z_s}{\sum_{s \neq e} N_s} \right) \left( \sum_s N_s z_s^2 \theta_s \right)^{1/2} \quad (4.10)
\end{aligned}$$

$$\frac{\partial \eta}{\partial T} = -\frac{3}{T} \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} = -1.5 \frac{1}{\theta_e T} \quad (4.11)$$

$$\frac{\partial \eta}{\partial V} = -2 \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} = -\frac{1}{\theta_e} \quad (4.12)$$

$$\frac{\partial x}{\partial T} = x \left\{ -\frac{3}{2T} + \left[ \theta_e - \frac{3F_{1/2}(\eta)}{F_{3/2}(\eta)} + \frac{N_e \theta'_e}{2 \sum_s N_s z_s^2 \theta_s} \right] \frac{\partial \eta}{\partial T} \right\} \quad (4.13)$$

$$\frac{\partial x}{\partial V} = x \left\{ -\frac{1}{2V} + \left[ \theta_e - \frac{3F_{1/2}(\eta)}{F_{3/2}(\eta)} + \frac{N_e \theta'_e}{2 \sum_s N_s z_s^2 \theta_s} \right] \frac{\partial \eta}{\partial V} \right\} \quad (4.14)$$

## IV. Atomic Internal Structure Contribution

### (Ionization and Excitation)

If we set  $E_{o,1} = 0$  (neutral ground state), then the internal contribution may be expressed as

$$E_4 = \sum_{s \neq e}^Z N_s E_{s,1} + \sum_{s \neq 1}^Z \left[ \sum_i N_{s,i} (E_{s,i} - E_{s,1}) \right]. \quad (4.15)$$

If we set  $E_{Z,1} = 0$  (fully ionized), then

$$E_4 = \sum_{s \neq e}^Z N_s (E_{s,1} - E_{o,1}) + \sum_{s \neq 1}^Z \left[ \sum_i N_{s,i} (E_{s,i} - E_{s,1}) \right] \quad (4.16)$$

where  $s$  is the index for ionization degrees with  $s = 0$  for neutral, and  $i$  is the index for energy levels.

## 5. Calculations of Radiative Properties

### 5.1. Absorption, emission, and scattering coefficients

The radiative properties of the plasma are calculated using cross sections obtained from detailed atomic physics calculations (e.g., ATBASE and ATTABLE). The absorption and emission coefficients include contributions from free-free (bremsstrahlung), bound-free (photoionization), and bound-bound (photoexcitation) transitions.

The general forms for the absorption coefficient and emissivity can be written respectively as [Mihalas, 1978]

$$\begin{aligned} \kappa_\nu = & \sum_k \sum_j \left\{ \sum_n \sum_{m>n} \left[ n_{njk} - \left( \frac{g_{njk}}{g_{mjk}} \right) n_{mjk} \right] \alpha_{nm}^{bb}(\nu) \right. \\ & \left. + \sum_{n>n'} [n_{njk} - n_{njk}^* e^{-h\nu/k_B T}] \alpha_n^{bf}(\nu) + n_e n_{j+1,k} \alpha^{ff}(\nu) (1 - e^{h\nu/k_B T}) \right\} \quad (5.1) \end{aligned}$$

and

$$\eta_\nu = \left( \frac{2h\nu^3}{c^2} \right) \sum_k \sum_j \left\{ \sum_n \sum_m \left( \frac{g_{njk}}{g_{mjk}} \right) n_{mjk} \alpha_{nm}^{bb}(\nu) + \sum_{n>n'} [n_{njk} - n_{njk}^* e^{-h\nu/k_B T} \alpha_n^{bf}(\nu) + n_e n_{j+1,k} \alpha^{ff}(\nu) e^{h\nu/k_B T}] \right\} \quad (5.2)$$

where  $n'$  is determined by the photoionization cutoff energy  $h\nu_{n'} = \Phi_{jk}(n_0/n')^2$ , and

$$n_{njk}^* = n_{0,j+1,k} n_e (1.66 \times 10^{-22}) \times \left( \frac{g_{njk}}{g_{0,j+1,k}} \right) T^{-3/2} e^{(\Phi_{jk} - \Delta E_{mn0})/T}$$

is the LTE population of state  $n_{njk}$  using the computed ion density of the post-ionization ground state. The  $\alpha$ 's represent the cross sections of the various transitions and are defined below. The indices  $j$  and  $k$  again refer to the ionization state and gas species, respectively.  $h$ ,  $c$ ,  $k_B$ , and  $\nu$  as usual represent Planck's constant, the speed of light, Boltzmann's constant, and the photon frequency,  $\alpha^{bb}$ ,  $\alpha^{bf}$ , and  $\alpha^{ff}$  are the absorption cross sections for bound-bound, bound-free, and free-free processes, respectively. All other symbols have been defined in previous sections.

The terms from left to right in equations (5.1) and (5.2) represent the contributions from bound-bound, bound-free, and free-free transitions. The second term inside each of the square brackets in eq. (5.1) is the contribution from stimulated (induced) emission to the absorption coefficient. Note that in the high density limit (i.e. LTE),  $n_m = n_n (g_m/g_n) \exp(-\Delta E/T)$  and  $n_n = n_n^*$ . Thus, the correction for stimulated emission for all 3 transitions reduces to the LTE form,  $1 - \exp(-h\nu/k_B T)$ , and the relation between the absorption coefficient and emissivity is given by the well-known Kirchoff-Planck relation,  $\eta_\nu = \kappa_\nu B_\nu$  (where  $B_\nu$  is the Planck function). Because this relation will not be true in general, EOSOPC tabulates the opacities for absorption and emission separately.

The cross section for free-free transitions in the hydrogenic approximation is

$$\alpha^{ff}(\nu) = \frac{(2.40 \times 10^{-37} \text{cm}^5)(Z)^2 \overline{g_{ff}}}{(h\nu)^3 T^{1/2}}, \quad (5.3)$$

where  $h\nu$  is the photon energy in eV. For the free-free Gaunt factor, we use a fitting formula for the results of Karzas and Latter. The bound-free cross sections are calculated with the Hartree-Fock model (dipole approximation). For highly excited Rydberg states, a hydrogenic approximation is used.

The bound-bound cross section is a function of the oscillator strength,  $f_{nm}$ , and the line shape function  $L(\Gamma, \nu)$ :

$$\alpha_{nm}^{bb} = (2.65 \times 10^{-2} \text{cm}^2 \text{s}) f_{nm} L(\Gamma, \Delta\nu). \quad (5.4)$$

EOSOPC will compute the line shapes using either a Lorentzian profile or a Voigt profile (default). The expression for the Lorentzian profile is

$$L_L(\Gamma \Delta\nu) = \frac{\Gamma/4\pi^2}{(\Delta\nu)^2 + (\Gamma/4\pi)^2},$$

where  $\Delta\nu$  is the photon frequency shift from the line center, and  $\Gamma$  is the damping factor due to natural, Doppler (thermal), and Stark broadening:

$$\Gamma = \Gamma_{\text{nat}} + \Gamma_{\text{Dop}} + \Gamma_{\text{Stark}}.$$

The Voigt line profile is

$$L_V(\Gamma, \Delta\nu) = H(\Gamma, \Delta\nu \Delta\nu_D) / (\pi^{1/2} \Delta\nu_D),$$

where  $\Delta\nu_D$  is the Doppler shift, and  $H(\Gamma, \Delta\nu/\Delta\nu_D)$  is the Voigt function, which depends on the frequency shift and the ratio of the Doppler damping factor to the sum of the natural plus collisional damping factors.

The scattering coefficient is used in calculating the radiative transport properties of the plasma. EOSOPC considers contributions from Thomson electron scattering and plasma waves. We use the classical form of the Thomson cross section, which is reliable for low to moderate X-ray energies ( $\lesssim 10^4$  eV):

$$S_\nu^T = \frac{8\pi e^4}{3m^2 c^4} n_e^\dagger, \quad (5.5)$$

where  $n_e^\dagger$  is the effective electron density in  $\text{cm}^{-3}$ , which includes contributions from each bound electron for which the photon energy is greater than its binding energy. Thomson scattering becomes a dominant contributor to the Rosseland opacity at relatively high temperatures and low densities.

The scattering of photons by plasma oscillations can occur at low photon energies and high electron densities ( $\gtrsim 10^{19} \text{cm}^{-3}$ ). The plasma wave scattering coefficient can be written as

$$S_\nu^p = \begin{cases} (w_P^2 - w^2)^{1/2}/c, & \text{if } h\nu \leq hw_P, \\ 0, & \text{if } h\nu > hw_P, \end{cases} \quad (5.6)$$

where

$$w_P = (4\pi^2 n_e / m_e)^{1/2}$$

is the plasma frequency,  $e$  is the electron charge, and  $m_e$  is the electron mass.

## 5.2. Opacity calculations

The Rosseland and Planck mean opacities are obtained by integrating the absorption, emission, and scattering coefficients over the photon energy. The Rosseland mean opacities are generally used in determining the transport characteristics of radiation through a medium, while the Planck mean opacities are used to calculate the rates of energy exchange between the plasma and radiation. EOSOPC computes Planck and Rosseland mean group opacities for up to 50 photon energy bins. This limitation can be easily lifted by changing the array parameters. Planck mean opacities for absorption and emission are computed separately because local thermodynamic equilibrium cannot be assumed.

The Planck mean group opacities for absorption and emission in the photon energy range from  $x_g \equiv h\nu_g/k_B T$  to  $x_{g+1} \equiv h\nu_{g+1}/k_B T$  are defined by

$$\sigma_{P,g}^A = \frac{1}{\rho} \frac{\int_{x_g}^{x_{g+1}} dx B_\nu(T_R) \kappa_\nu}{\int_{x_g}^{x_{g+1}} dx B_\nu(T_R)} \quad (5.7)$$

and

$$\sigma_{P,g}^A = \frac{1}{\rho} \frac{\int_{x_g}^{x_{g+1}} dx B_\nu \eta_\nu}{\int_{x_g}^{x_{g+1}} dx B_\nu(T_R)} \quad (5.8)$$

where  $\rho$  is the mass density, and  $\kappa_\nu$  and  $\eta_\nu$  are defined in eqs. (5.1) and (5.2).  $B_\nu(T_R)$  is the Planck function characterized by the radiation temperature  $T_R$ . The Rosseland mean group opacity is determined from a weighted average of the inverse of the total extinction coefficient,  $\kappa_\nu + x_\nu$ . In this case, the radiative coefficients are weighted by the temperature derivative of the Planck function:

$$\sigma_{R,g} = \frac{1}{\rho} \frac{\int_{x_g}^{x_{g+1}} dx \left( \frac{\partial B_\nu}{\partial T_R} \right)}{\int_{x_g}^{x_{g+1}} dx \left( \frac{\partial B_\nu}{\partial T_R} \right) \frac{1}{\kappa_\nu + s_\nu}}. \quad (5.9)$$

In most cases the absorption and emission coefficients are not smoothly varying functions of the photon energy. Thus, to evaluate the opacity integrals with the desired accuracy,  $\kappa_\nu$  and  $\eta_\nu$  must be evaluated at a number of strategically placed points. Examples of this include points on either side of each photoionization edge, and several points in the vicinity of each bound-bound transition energy.

The integration scheme employed to evaluate the group opacities is a trapezoidal method using logarithmic interpolation between adjacent points. By placing a reasonable number of mesh points near each line transition energy ( $\sim 5-10$ ) and photoionization edge (2), the numerical accuracy of the integration is approximately a few per cent. Thus, the numerical inaccuracies are smaller than the uncertainties introduced by our physical models with the consideration of the complexity of the problem.

The mean opacities integrated over all photon energies are computed by the group opacities:

$$\sigma_{\text{P.tot}} = \frac{\left[ \sum_g \sigma_{\text{P},g} \int_{x_g}^{x_{g+1}} dx B_\nu(T_R) \right]}{\int_0^\infty dx B_\nu(T_R)} \quad (5.10)$$

and

$$\sigma_{\text{R.tot}} = \frac{\int_0^\infty dx \left( \frac{\partial B_\nu}{\partial T_R} \right)}{\left[ \sum_g \sigma_{\text{R},g}^{-1} \int_{x_g}^{x_{g+1}} dx \left( \frac{\partial B_\nu}{\partial T_R} \right) \right]}. \quad (5.11)$$

## 6. Input/Output File Descriptions

The EOSOPC code uses 3 types of input files, 9 result output files, 2 types of debugging output files, and 1 scratch file. The files are listed in Table 6.1, along with their default logical unit numbers (LUN), names (for UNIX systems), types, and a brief description of their contents. There are two atomic data input files for each element: ATOMIC.DATn and PIXFIT.DATn. Here ‘n’ is the abundance order of the element in the mixture. For a plasma with a single element, n=1. For a plasma with M different elements, n=1 corresponds to the most abundant element in the mixture, n=2 corresponds to the second most abundant element, and so on. Both ATOMIC.DATn and PIXFIT.DATn are obtained by running the ATBASE suite of atomic physics codes.

The user defines the parameters of a problem with the namelist input file EOSOPC.INP. Through it, the user defines the composition of the plasma, sets up the temperature and density grid over which the physical properties of the plasma will be evaluated, requests plotting and debugging output, and overrides default values of various parameters. The names and a brief description of the namelist input variables are listed in Table 6.2.



**Table 6.1. Input/Output Files**

Default Unit Number	Default Name (UNIX)	Type	Description
1	EOSOPC.INP	Input	Namelist input file
2		Scratch	Scratch file
9	EOSOPC.OUT	Output	Standard formatted output file
12	CNRDEOS0	Output	Not used
13	CNRDEOS	Output	Output data table for CONRAD input
17	RATE.MATRIX	Output	Debugging output of $N \times N$ statistical equilibrium matrix
22	EOS1VSN.DAT	Output	Output EOS for plotting $x \rightarrow$ ion densities $y \rightarrow \bar{Z}$ , energy, pressure
23	EOS1VST.DAT	Output	Output EOS for plotting $x \rightarrow$ temperature $y \rightarrow \bar{Z}$ , energy, pressure
24	EPS2VST.DAT	Output	Output EOS for plotting $x \rightarrow$ temperature $y \rightarrow$ heat capacity $\frac{d\bar{Z}}{dT}, \frac{dP}{dT}$
25	ABSCO.DAT	Output	Output absorption coefficients for plotting $x \rightarrow$ photon energy $y \rightarrow$ B-B absorption coefficient B-F absorption coefficient $x \rightarrow$ F-F absorption coefficient Total absorption coefficient
26	EMICO.DAT	Output	Output emissivity coefficient for plotting $x \rightarrow$ photon energy $x \rightarrow$ B-B, B-F, F-F, Total
27	GOPATY.DAT	Output	Output multigroup opacities for plotting $x \rightarrow$ photon energy $y \rightarrow$ Planck emission opacity Planck absorption opacity Rosseland mean opacity
30-35	TOMIC.DATN	Input	Atomic data files for element “ $n$ ”
36-40	PIXFIT.DATN	Input	Photoionization cross sectn data file for element “ $n$ ”
41-45	ATOMIC.CHKN	Output	For checking atomic.datn
41-50	PIXFIT.CHKN	Output	For checking pixfix.datn

**Table 6.2. Namelist Input Variables**

Variable	Type	Default Value	Description
(1) Plasma Composition			
NGASES	IV	1	Number of gas species (maximum = 5)
NZGAS	IV	0	Atomic number of each gas (in the sequence of abundance)
ATOMWT	RV	0	Atomic weight of each gas (amu)
FRACSP	RV	0	Fractional abundance of each gas species
(2) Temperature and Density Grid			
NTEMP	IV	1	Number of plasma temperature (maximum = 20)
NDENS	IV	1	Number of densities (maximum = 20)
NTRD	IV	0	Number of radiation temperature (not used)
TPLSMA	RV	0	Plasma temperature (eV)
DENION	RV	0	Total ion density (1/cm <sup>3</sup> )
TRAD	RV	0	Radiation temperature (eV) (not used)
DLGTMP	RV	0	Logarithmic increment in plasma temperature
DLGDEN	RV	0	Logarithmic increment in density
DLGTRD	RV	0	Logarithmic increment in radiation temperature
DTHEAT	RV	0	Fractional temperature increment for specific heat and charge state derivative calculation
(3) Photon Energy Grid			
EIPHON	RV	0	Minimum photon energy to be considered (eV)
EIPHON	RV	0	Maximum photon energy to be considered (eV)
NGROPS	IV	0	Number of photon energy groups for multigroup opacity calculation (maximum = 50)
GROPBD	RV	0	Photon energy group boundaries
(4) Computational Options			
ICOMPT (1)	IV	0	= 0: Compute heat capacity and $\frac{dE}{dn}$ ; > 0: not compute
ICOMPT (2)	IV	0	= 0: Compute pressure derivative $\frac{dP}{dT}$ ; > 0: not compute
ICOMPT (3)	IV	0	= 0: Compute opacity > 0: Not compute

**Table 6.2. Namelist Input Variables (Continued)**

Variable	Type	Default Value	Description
(5) Model Selections			
IMODEL (1)	IV	3	= 1: Using Saha model = 2: Using Coronal model = 3: Solving steady-state rate equations
IMODEL (2)	IV	2	= 1: Using LTE to estimate level occupation probability = 2: Solving steady-state rate equations
IMODEL (3)	IV	2	= 1: No pressure ionization = 2: Using Mihalas-Hummer model for $w_{jm}$
IMODEL (5)	IV	0	= 0: Using $\bar{g} = 0.2$ for Stark broadening calculation > 0: On line calculation for $\bar{g}$
(6) Criterion			
CRITAS (1)	RV	$10^{-2}$	Convergent criterion in iterative calculations
(7) Output Options			
IOUTPT (1)	IV	0	=2: Output EOS and opacity data table in CONRAD input format
IPLOT (1)	IV	0	= 1: Output (EOS1 vs. N) for plotting = 0: no
IPLOT (2)	IV	0	= 1: Output (EOS1VST) for plotting = 0: No
IPLOT (3)	IV	0	= 1: Output (EOS2VST) for plotting = 0: No
IPLOT (4)	IV	0	= 1: Output absorption coefficient emissivity, and multigroup opacity for plotting
(8) Debugging Output			
IDEBUG (1)	iv	0	> 0: Dumping out input atomic data for checking = 0: No
IDEBUG (2)	IV	1	= 1: No debugging output in CRE calculation = 0: Yes

All results for equations of state and opacities are written to the formatted file EOSOPC.OUT. Equation of state and opacity data tables used for CONRAD (a radiation hydrodynamics code) input are written in the formatted file CNRDEOS. Additional output useful for plotting results is contained in files EOS1VSN.DAT, EOS1VST.DAT, EOS2VST.DAT, ABSCO.DAT, EMICO.DAT, and GOPATY.DAT.

## 7. Computational Procedures

(1) To calculate equations of state and opacities of plasmas by using EOSOPC, one should first run the ATBASE suite of atomic physics codes to generate related atomic data files: ATOMIC.DAT $n$  and PIXFIT.DAT $n$ . In generating ATOMIC.DAT $n$  by using ATTABLE code, one should be remember that the maximum temperature grid point is 10 and the maximum density grid point is 4. This limitation may be lifted in a later version by changing some of the array parameters.

(2) Check the abundance of each element in the mixture, and assign an index ' $n$ ' for it. ' $n$ ' is the array index of the element in array NZGAS, ATOMWT, and FRACSP. ' $n$ ' should be the order of the abundance, i.e.,  $n = 1$  for the most abundant species,  $n = 2$  for the second abundant species, and so on.

(3) Design a temperature and density grid over which the physical properties of the plasma will be evaluated. For the current version of EOSOPC, the maximum temperature and density grid points is set to 20. But this limitation can easily be expanded by changing the array parameter 'MXTEMP' and 'MXDENS'. The user should keep in mind that this code does not include molecular effects, hence it may provide incorrect results for low temperature and high density cases where molecular effects are important.

(4) Determine the range of photon energy over which radiative properties will be evaluated.

(5) Design a group structure of photon energy for multigroup opacity calculations. The EOSOPC can set up the group structure automatically in a prudent manner. It checks every important ionization edge carefully and uses these important edges as the group boundaries.

(6) Select proper models for the calculations. This is the most crucial step of the calculation. Here, we list several most often used model selections:

- **Saha-Boltzmann model without pressure ionization:**  $\text{imodel}(1)=3$ ,  $\text{imodel}(2)=1$ ,  $\text{imodel}(3)=1$ ,  $\text{imodel}(5)=0$ .
- **Saha-Boltzmann model with pressure ionization:**  $\text{imodel}(1)=3$ ,  $\text{imodel}(2)=1$ ,  $\text{imodel}(3)=2$ ,  $\text{imodel}(5)=0$ .
- **Coronal model without pressure ionization:**  $\text{imodel}(1)=2$ ,  $\text{imodel}(2)=1$ ,  $\text{imodel}(3)=1$ ,  $\text{imodel}(5)=0$ .
- **Coronal model with pressure ionization:**  $\text{imodel}(1)=2$ ,  $\text{imodel}(2)=1$ ,  $\text{imodel}(3)=2$ ,  $\text{imodel}(5)=0$ .

The user should keep in mind that the Coronal model assumes that all ions are in the ground state; it can not provide information for emissivity. Hence this model is inadequate for opacity calculations.

- **CRE model without pressure ionization:**  $\text{imodel}(1)=3$ ,  $\text{imodel}(2)=2$ ,  $\text{imodel}(3)=1$ ,  $\text{imodel}(5)=0$ .
- **CRE model with pressure ionization:**  $\text{imodel}(1)=3$ ,  $\text{imodel}(2)=2$ ,  $\text{imodel}(3)=2$ ,  $\text{imodel}(5)=0$ .

(7) Edit namelist file.

(8) Run EOSOPC

## 8. Subroutine and Common Block Descriptions

A schematic flow diagram for EOSOPC is shown in Fig. 8.1. This code is written in standard FORTRAN 77 and is easy to implement on various different computer systems. In what follows, subroutines and common blocks are described for EOSOPC.

### *Main program*

The main program in this code is EOSOPC. It does no detailed calculations itself but leads the whole code from accepting input through the calculations to the printing and storing of results. It should be noted that the main program also controls the loops over temperatures, densities and photon energy groups.

Subroutine Called: TITLE, PARAM, INPUT, FILES, EOS, HVGROP, HVMESH, ABEMCO, OPACTY, WRIOUT, and RESULT.

### *Subroutines*

**ABEMCO:** This subroutine calculates the absorption and emission coefficients for values of the photon energy in a particular energy group.

Called from: Main program

Subroutines called: BBSTMP, BFSTMP, FFSPTM, SCSPTM.

**ATDATA:** This subroutine does interpolation for rate coefficients of various atomic collisional/radiative processes at a particular temperature/density points. Linear interpolation method is used.

Called from: ENERGY, NONLTE.

Subroutine called: none.

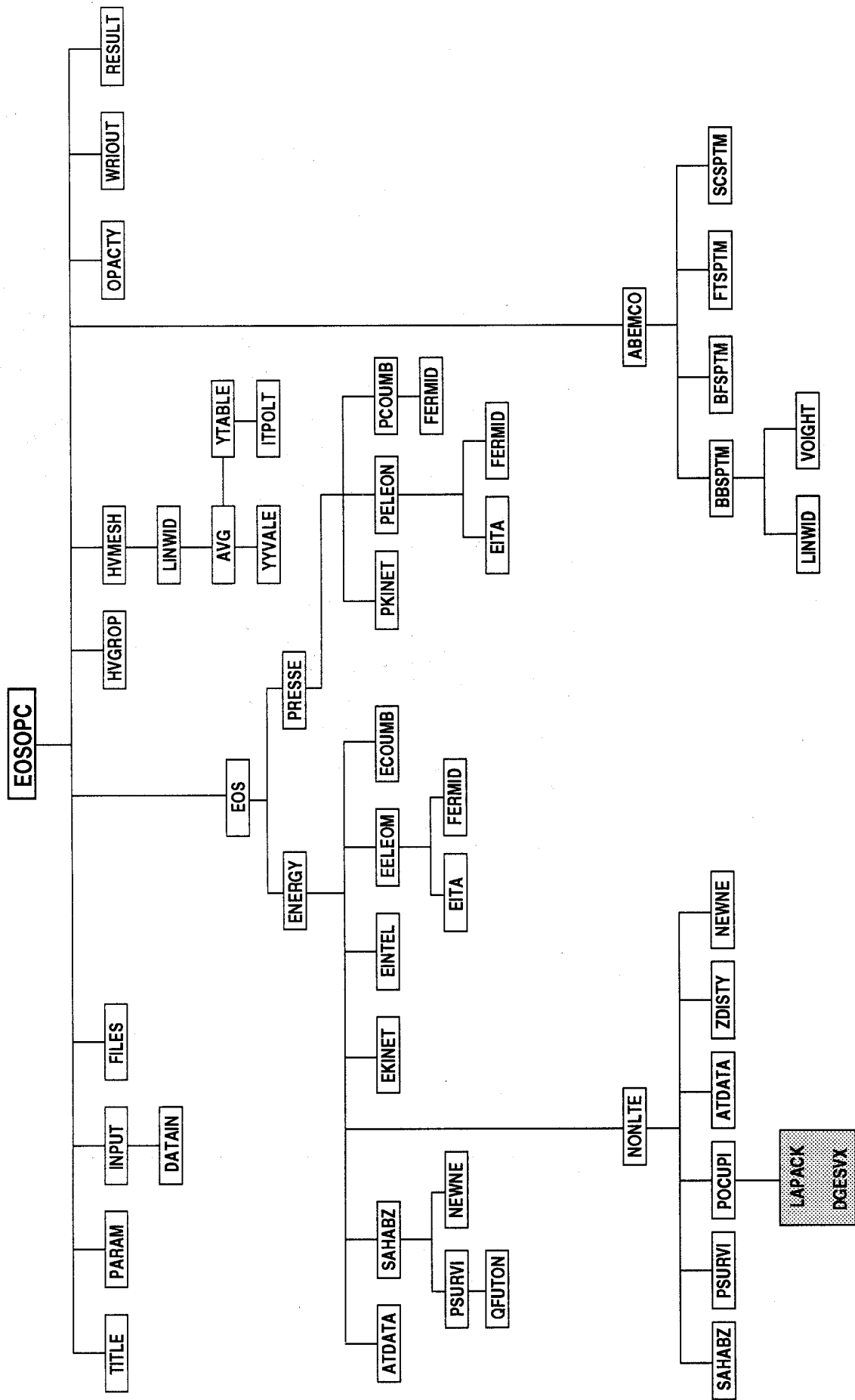


Figure 8.1. Flow diagram for EOSOPC.

**AVG:** This subroutine calculates the average f-f Gaunt factor which is used for the Stark broadening calculation.

Called from: LINWID.

Subroutines called: YYVALUE, EXTROP.

**AVGFF:** This subroutine interpolates Karzas and Latter's data table for radiative free-free Gaunt factor.

Called from: FFSPTM.

Subroutines called: none.

**BBSPTM:** This subroutine calculates bound-bound radiative absorption and emission coefficients.

Called from: ABEMCO.

Subroutines called: LINWID.

**BFSPTM:** This subroutine calculates bound-free radiative absorption (photoionization) and emission coefficients.

Called from: ABEMCO.

Subroutines called: none

**BESSEL:** This routine evaluates the values of the modified Bessel function.

Called from: YVALUE.

Subroutine called: none.

**BESSEP:** This routine evaluates the values of derivative the modified Bessel function.

Called from: YVALUE.

Subroutine called: none.

**DATAIN:** This routine reads and stores all the relevant atomic data tables generated from the ATBASE suite of atomic physics calculation codes.

Called from: INPUT.

Subroutines called: none



**ECOUMB:** This subroutine calculates the Debye-Hückel correction term to the plasma energy.

Called from: ENERGY.

Subroutines called: EITA, FERMID.

**EELEON:** This routine calculates the contribution of a partially degenerate electron gas to the plasma energy.

Called from: ENERGY.

Subroutines called: EITA.

**EINTEL:** This subroutine calculates the internal contributions (excitation and ionization) to the energy of plasma.

Called from: ENERGY.

Subroutines called: none.

**EKINET:** This subroutine calculates the translation energy of atoms/ions in the plasma.

Called from: ENERGY.

Subroutines called: none.

**EITA:** This routine calculates the degeneracy factor of a partially degenerate electron gas.

Called from: ECOUMB, EELEON, PCOUMB, PELEON.

Subroutines called: none.

**ENERGY:** This routine controls the calculations of energy of the plasma.

Called from: EOS.

Subroutines called: ATDATA, SAHSBZ, NONLTE, EKINET, EINTEL, EELEON, ECOUMB.

**EOS:** This subroutine controls the calculations of equations of state.

Called from: Main program.

Subroutines called: ENERGY, PRESSE

**EXTROP:** This routine does extrapolation for a specific function.

Called from: AVG.

Subroutines called: none.

**FERMID:** This routine evaluates the values of the Fermi-Dirac integrals of orders  $-1/2$ ,  $1/2$ ,  $3/2$ , and the derivative of order  $-1/2$  by using the Rational Chebyshev approximation.

Called from: ECOUMB, EELEON, PCOUMB, PELEON, EITA.

Subroutines called: none.

**FILES:** This routine opens files for storing output data.

Called from: Main program.

Subroutine called: none.

**FFSPTM:** This routine calculates radiative free-free absorption and emission coefficients.

Called from: ABEMCO.

Subroutine called: AVGFF.

**HVGROP:** This routine sets up group structure of photon energy for multigroup opacity calculations.

Called from: Main program.

Subroutine called: none.

**HVMESH:** This routine constructs a mesh of photon energy for evaluating radiative absorption and emission coefficients.

Called from: Main program.

Subroutine called: LINWID.

**ITPOLT:** This routine does interpolation for a specific function.

Called from: YTABLE.

Subroutine called: none.

**INPUT:** This routine controls the primary input of the code.

Called from: Main program.

Subroutines called: DATAIN.

**LINWID:** This subroutine evaluates line widths for bound-bound transitions.

Called from: BBSPTM, HVMESH.

Subroutines called: AVG.

**NEWNE:** This routine determines new electron density for next iteration calculation.

Called from: SAHABZ, NONLTE.

Subroutines called: none.

**NONLTE:** This routine controls the whole CRE calculation with the inclusion of pressure ionization effects.

Called from: ENERGY.

Subroutines called: SAHABZ, PSURVI, POCUPI, ATDATA, ZDISTY, NEWNE.

**OPACTY:** This routine does integration for absorption and emission coefficients to obtain group opacity for a specific group.

Called from: Main program.

Subroutines called: none.

**PARAM:** This routine assigns some important parameters for the calculations.

Called from: Main program.

Subroutines called: none.

**PCOUMB:** This subroutine calculates the Debye-Hückel correction term to the plasma pressure.

Called from: PRESSE.

Subroutines called: EITA, FERMID.

**PELEON:** This routine calculates the contribution of a partially degenerate electron gas to the plasma pressure.

Called from: PRESSE.

Subroutines called: EITA.

**PKINET:** This subroutine calculates the pressure coming from the translational motion of atoms/ions in the plasma.

Called from: PRESSE.

Subroutines called: none.

**PRESSE:** This routine controls the calculation of pressure in a plasma.

Called from: EOS.

Subroutine called: PCOUMB, PELEON, PKINET

**POCUPI:** This routine solves rate equations to determine the level occupation probabilities.

Called from: NONLTE.

Subroutines called: LAPACK package.

**PSURVI:** This routine calculates level survival probabilities under specific plasma conditions by using the Mihalas-Hummer model.

Called from: SAHABZ, NONLTE.

Subroutines called: QFUTON.

**QFUTON:** This subroutine evaluates the values of Q function which is used for describing microfield distribution in plasmas.

Called from: PSURVI.

Subroutines called: none.

**RESULT:** This subroutine organizes and writes out EOS and multigroup opacity results in the format of CONRAD input file.

Called from: Main program.

Subroutines called: none.

**SCSPTM:** This subroutine calculates the electron scattering coefficient.

Called from: ABEMCO.

Subroutines called: none.

**SAHABZ:** This subroutine calculates ionization distribution and level populations using Saha-Boltzmann model.

Called from: ENERGY, NONLTE.

Subroutines called: PSURVI, NEWNE.

**TITLE:** This routine marks the title of the code.

Called from: Main program.

Subroutines called: none.

**VOIGT:** This routine calculates spectrum line shape by using the Voigt profile.

Called from: BBSPTM.

Subroutines called: none.

**WRIOUT:** This routine organizes and outputs results at each temperature and density loop.

Called from: Main program.

Subroutines called: none.

**YVALUE:** This routine evaluates the values of Y function which is proportional to the electron collisional bound-bound excitation cross section.

Called from: AVG.

Subroutines called: YTABLE, BESSEL, BESSEP.

**YTABLE:** This routine does interpolation for Y function.

Called from: YVALUE.

Subroutines called: ITPOLT.

**ZDISTY:** This routine determines ionization distribution of the plasma using average rate coefficients.

Called from: NONLTE.

Subroutine called: none.

## 9. Common Blocks

Listed in Table 8.1 are the common blocks used in EOSOPC. For each common block, the variable name, type, dimensions, and brief description of each variable is provided. In most cases, the dimensions of variables are specified by quantities defined in parameter statements. These parameters are:

Parameter	Description
MXGASS	Maximum number of gas species
MXATOM	Maximum number of ionization stages (per gas species)
MXSHEL	Maximum number of subshells in an electronic configuration
MXLEVL	Maximum number of atomic levels
MXTRAN	Maximum number of atomic transitions
MXTEMP	Maximum number of temperature grid points
MXDENS	Maximum number of density grid points
MXGROP	Maximum number of photon energy groups
MXHVPT	Maximum number of grid point in photon energy mesh per group

Table 8.1. Common Blocks

COMMON/GASES/

Variable	Type	Dimensions	Units	Description
NGASES	I*4	—	—	Number of gas species in the problem
NZGAS	I*4	MXGASS	—	Atomic number of each gas species
ATOMWT	R*8	MXGASS	amu	Atomic weight of each gas species
AVGATW	R*8	—	amu	Average atomic weight of the plasma
<b>COMMON/ATOMST/</b>				
LVMX	I*4	MXGASS	—	Number of levels of each gas species
IONBOD	I*4	MXGASS MXATOM	—	The first level index of each ion in a specific gas species
ILMBDI	I*4	MXGASS	—	The first level index of each gas species
LVID	I*4	MXLEVL	—	Atomic energy level index
IONSTG	I*4	MXLEVL	—	Ionization stage to which each level belongs
CONFIG	C*40	MXLEVL	—	Electronic configuration of each level
TERM	C*6	MXLEVL	—	LS term expression of each level
EVVV	R*8	MXLEVL	eV	Atomic energy of each level
GGGG	R*8	MXLEVL	—	Degeneracy of each level
MSHELL	I*4	MXLEVL	—	Number of shell of each electronic configuration

COMMON/ATOMST/ (Continued)

Variable	Type	Dimensions	Units	Description
EBIND	R*8	MXLEVL MXSHEL	2*Ry	Binding energy of each shell
VVJ	R*8	MXLEVL	—	J value of each level. If there is no fine structure, VVJ < 0.
RBAR	R*4	MXLEVL MXSHEL	$a_0$	Orbit radius of each atomic shell: $\bar{r}$
RZBAR	R*4	MXLEVL MXSHEL	$a_0^2$	$\bar{r}^2$
<b>COMMON/FUALUS/</b>				
MXFVN	I*4	MXGASS	—	Number of oscillator strengths of each gas species
ILMBD2	I*4	MXGASS	—	The start point of oscillator strength of each gas species in storing array
IDHLOS	I*4	MXTRAN	—	Transition index of each transition (upper *10000 + lower)
FLH	R*8	MXTRAN	—	Absorption oscillator strength
SPONHL	R*8	MXTRAN	s <sup>-1</sup>	Radiative spontaneous DECAY RATE



## COMMON/PHOTCS/

Variable	Type	Dimensions	Units	Description
PII0	R*8	MXLEVL * MXSHEL	eV	Ionization threshold of each subshell
CS0	R*8	MXLEVL * MXSHEL	MB	Photoionization cross section at threshold
BETA	R*8	MXLEVL * MXSHEL	—	Fitting parameter $\beta$ for photoionization cross section
SPH	R*8	MXLEVL * MXSHEL	—	Photoionization cross section fitting parameter $\phi$

\*Photoionization cross sections are fit to:

$$\sigma(\nu) = \sigma(\nu_1) \left\{ \beta \left( \frac{\nu}{\nu_1} \right)^\phi + (1 - \beta) \left( \frac{\nu}{\nu_1} \right)^{\phi+1} \right\}, \quad \nu \geq \nu_1$$

## COMMON/COEFFS/

Variable	Type	Dimensions	Units	Description
NTTEMP	I*4	MXGASS	—	Number of temperature points in rate coefficient table of each gas species
NTNDEN	I*4	MXGASS	—	Number of electron density points in rate coefficient table of each gas species
TEMPTB	R*8	MXGASS*11	eV	Temperature mesh points in rate coefficient table
DENETB	R*8	MXGASS*11	cm <sup>-3</sup>	Electron density mesh points in rate coefficient table
MXCBB	I*4	MXGASS	—	Total number of bound-bound transitions in each gas species
ILMBD3	I*4	MXGASS	—	The start point of bound-bound transition data of each gas species in storing array
IDHLBB	I*4	MXTRAN	—	Bound-bound transition index (upper * 10000 + lower)
EXITBB	R*8	MXTRAN*11	cm <sup>3</sup> s <sup>-1</sup>	Electron collisional excitation coefficient
DXITBB	R*8	MXTRAN*11	cm <sup>3</sup> s <sup>-1</sup>	Electron collisional deexcitation coefficient
MCXBF	I*4	MXGASS	—	Total number of bound-free transitions in each gas species
ILMBD4	I*4	MXGASS	—	The start point of bound-free transition data of each gas species in storing array
IDHLBF	I*4	MXTRAN	—	Bound-free transition index (10000 * upper + lower)
COLLBF	R*8	MXTRAN*11	cm <sup>3</sup> s <sup>-1</sup>	Electron collisional ionization rate coefficient
COLLBF	R*8	MXTRAN*11	cm <sup>3</sup> s <sup>-1</sup>	Electron collisional recombination rate coefficient
RADIFB	R*8	MXTRAN*11	cm <sup>3</sup> s <sup>-1</sup>	Radiative recombination rate coefficient
DIELFB	R*8	MXTRAN*11*5	cm <sup>3</sup> s <sup>-1</sup>	Dielectronic recombination rate coefficient

**COMMON/SKPARM/**

Variable	Type	Dimensions	Units	Description
DECC	R*8	MXLEVL	2*Ry	Transition energy to the closest neighbor level
RJI	R*8	MXLEVEL	$a_0$	$\bar{\nu}$ of the initial state
RFF	R*8	MXLEVEL	$a_0$	$\bar{\nu}$ of the final state
GRATIO	R*8	MXLEVEL	—	Ratio of degeneracies of initial and final states

**COMMON/TDMESH/**

NTEMPE	I*4	—	—	Number of electron temperature grid points
NDENST	I*4	—	—	Number of ion density grid points
NTRAD	I*4	—	—	Number of radiation temperature grid points
DLGTMP	R*8	—	—	Log 10 increment in temperature mesh
DLGDEN	R*8	—	—	Log 10 increment in ion density mesh
DLGTRD	R*8	—	—	Log 10 increment in radiation temperature mesh
TFLSMA	R*8	MXTEMP	eV	Plasma temperature grid
DENION	R*8	MXDENS	cm <sup>-3</sup>	Ion density grid
TRAD	R*8	MXTEMP	eV	Radiation temperature grid
DTHEAT	R*8	—	—	Percentage increment of temperature/density for $\frac{dE}{dT}, \frac{dP}{dT}, \frac{dE}{dn}, \frac{dP}{dn}$ calculation

COMMON/COEFFS/

Variable	Type	Dimensions	Units	Description
EEEE	R*8	MXTEMP*MXDENS	3/G	Specific energy
PPPP	R*8	MXTEMP*MXDENS	dyne cm <sup>-2</sup>	Pressure
AVZZ	R*8	MXTEMP*MXDENS	—	Average charge state
EITI	R*8	MXTEMP*MXDENS	—	Degeneracy factor for a partially degenerate electron gas
DEDT	R*8	MXTEMP*MXDENS	3 g <sup>-1</sup> eV <sup>-1</sup>	$\frac{dE}{dT}$
DEDN	R*8	MXTEMP*MXDENS	3 cm <sup>3</sup> g <sup>-1</sup>	$\frac{dE}{dn}$
DZDT	R*8	MXTEMP*MXDENS	eV <sup>-1</sup>	$\frac{dZ}{dT}$
DNEE	R*8	MXTEMP*MXDENS	cm <sup>-3</sup>	Electron density
DPDT	R*8	MXTEMP*MXDENS	dyne cm <sup>-2</sup> eV <sup>-1</sup>	$\frac{dP}{dT}$
DPDN	R*8	MXTEMP*MXDENS	dyne cm	$\frac{dP}{dn}$

## COMMON/OPACS/

Variable	Type	Dimensions	Units	Description
NGROPS	I*4	—	—	Number of photon energy groups
GROBPD	R*8	MXGGROP+1	eV	Group boundaries
EIPHON	R*8	—	eV	Minimum photon energy in the calculation
EFPHON	R*8	—	eV	Minimum photon energy in the calculation
HV	R*8	MXHVPT	eV	Photon energy mesh for absorption and emission coefficients calculations
MESHPT	I*4	—	—	Number of mesh points in photon energy mesh
ABBBCO	R*8	MXHVPT	cm <sup>-1</sup>	Absorption coefficient (b-b)
EMBBCO	R*8	MXHVPT	cm <sup>-1</sup>	b-b emission coefficient
ABBFCO	R*8	MXHVPT	cm <sup>-1</sup>	b-f absorption coefficient
EMBFCO	R*8	MXHVPT	cm <sup>-1</sup>	b-f emission coefficient
ABFFCO	R*8	MXHVPT	cm <sup>-1</sup>	f-f absorption coefficient
EMFFCO	R*8	MXHVPT	cm <sup>-1</sup>	f-f emission coefficient
SCATTCO	R*8	MXHVPT	cm <sup>-1</sup>	Electron scattering coefficient
ABTOT	R*8	MXHVPT	cm <sup>-1</sup>	Total absorption coefficient
EMTOT	R*8	MXHVPT	cm <sup>-1</sup>	Total emission coefficient
OPAC1	R*8	MXGGROP	cm <sup>2</sup> g <sup>-1</sup>	Planck mean group opacity (absorption)
OPAC2	R*8	MXGGROP	cm <sup>2</sup> g <sup>-1</sup>	Planck mean group opacity (emission)
OPAC3	R*8	MXGGROP	cm <sup>2</sup> g <sup>-1</sup>	Rosseland mean group opacity
OPTOT1	R*8	MXTEMP*MXDENS	cm <sup>2</sup> g <sup>-1</sup>	Total Planck mean opacity (absorption)
OPTOT2	R*8	MXTEMP*MXDENS	cm <sup>2</sup> g <sup>-1</sup>	Total Planck mean opacity (emission)
OPTOT3	R*8	MXTEMP*MXDENS	cm <sup>2</sup> g <sup>-1</sup>	Total Rosseland mean opacity

## COMMON/OPASS/

Variable	Type	Dimensions	Units	Description
OPGRA	R*8	MXTEMP*MXDENS* MXGROP	cm <sup>2</sup> g <sup>-1</sup>	Rosseland group mean opacity
OPGPA	R*8	MXTEMP*MXDENS* MXGROP	cm <sup>2</sup> g <sup>-1</sup>	Planck group mean opacity (absorption)
OPGPE	R*8	MXTEMP*MXDENS* MXGROP	cm <sup>2</sup> g <sup>-1</sup>	Planck group mean opacity (emission)

## COMMON/DISTRI/

FRACSP	R*8	MXGASS	—	Fractional abundance of different gas species
FRACIZ	R*8	MXGASS*MXATOM	—	Fractional abundance of ionization stages
FRACLV	R*8	MXLEVL	—	Fractional occupation probabilities of each level

## COMMON/CONTRL/

IMODEL	I*4	10	—	Switch for model selections
ICOMPT	I*4	10	—	Switch for computation processes selections
IOUTPT	I*4	10	—	Switch for output data selections
ORITAS	I*4	10	—	Computation criterion
IPLOT	I*4	10	—	Plotting output selections
IDEBUG	I*4	10	—	Debugging output selections

## Acknowledgments

Funding has been provided by Kernforschungszentrum Karlsruhe through Fusion Power Associates.

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