Calculation of Neutral Beam Deposition Accounting for Excited States

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1 Abstract

Large-scale neutral-beam auxillary heating of plasmas has led to new plasma operational regimes which are often dominated by fast ions injected via the absorption of an energetic beam of hydrogen neutrals. An accurate simulation of the slowing down and transport of these fast ions requires an intimate knowledge of the hydrogenic neutral deposition on each flux surface of the plasma. As a refinement to the present generation of transport codes, which base their beam deposition on ground-state reaction rates, a new set of routines, based on the excited states of hydrogen, is presented as mechanism for computing the attenuation and deposition of a beam of energetic neutrals. Additionally, the numerical formulations for the underlying atomic physics for hydrogen impacting on the constituent plasma species is developed and compiled as a numerical database. Sample results based on this excited state model are compared with the ground-state model for simple plasma configurations.

2 Introduction

As new operational plateaus (H-mode and supershot) have been reached in tokamaks, plasma simulation codes (TRANSP and SNAP) have been required to refine their underlying physics models to accurately reproduce experimental diagnostic measurements. One significant change in these regimes over the previous L-mode and ohmic plasmas has been an increase in the importance of fast ion populations injected via the neutral heating beams. While these fast ion populations may not explain the physics of the transport and confinement of these regimes, an accurate simulation of these regimes cannot be completed without an improved treatment of the spatial absorption of the energetic neutral atoms in the plasma.

Under the present generation of transport codes, the neutral beam attenuation is nominally based on simple models that allow only for ionization or

charge exchange events via the ground state of the beam atoms. While such models have advantages in both speed and ease of implementation, recent modelling, which includes the effect of the beam excited state populations in the calculation of the beam attenuation, indicates that their inclusion can significantly alter the beam deposition. [1] In the past, such large uncertainties did not alter simulation results, because beam ions represented only a small fraction of the total ion population in the plasma. Furthermore, the computational effort associated with the inclusion of the neutral beam excited state populations represented a sizable increase in code run time, which, when coupled to the small uncertainties, did not strongly motivate their inclusion in the simulations. While this computational effort may still pose a problem, the uncertainties in the beam neutral populations are believed to be no longer acceptable.

To facilitate the inclusion of the beam neutral excited states in the computation of the neutral beam attenuation through the plasma, a new set of codes has been developed. These codes are divided into two packages: 1) a pre-processor package for generating a database of the underlying atomic physics; and 2) a beam-attenuation package for computing beam deposition into ionization and charge exchange channels. Inherent in the design of these codes was the need to insure computational speed, but yet to retain a measure of flexibility. Speed was required to insure routines that would not significantly increase the computational load associated with the present generation of transport codes. Flexibility was deemed necessary to handle variations in plasma species mix, species temperature, and different beam energy components, as well as to allow the introduction of updated atomic physics cross-sections. These features have been achieved by pre-processing the atomic physics for each plasma species into databases for the reaction rates of interest, i.e., ionization, charge exchange, excitation, de-excitation, and radiative decay. Interpolation within these tables provides a rapid mechanism for computing reaction rates for subsequent use in the numerical solutions of the beam deposition. Further increases in speed are obtained by the use of efficient algorithms for the numerical solution of the coupled, ordinary-differential-equations associated with the beam deposition calculation.

Ultimately, the beam attenuation code returns a "zone-averaged" set of reaction rates that relate the ionization and charge exchange rates for each plasma species to the results of a simple ground state calculation for the zone. This ratio isolates the reaction rates used in this code, so that if alternate reaction rates are used in a different transport code, they may be re-scaled to include this effect.

3 ATOMIC PHYSICS DATA-BASE

The atomic physics reaction rates for the beam-deposition routine are generated with two codes for plasma species impact processes, *erate.f* and *prate.f*, and one

code for neutral hydrogen radiative decay, *rrate.f*. The general philosophy of these codes is that each generates appropriate output files in ASCII format for ionization, charge exchange and excitation/de-excitation events associated with a particular plasma species. The rates are computed based on an isotropic, Maxwellian plasma population and a mono-directional, mono-energetic neutral beam population and are given by

$$\langle \sigma v \rangle = \frac{1}{2} \int_0^\infty dE_p f(E_p) \int_{-1}^1 d\mu \sigma(E_c) (v_p^2 + v_o^2 - 2\mu v_p v_o), \quad (1)$$

where $f(E_p)$ is a Maxwellian energy distribution for a plasma species at temperature T (eV),

$$f(E_p) = \frac{2E_p^{1/2}}{\pi^{1/2} T^{3/2}} \exp(-E_p/T), \quad (2)$$

$\sigma(E_c)$ is the cross-section for the reaction of interest, with E_c as the effective collision energy,

$$E_c = E_p + \frac{A_o}{A_p} E_o + 2\mu \left(\frac{A_o A_p E_p}{E_o} \right)^{1/2}, \quad (3)$$

and μ as the $\cos \theta$ angle in velocity space. The variable v_p is the plasma particle velocity at energy E_p ,

$$v_p = \left(\frac{2E_p}{A_p} \right)^{1/2}, \quad (4)$$

and v_o is the velocity of the beam at energy E_o ,

$$v_o = \left(\frac{2E_o}{A_o} \right)^{1/2}, \quad (5)$$

where A_p is the atomic number of the plasma particle and A_o is the atomic number of the beam species. All generated rates are in units of $\text{cm}^3 \text{s}^{-1}$.

The integration is completed by Laguerre and Gaussian quadratures over the energy and the angular integrals, respectively. The reaction rates are relatively insensitive to the choice of integration order, except for cases when the beam energy and plasma temperatures are comparable. Typically, 16 point Laguerre and 8 point Gaussian quadrature have proven sufficient to generate accurate reaction rates, especially when compared to the inherent uncertainties in the present set of cross-sections. The total number of reaction rates within each file is dictated by the choice of the maximum number of states, *nmaz*, which is determined by the Lorentz ionization limit, memory requirements, and speed. These factors bear directly on the operational aspects of the beam-deposition code and will be discussed later.

The first file generated by each of the impact process codes is comprised of reaction rates for impact ionization events and represents a single vector of

reaction rates for each quantum state of the beam up to the prescribed maximum state (a total of $nmax$ reaction rates at each beam energy and temperature value in a table). The second file generated (but only for the ion species) is comprised of a vector of charge exchange reaction rates (again, a total of $nmax$ reaction rates per table location). These charge exchange rates do not attempt to track the excited-states of the plasma particle after the charge exchange event, but instead represent the total probability of charge exchange with a plasma species. The final file generated is a matrix which contains rates for excitation and de-excitation events (a total of $nmax^2$ reaction rates per table location). The diagonal of this matrix is comprised of a sum over excitation events which move particles to states above the prescribed maximum state, and ultimately contribute to the ionization reaction rate. The total number of reaction rates at each beam energy and plasma temperature table location contains $nmax(nmax + 2)$ distinct rates.

The first impact process code, *erate.f*, computes tables of Maxwellian averaged reaction rates, $\langle\sigma v\rangle_{nkl}$ (cm^3s^{-1}), for electrons interacting with a mono-energetic hydrogen beam. Three subscripts n, k, l refer to reaction rate locations within a table corresponding to the quantum state of the neutral hydrogen beam, the electron temperature, and the beam energy, respectively. Choices for the electron temperature T_k within the table are based on a log spacing between the minimum and maximum table temperatures and are required input values. However, because the electron velocities far exceed the beam velocity, no actual beam energy dependence appears in the calculation of these electron reaction rates. But, for convenience and consistency with other reaction rate tables, the tables for the electron species are dimensioned to have a beam energy dependence. Consequently, all reaction rates within the table are set to zero except for those which correspond to the lowest beam energy component, $l = 1$.

The first file *erate.f* returns contains an array of ionization reaction rates at temperature T_k for each quantum state n . The analytical form of the cross-sections for the electron impact ionization process (and also for the excitation reactions) allows Eq. (1) to be integrated analytically so that the reaction rates are given by [2]

$$\langle\sigma v\rangle_{nkl} = 9.56(10^{-6}) \frac{\exp(-E_n)}{(E_n^{2.33} + 4.38E_n^{1.72} + 1.32E_n)T_k^{1.5}}, \quad (6)$$

where

$$E_n = \frac{13.598}{T_k n^2}, \quad (7)$$

and T_k is the electron temperature (eV).

The final file generated corresponds to a matrix of reaction rates, $\langle\sigma v\rangle_{mnkl}$, for electron excitation and de-excitation of neutral hydrogen. The additional subscript m refers to an event in which electron impact causes the transition of a beam particle from an initial quantum state given by m to a final quantum

state given by n . For excitation between the states $1s \rightarrow 2s$, $1s \rightarrow 2p$, $1 \rightarrow 3$, and $2 \rightarrow 3$, the reaction rates are computed via [3]

$$\langle \sigma v \rangle_{mnkl} = \exp \left\{ \sum_{i=1}^8 A_{imn} (\log T)^i \right\}, \quad (8)$$

where the A_{imn} are a set of fitting coefficients, which are listed in the subroutine *sigvee* in Appendix A. While the rates for the reactions $1s \rightarrow 2s$ and $1s \rightarrow 2p$ are computed, these rates are always combined into a single $1 \rightarrow 2$ rate. All other excitation rates are given by [2]

$$\langle \sigma v \rangle_{mnkl} = 5.19(10^{-6}) E_{mi}^{1.5} \frac{\exp(-E_{mn})}{T E_{ni}^{2.33}}, \quad (9)$$

where

$$E_{mi} = \frac{13.589}{m^2 T}, \quad (10)$$

and

$$E_{ni} = \frac{13.589}{n^2 T}, \quad (11)$$

and

$$E_{mn} = E_{mi} - E_{ni}. \quad (12)$$

The de-excitation rates are computed via the principle of detailed balance which relates a forward reaction to its reverse reaction. Hence, the de-excitation rates are given by [2]

$$\langle \sigma v \rangle_{mnkl, dexc} = \langle \sigma v \rangle_{nmkl, exc}(T') \frac{T' n^2}{T m^2}, \quad (13)$$

where

$$T' = T - E_{mn}, \quad (14)$$

and E_{mn} is given by Eq. (12).

Finally, the diagonal elements of this matrix represent excitation events above the maximum table value, n_{max} , and are given by

$$\langle \sigma v \rangle_{mnkl} = \sum_{n=n_{max}+1}^{n_{max}+n_{more}} \langle \sigma v \rangle_{mnkl}, \quad (15)$$

where n_{more} is an input value which dictates the number of extra reaction rates to include in the sum above the maximum value. At a value of $n_{more}=80$, the summation appears to change by no more than a 0.1% per additional term. Any additional benefit or accuracy gained by increasing the value of n_{more} is probably overshadowed by the uncertainties in the cross-sections themselves and represent an unnecessary increase in the computational load.

The second impact process code, *prate.f*, produces an array of Maxwellian averaged reaction rates for a hydrogenic ($Z=1$) plasma species interacting with a hydrogenic neutral beam. The reaction rates ($cm^3 s^{-1}$) are tabulated versus T/A and E_b/A_b , where T is the plasma species temperature (eV), A is the plasma species atomic number (amu), E_b is the beam energy (eV), and A_b is the beam atomic number (amu). Choices for E_b/A_b and T/A are based on a log spacing between the minimum and maximum input values for each parameter. This scaling facilitates the use of a single table for proton, deuterium and tritium plasma and beam species and as will be explained later allows for scaling to impurity species.

The first file this routine creates is a table of reaction rates for the impact ionization of the beam particles. This rate for each quantum state n is computed by substituting into Eq. (1) the expression for the ionization cross-section. The ground-state ionization cross-section is given by [1]

$$\sigma_{gs,ion} = 1.76(10^{-6})n^4 \left[1.6160D_\beta \left(\frac{1.0999(10^4)}{n^2 E} \right) + 0.2487D_\beta \left(\frac{6.9284(10^3)}{n^2 E} \right) \right], \quad (16)$$

where D_β is a tabulated function [4] that is listed in the subroutine *dbeta* of Appendix B and E is in units of eV/amu . One caveat to the use of this form of the ionization cross-section is the necessity to set to zero any non-physical, negative cross-section values. The ionization cross-sections for the higher excited states are computed based on scaling this ground state cross-section as per the loss cross-section which is discussed below. While such a scaling is valid for regions in which the loss cross-section is strongly dominated by ionization, the validity in the region where charge exchange becomes important has not been proven and is beyond the scope of this report. The ionization cross-section for the higher excited states is then

$$\sigma_{n,ion} = \sigma_{gs,ion} n^2 \left\{ \frac{1 - \exp[-0.10799(10^{-3})n^{-2}E^{-1}]}{1 - \exp[-0.10799(10^{-3})E^{-1}]} \right\}, \quad (17)$$

where E is the collision energy in eV/amu .

The second file generated by *prate.f* is a table of charge exchange rates. The generation of this table has been hampered by the un-availibilty of a complete set of cross-sections for the full range of quantum states required in the beam deposition code. As a consequence, the computation of charge exchange cross-sections are computed by first calculating a loss cross-section which includes both ionization and charge exchange and by then subtracting the ionization cross-section of Eqs. (16) or (17). This loss cross-section from a quantum state n is given by [1]

$$\sigma_{n,loss}(E) = 1.467(10^{-11})n^2 E^{-1} [1 - \exp(-0.10799(10^{-3})n^2 E)]. \quad (18)$$

Thus, the charge exchange cross-section is given by

$$\sigma_{n,cx}(E) = \sigma_{n,loss}(E) - \sigma_{n,ion}(E) \quad (19)$$

where if $\sigma_{n,cx}(E) < 0$, this cross-section is set to zero.

The final file that *prate.f* generates is a table of collisional excitation and de-excitation rates. In the interest of brevity and due to the complexity of these excitation cross-sections, the form for these reactions may be found in the subroutine *sigpnm* of Appendix B.[3], [5] As with the electrons, the de-excitation rates are computed using the principle of detailed balance. Hence, the cross-section for the de-excitation reaction $m \rightarrow n$, where $n < m$, is given by

$$\sigma_{mnkl}(E) = \sigma_{nmkl}(E_m) \frac{n^2 E_m}{m^2 E}, \quad (20)$$

where

$$E_m = E + E_{nm}, \quad (21)$$

with

$$E_{nm} = 13.598 (n^{-2} - m^{-2}) A^{-1}, \quad (22)$$

and A is the atomic number of the plasma species. Finally, the diagonal of this matrix represents a summation of reaction rates for excitation events that lead to states not explicitly contained within the table and is given by Eq. (15).

The final set of impact processes concern impurity reaction rates. A separate code has not been provided for these impurity reaction rates, because a reasonable approximation is to simply scale the hydrogenic reaction rates with the Z -number of the impurity (i.e., fully stripped He with $Z=2$). Such a scaling is possible, because the cross-sections for impurity impact processes may be normalized to Z [1], i.e.,

$$\sigma \left(\frac{E}{A} \right) = Z \sigma_z \left(\frac{E}{AZ} \right). \quad (23)$$

Based on this scaling, interpolation within the hydrogenic reaction rate tables is completed based on a temperature of $T/(AZ)$ and a beam energy of $E_b/(A_b Z)$. The true reaction rate for the impurity species is then this interpolated value multiplied by $Z^{3/2}$. As better cross-sections become available, the routine *prate.f* could readily be modified to generate a separate set of reaction rates for each of the impurities.

The final atomic physics code, *rrate.f*, computes a table of radiative decay rates for the various excited states of neutral hydrogen. No beam energy or plasma temperature dependence occurs in this table. Hence, with a dependence only on an initial and final quantum states, the table contains only n_{max}^2 elements. The radiative decay rates, $A_{mn}(s^{-1})$, for the transition $m \rightarrow n$ are given by [6]

$$A_{mn} = 8.02862(10^8) f_{mn} (n^{-2} - m^{-2}) n^2 m^{-2}, \quad (24)$$

where f_{nm} is the oscillator strength of the transition and is given by [7]

$$f_{mn} = 1.960281 nG [m(1 - n^2 m^{-2})]^{-3}, \quad (25)$$

where G is a Gaunt factor and is given by [7]

$$G = G_o + G_1 (1 - n^2 m^{-2})^{-1} + G_2 (1 - n^2 m^{-2})^{-2}, \quad (26)$$

with

$$G_0 = \begin{cases} 1.1330 & , n = 1 \\ 1.0785 & , n = 2 \\ 0.9935 + 0.2328n^{-1} - 0.1296n^{-2} & , n \geq 3 \end{cases}, \quad (27)$$

$$G_1 = \begin{cases} -0.4059 & , n = 1 \\ -0.2319 & , n = 2 \\ -0.6282n^{-1} + 0.5598n^{-2} - 0.5299n^{-3} & , n \geq 3 \end{cases}, \quad (28)$$

and

$$G_2 = \begin{cases} 0.0714 & , n = 1 \\ 0.02947 & , n = 2 \\ 0.3887n^{-2} - 1.181n^{-3} + 1.470n^{-4} & , n \geq 3 \end{cases}. \quad (29)$$

In summary, three codes must be run prior to use of the beam deposition code: *erate.f*, *prate.f* and *rrate.f*. These routines have been written in FORTRAN, and should be compiled with an appropriate flag set to continue code operation beyond underflow errors. With DEC-FORTRAN this amounts to the inclusion of a `-fpe3` as a compiler option. Once these codes have been run, the generated ASCII data files preclude the necessity of re-running the codes again except as revisions are made to the underlying atomic physics.

The total number of reaction rates generated by each program for $ntemp$ temperature locations, $nbeam$ beam locations and $nmax$ quantum states is:

Electron Ionization	$nbeam \cdot ntemp \cdot nmax$
Electron Charge Exchange	0
Electron Excitation	$nbeam \cdot ntemp \cdot nmax \cdot nmax$
Ion Ionization	$nbeam \cdot ntemp \cdot nmax$
Ion Charge Exchange	$nbeam \cdot ntemp \cdot nmax$
Ion Excitation	$nbeam \cdot ntemp \cdot nmax \cdot nmax$
Radiative Decay	$nmax \cdot nmax$

The total number of reaction rates is therefore

$$ntotal = nbeam \cdot ntemp \cdot nmax(3 + 2nmax) + nmax^2$$

with an additional $nbeam \cdot ntemp \cdot nmax(2 + nmax)$ rates for each additional impurity reaction rate table not based on the program *prate.f*.

4 DEPOSITION CODE

The zonal deposition routine, *exc_dep*, has been developed to compute the transfer of beam particles into plasma ionization and charge exchange channels, but with the inclusion of excited state populations up to either the Lorentz ionization limit or to the maximum number of reaction rates available in the tables. To isolate the under-lying atomic physics, the routine generates a set of “enhancement” factors that represent the ratio of ionization (or charge exchange) based on the excited-state model relative to a similiar calculation based on a ground-state model. The ground-state model, which is commonly used by the present generation of transport codes, assumes that the excited states instantaneously decay, so that the dynamics of the beam attenuation depend solely on ground-state ionization and charge exchange reaction rates. By introducing the “enhancement” factors, only minor modification of existing transport codes is required to include this effect in the beam deposition calculation. Additionally, an extensive revamping of the potentially different atomic physics associated with a transport code is no longer necessary.

The routine, in the present incarnation, is designed to be used with a neutral particle tracker. The tracker would supply zone-averaged plasma species mix, densities, and temperatures, as well as, beam energy, initial excited state populations, and the zonal width parameters. In this context, the zonal width is the travel distance of the beam across a region (typically between flux surfaces) through which the plasma parameters are deemed constant. The underlying physics is modelled by a convective differential equation for each of the quantum states of the beam, i.e.,

$$\frac{\partial I_n}{\partial t} + v_b \frac{\partial I_n}{\partial x} = \sum_{m=1}^{nord} Q'_{nm} I_m, \quad (30)$$

where I_n is the population intensity of the n -th excited state, v_b is the neutral beam velocity, *nord* is the number of states below the Lorentz ionization limit, and Q'_{nm} is the total reaction rate matrix for the zone. However, for beam deposition and attenuation, only the steady-state portion of the convective-differential equation need be considered. Therefore, Eq. (31) reduces to the ordinary differential equation

$$\frac{dI_n}{dx} = \sum_{m=1}^{nord} Q_{nm} I_m, \quad (31)$$

where the matrix Q_{nm} is given by

$$Q_{nm} = \frac{1}{v_b} \begin{cases} \sum_{\alpha=1}^{nspec} n_{\alpha} \langle \sigma v \rangle_{\alpha mn, ez} & m < n \\ - \left\{ \sum_{l=1}^{m-1} A_{ml, rad} + \sum_{\alpha=1}^{nspec} n_{\alpha} \left[\langle \sigma v \rangle_{\alpha m, ion} + \langle \sigma v \rangle_{\alpha m, cz} + \sum_{l=1}^{nmax} \langle \sigma v \rangle_{\alpha ml, ez} \right] \right\} & m = n \\ A_{mn, rad} + \sum_{\alpha=1}^{nspec} n_{\alpha} \langle \sigma v \rangle_{\alpha mn, ez} & m > n \end{cases} \quad (32)$$

where $A_{mn, rad}$ are the radiative decay rates, $\langle \sigma v \rangle_{\alpha mn, ez}$ is the Maxwellian averaged reaction rate for impact excitation or de-excitation due to species α , $\langle \sigma v \rangle_{\alpha mn, ion}$ is the Maxwellian averaged reaction rate for impact ionization due to species α , $\langle \sigma v \rangle_{\alpha mn, cz}$ is the Maxwellian averaged reaction rate for charge exchange with species α , n_{α} is the density of species α , $nspec$ is the number of plasma species, and $nmax$ is the total number of states in the reaction rate tables (as opposed to $nord$, the Lorentz limit).

The total number of states, $nmax$, relates to the total number of quantum states in the atomic physics databases and as such is simply a convenient value to terminate the tables. However, $nord$ is an estimate of the first quantum state of the neutral beam atoms which resides in the continuum. Excited state populations which fall into this or higher states may be treated as instantly auto-ionized. The value of the Lorentz ionization limit may be estimated by considering excited beam atoms moving at a velocity v_b in a magnetic field B . Such particles are subject to ionization by the Lorentz field $E_{L,c} = v_b \times B$. [1]

The critical field at which the ionization becomes unity for the Stark component with the strongest dipole field is given by

$$E_{L,c} = \frac{\epsilon_o}{16n^4}, \quad (33)$$

where ϵ_o is the classical electric field of the nucleus evaluated at the first Bohr radius. Hence, for a given beam velocity and magnetic field, the value of the highest level $nord$ above which levels may be treated as lying in the continuum is

$$nord = \frac{1}{2} \left(\frac{\epsilon_o}{|v_b \times B|} \right)^{1/4}. \quad (34)$$

The differentiation between $nord$ and $nmax$ is important to compute correctly the ionization rates in the excited state model.

Since the plasma parameters and therefore the reaction rates are constant throughout a zone, the calculation of the "enhancement" factors requires an integration of the population intensities across the zonal width. These integrated

intensities are folded into the ionization or charge exchange reaction rates to generate total loss rates for each plasma species channel. The loss rate F_α for charge exchange is

$$F_{\alpha,cx} = \sum_{m=1}^{nord} n_\alpha \langle \sigma v \rangle_{\alpha m, cx} \int_0^{w_z} dx I_m(x), \quad (35)$$

where n_α is the density of the plasma species α , $\langle \sigma v \rangle_{\alpha, m}$ is the charge exchange reaction rate for the plasma species α , $I_m(x)$ is the population intensity of the m -th quantum state across the zone, and w_z is the travel distance of the beam through the zone. The same general form applies to the calculation of the ionization rate, but the possibility of excitation events above the Lorentz ionization limit must also be included. Hence, the loss rate F_α for ionization is

$$F_{\alpha, ion} = \sum_{m=1}^{nord} n_\alpha \left\{ \langle \sigma v \rangle_{\alpha m, ion} + \langle \sigma v \rangle_{\alpha m m, ex} + \sum_{n=nord+1}^{nmax} \langle \sigma v \rangle_{\alpha m n, ex} \right\} \int_0^{w_z} dx I_m(x), \quad (36)$$

where $\langle \sigma v \rangle_{\alpha m, ion}$ is the ionization reaction rate for species α , $\langle \sigma v \rangle_{\alpha m m, ex}$ is the ionization reaction rate due to excitation events above the highest state available in the reaction rate tables ($> nmax$), and $\langle \sigma v \rangle_{\alpha m n, ex}$ is the ionization reaction rate due to excitation events above the Lorentz ionization limit, $nord$, but less than the maximum table value, $nmax$. The Lorentz ionization limit also introduces the possibility of a loss channel not due to any plasma species, but due to the auto-ionization of non-zero excited state populations which are above the Lorentz ionization limit as they enter a new zone. This loss rate is dealt with by summing these populations together and storing them as a separate ionization loss rate for the zone.

Finally, to complete the calculation of the enhancement factor, the loss rate via the ground state model must also be computed and then ratioed to the result of Eq.(35) or (36) as appropriate. The initial vector of excited states $I_m(x=0)$, which represents the population intensities of the beam entering the zone, is summed to find the initial beam intensity I_o , i.e.,

$$I_o = \sum_{m=1}^{nord} I_m(x=0). \quad (37)$$

This beam intensity is then used with the total charge exchange and ionization reaction rate for the ground-state, which is given by

$$\sigma_{tot, gs} = \frac{1}{v_b} \sum_{\alpha=1}^{nspec} n_\alpha [\langle \sigma v \rangle_{\alpha 1, ion} + \langle \sigma v \rangle_{\alpha 1, cx}], \quad (38)$$

where v_b is the beam velocity, and $\langle\sigma v\rangle_{\alpha 1, ion}$ and $\langle\sigma v\rangle_{\alpha 1, cx}$ are the ionization and charge exchange rates, respectively, for the collisions of the groundstate of the beam atom with plasma species α . This ground-state reaction rate is independent of the Lorentz ionization limit and ignores the effect of all excitation events above the Lorentz limit. The total beam population across the zone is then

$$I(x) = I_o \exp(-\sigma_{tot,gs}x). \quad (39)$$

Equation (39) is then integrated across the zone and combined with the ground-state charge exchange and ionization reaction rates to generate loss rates for each of the plasma species channels. Therefore, the charge exchange rate with species α is given by

$$F_{\alpha, cx, gs} = n_{\alpha} \langle\sigma v\rangle_{\alpha 1, cx} \frac{I_o}{\sigma_{tot,gs}} [1 - \exp(-\sigma_{tot,gs}w_z)], \quad (40)$$

and the ionization rate is given by

$$F_{\alpha, ion, gs} = n_{\alpha} \langle\sigma v\rangle_{\alpha 1, ion} \frac{I_o}{\sigma_{tot,gs}} [1 - \exp(-\sigma_{tot,gs}w_z)], \quad (41)$$

Finally, the enhancement factors are given by

$$f_{\alpha, ion} = \frac{F_{\alpha, cx}}{F_{\alpha, cx, gs}}, \quad (42)$$

and

$$f_{\alpha, cx} = \frac{F_{\alpha, ion}}{F_{\alpha, ion, gs}}, \quad (43)$$

where species $\alpha = 0$ of the ionization enhancement factors is reserved for the sum of auto-ionized initial populations that were above the Lorentz limit upon entering the zone.

The flow diagram in Fig. 1 illustrates the operational aspects of the above formalism as implemented in the FORTRAN code *exc_dep*. As with the atomic physics codes, this routine should be compiled with a flag set which allows program execution to continue beyond underflow errors. Prior to the first call to *exc_dep*, a call must be made to the routine *QREAD* to initialize and store the reaction rate matrices in the common block */TRRATE/*. In addition to initializing */TRRATE/*, the variables in the common block */gquad/* should be initialized by setting the zone quadrature order *ngmax* and by supplying the associated set of Gaussian quadrature ordinates and weights. Once the initialization is complete, the routine *exc_dep* may be called by specifying the zone plasma conditions via the variables of the common block */SPECI/* and the variables in the declaration of the subroutine. An explanation of each of the above variables and common blocks is provided either in the program file *exc_dep* of Appendix E or in the include file, *exc_dep.com* of Appendix F. After

a succesful calculation, the routine will return a value of $ierr=0$, the common block `/fficx/` will contain the enhancement factors for the zone, and the state intensity vector will contain the excited state populations at the zone edge. Within this common block, the variable `ffii(0)` is reserved for the instantaneous ionization associated with any of the excited state populations above the Lorentz limit.

5 RESULTS

Figure 2 illustrates typical ionization enhancement factors for a 60 keV/amu hydrogen beam impacting normally on a two species plasma composed of electrons and hydrogen. The plasma temperature ($T_e = T_i$) is parabolic with a peak temperature of 10 keV and an edge temperature of 90 eV at a minor radius of 80 cm. Likewise, the density profile ($n_e = n_i$) is parabolic with a centerline density of 10^{14} cm^{-3} and an edge density of 10^{13} cm^{-3} . The plasma is divided into 5 cm radial zones with a uniform magnetic field across the entire plasma. For this particular model, the enhancement factors start at ~ 1 at the plasma edge and then gradually rise as the beam passes into the plasma core to ~ 2.2 for the electron species and ~ 1.1 for the proton species. The enhancement factors begin near one because initially only the ground-state of the beam is populated. The increase can then be related to the equilibration of the ground-state with the excited states and the larger ionization reaction rates associated with these excited states. The large enhancement factor (~ 2.2) for the electron species should not be construed as a radical change in the overall ionization rate within the zone, because the electron impact ionization is normally small except for regions near the plasma edge. However, the enhancement factor for the proton species, which is much smaller (~ 1.1) can significantly affect the deposition profile since the overall ionization is strongly dominated by ion impact processes.

Figure 2 also addresses the sensitivity of the enhancement factor to the Lorentz ionization limit and hence the magnitude of the magnetic field. In particular, the magnetic field has been adjusted to 6, 0.5, and 0.01 T such that the number of excited states, *nord*, takes on values of 5, 10, and 15, respectively. As the number of excited states is increased, the magnitude of the enhancement factor for all the zones increases for the ion species but decreases for the electron species. Several effects interplay with each other to produce these trends. First, excitation events that previously led to states above the Lorentz limit are no longer ionization events and will therefore no longer contribute to the ionization enhancement factor. Second, the ionization rates for these higher excited states are much stronger than any of the preceeding lower excited states and will therefore increase the ionization when these states are strongly populated. Finally, increases in the overall attenuation of the beam populations may lead to decreases in those enhancement factors that contribute weakly to the overall

attenuation of the beam. With these observations, the increase in the ion ionization enhancement factor relates to the strong excitation of beam populations to the higher excited states and their subsequent rapid ionization. By a similar argument, the enhancement factor for the electron species is expected to also exhibit a comparable increase. However, since the beam attenuation is strongly dominated by ion impact processes, the large increase in the ion enhancement factor is indicative of an overall decline in the beam populations. This decline in beam populations manifests itself as a lower enhancement factor for the electron species.

Figure 3 illustrates typical ionization enhancement factors for the previously described plasma and beam conditions, but with the added complication of a helium species with $Z_{eff} = 1.5$. As with the previously described problem, the enhancement factor for all three species begins near one at the plasma edge and then gradually rises as the beam moves into the core regions. Likewise, decreases in the magnetic field cause an increase in the ionization enhancement factor for both the hydrogen and helium species, but a decrease in the enhancement factor for the electron species. Surprisingly, the enhancement factors for hydrogen and helium do not deviate from the same value until the magnetic field becomes relatively small. Additionally, the introduction of the new species causes a moderate decrease in the ionization enhancement factor for both the hydrogen and for the electron species. This decline is related to the additional attenuation of the beam populations caused by the helium species.

A significant complication of adding the excited states into a beam deposition model is potential for a sizable increase in the computational time. Table I illustrates typical timing information based on the previously described plasma and beam conditions. As expected, the run time appears to increase in a nearly linear manner as the number of species is increased. However, the run time appears to increase cubically with the number of excited states *per* species. Consequently, for a true heating beam which passes through edge zones with a strong perpendicular magnetic field and through core zones with a weak perpendicular magnetic field, the actual computation time is a sum over these times weighted for zone width. Furthermore, since the generated deposition represents only a single beam line, the increase in time will directly relate to the total number of beam lines used in any associated transport code.

6 Acknowledgements

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TABLE I. Average user time per 5 cm zone versus the perpendicular magnetic field and the number of plasma species in the zone. User time refers to the output from the *time* command during program execution on a DECstation 5000 under Ultrix 4.2. The test program was compiled with full optimization with DEC Fortran for ULTRIX RISC Systems Version 3.1.

		Average System Time per Zone (s)		
B_{perp} (T)	$nord$	2 species	3 species	4 species
6	5	0.16	0.17	0.18
0.5	10	0.39	0.48	0.56
0.01	15	1.98	2.58	3.04

FIGURE 1. Flow diagram of the routine exc_dep with a connection to a neutral beam particle tracker and associated transport code. The routine requires zone quadrature data and the reaction rate matrices to be passed via the transport code. Each call to the routine computes the enhancement factor for a single zone with associated beam and plasma conditions.

FIGURE 2. Impact ionization scale factor for a 60 keV/amu hydrogen beam impinging on a two species plasma composed of electrons and hydrogen. The plasma has a minor radius of 80 cm and each zone is 5 cm in width. The temperature profile is parabolic with a peak temperature of 10 keV and an edge temperature of 90 eV. The number n refers to the Lorentz ionization limit and is the total number of equations retained in the calculation.

FIGURE 3. Impact ionization scale factor for a 60 keV/amu hydrogen beam impinging on a three species plasma composed of electrons, hydrogen, and helium. The plasma has a Z_{eff} :1.5 over the entire plasma. The plasma has a minor radius of 80 cm and each zone is 5 cm in width. The temperature profile is parabolic with a peak temperature of 10 keV and an edge temperature of 90 eV. The number n refers to the Lorentz ionization limit and is the total number of equations retained in the calculation.

A Electron Reaction Rate Code *erate.f*

```

c   Program generates two ASCII files for electron impact
c   ionization of neutral hydrogen and electron impact
c   excitation of neutral hydrogen. The files contain
c   reaction rates ( $\text{cm}^3 \text{s}^{-1}$ ) for a Maxwellian electron
c   temperature and stationary hydrogen atom. The same
c   reaction rates may be readily used for non-stationary
c   hydrogen due to the large relative velocity of the electrons.
c
c   Parameters:
c   nsize -i number of grid electron temperature locations.
c   nord  -i number of hydrogen principal quantum states.
c
implicit real*8(a-h,o-z)
PARAMETER (NSIZE=10,NORD=10)
CHARACTER *64 FILEE,FILEI
C
c   get input data for program run
CALL INPUT(NMORE,FILEE,FILEI)
c   generate reaction rates
CALL ERATE(NMORE)
c   store electron ionization reaction rates
CALL OUTI(FILEI)
c   store electron excitation reaction rates
CALL OUTE(FILEE)
END

SUBROUTINE OUTI(FILE)
C   ROUTINE DUMPS ELECTRON IONIZATION ARRAY IN ASCII FORMAT
C   PARAMETERS:
C   FILE - name of output file
C
implicit real*8(a-h,o-z)
CHARACTER *64 FILE
PARAMETER (NSIZE=10,NORD=10)
DIMENSION IDIMSIZ(3)
COMMON/PARAM/TMIN,TMAX,TPOINT(NSIZE),NIMAX,NTGRID,
1 IROW(NORD)
COMMON/SIGV/ SVE(NSIZE,NSIZE,NORD,NORD),
1 SVI(NSIZE,NSIZE,NORD)
NTGRID=NSIZE
NIMAX=NORD
C
C   SET ARRAY SIZES FOR IONIZATION FILE DUMP
IDIMSIZ(1)=NTGRID
IDIMSIZ(2)=NTGRID
IDIMSIZ(3)=NIMAX
C   STORE DATA
irank=3
zero=0.0d+00
open(3,file=file,status='new')
write(3,*)irank
C
write(3,*)idimsiz(1)
write(3,*)idimsiz(2)
write(3,*)idimsiz(3)
do 20 i=1,idimsiz(1)
20  write(3,999)tpoint(i)
do 30 i=1,idimsiz(2)
30  write(3,999)zero
do 40 i=1,idimsiz(3)
40  write(3,*)i
C

```

```

      do 70 i=1,idimsiz(1)
        do 60 j=1,idimsiz(2)
          do 50 k=1,idimsiz(3)
50      write(3,999)SVI(i,j,k)
60      continue
70      continue
999    format(d12.5)
      RETURN
      END

```

```

      SUBROUTINE OUTE(FILE)
C      ROUTINE DUMPS ELECTRON EXCITATION ARRAY IN ASCII FORMAT
C      PARAMETERS:
C      FILE - OUTPUT FILE
C

```

```

      implicit real*8(a-h,o-z)
      CHARACTER *64 FILE
      PARAMETER (NSIZE=10,NORD=10)
      DIMENSION IDIMSIZ(4)
      COMMON/PARAM/TMIN,TMAX,TPOINT(NSIZE),NIMAX,NTGRID,
1      IROW(NC,RD)
      COMMON/SIGV/ SVE(NSIZE,NSIZE,NORD,NORD),
1      SVI(NSIZE,NSIZE,NORD)
      NTGRID=NSIZE
      NIMAX=NORD
C

```

```

C      SET ARRAY SIZES FOR EXCITATION FILE DUMP
C      IDIMSIZ(1)=NTGRID
C      IDIMSIZ(2)=NTGRID
C      IDIMSIZ(3)=NIMAX
C      IDIMSIZ(4)=NIMAX
C

```

```

      irank=4
      zero=0.0d+00
      open(3,file=file,status='new')
      write(3,*)irank
      do 10 i=1,irank
10     write(3,*)idimsiz(i)
C

```

```

      do 20 i=1,idimsiz(1)
20     write(3,999)tpoint(i)
      do 30 i=1,idimsiz(2)
30     write(3,999)zero
      do 40 i=1,idimsiz(3)
40     write(3,*)i
      do 45 i=1,idimsiz(4)
45     write(3,*)i
      do 70 i=1,idimsiz(1)
        do 60 j=1,idimsiz(2)
          do 50 k=1,idimsiz(3)
            do 49 l=1,idimsiz(4)
49      write(3,999)SVE(i,j,k,l)
50      continue
60      continue
70      continue
999    format(d12.5)
      RETURN
      END

```

```

      SUBROUTINE INPUT(NMORE,FILEE,FILEI)
C      ROUTINE INPUTS RELEVANT PROGRAM INFORMATION
C      PARAMETERS:
C      NIMAX - NUMBER OF EXCITATION GROUPS

```

```

C      NMORE - NUMBER OF ENHANCEMENT GROUPS
C      TMIN  - MINIMUM PLASMA TEMPERATURE
C      TMAX  - MAXIMUM PLASMA TEMPERATURE
C      NTGRID - NUMBER OF LOG SPACED ELECTRON
C              TEMPERATURE POINTS
C      TPOINT - ARRAY OF LOG SPACED TEMPERATURES
C      FILEE - ELECTRON EXCITATION FILENAME
C      FILEI - ELECTRON IONIZATION FILENAME
C
C      implicit real*8(a-h,o-z)
C      CHARACTER *64 FILEE,FILEI
C      PARAMETER (NSIZE=10,NORD=10)
C      COMMON/PARAM/TMIN,TMAX,TPOINT(NSIZE),NIMAX,NTGRID,
1      IROW(NORD)
C      WRITE(*,*)'INPUT THE MAXIMUM NUMBER OF STATES'
C      READ(5,*)NIMAX
C      DO 5 I=1,NORD
5      IROW(I)=I
C      WRITE(*,*)'INPUT THE NUMBER OF ENHANCEMENT STATES'
C      READ(5,*)NMORE
C      WRITE(*,*)'INPUT THE MINIMUM ENERGY GROUP (eV)'
C      READ(5,*)TMIN
C      WRITE(*,*)'INPUT THE MAXIMUM ENERGY GROUP (eV)'
C      READ(5,*)TMAX
C      WRITE(*,*)'INPUT THE NUMBER OF LOG SPACED TEMPS'
C      READ(5,*)NTGRID
C      AMULT=DEXP( (DLOG(TMAX)-DLOG(TMIN)) / (NTGRID-1))
C      TPOINT(1)=TMIN
C      DO 10 I=2,NTGRID
10      TPOINT(I)=TPOINT(I-1)*AMULT
C      WRITE(*,*)'READ OUTPUT FILENAME FOR EXCITATION'
C      READ(*,9999)FILEE
C      WRITE(*,*)'READ OUTPUT FILENAME FOR IONIZATION'
C      READ(*,9999)FILEI
C      RETURN
9999 FORMAT(A15)
C      END

C      SUBROUTINE ERATE(NMORE)
C      ROUTINE FILLS ELECTRON IMPACT REACTION RATE MATRIX
C      THOMAS A GIANAKON 7-5-90
C      PARAMETERS:
C      T      - ELECTRON TEMPERATURE (eV)
C      NIMAX  - LARGEST EXCITATION GROUP
C      NTGRID - TEMPERATURE ARRAY SIZE
C      SVE(,,) - EXCITATION REACTION RATE MATRIX
C      SVI(,,) - IONIZATION REACTION RATE
C
C      implicit real*8(a-h,o-z)
C      PARAMETER (NSIZE=10,NORD=10)
C      COMMON/SIGV/ SVE(NSIZE,NSIZE,NORD,NORD),
1      SVI(NSIZE,NSIZE,NORD)
C      COMMON/PARAM/TMIN,TMAX,T(NSIZE),NIMAX,NTGRID,
1      IROW(NORD)
C
C      COMPUTE REACTION RATE AT EACH TEMPERATURE
C      DO 500 L=1,NTGRID
C      COMPUTE THE ELECTRON IMPACT EXCITATION RATE
C      DO 20 M=1,NIMAX-1
C      DO 10 N=M+1,NIMAX
10      SVE(L,1,M,N)=SIGVEE(M,N,T(L))
20      CONTINUE
C
C      COMPUTE THE ELECTRON IMPACT DE-EXCITATION RATE

```

```

DO 40 M=2,NIMAX
DO 30 N=1,M-1
30   SVE(L,1,M,N)=SIGVED(M,N,T(L))
40   CONTINUE
C
C   COMPUTE THE ELECTRON IMPACT IONIZATION RATE
C   CALCULATE THE CONTRIBUTION OF EXCITATION TO  $i_{NIMAX}$ 
C   AND STORE ON DIAGONAL
IF(NMORE.NE.0)THEN
DO 190 M=1,NIMAX
SUML=0.0
SVI(L,1,M)=SIGVEI(M,T(L))
DO 185 JN=NIMAX+1,NIMAX+NMORE
185   SUML=SUML+SIGVEE(M,JN,T(L))
190   SVE(L,1,M,M)=SUML
ELSE
DO 191 M=1,NIMAX
SVI(L,1,M)=SIGVEI(M,T(L))
191   SVE(L,1,M,M)=0.0
END IF
C
500 CONTINUE
RETURN
END

```

```

FUNCTION SIGVEI(N,T)
c   Function computes the electron impact ionization
c   reaction rate of neutral hydrogen atom with
c   principal quantum number N integrated over a
c   Maxwellian electron temperature distribution.
c   The kinetic energy of the beam is neglected due
c   to the small hydrogen velocity relative to the
c   velocity of the plasma electrons.
C   REF. VRIENS & SMEETS
C   VALID AT ALL TEMPERATURES
C   PARAMETERS:
C   N - PRINCIPAL QUANTUM NUMBER OF THE NEUTRAL H
C   T - ELECTRON TEMPERATURE OF THE PLASMA (eV)
C
implicit real*8(a-h,o-z)
ENI=13.598/(N*N*T)
DENOM=(ENI**2.33+4.38*ENI**1.72+1.32*ENI)*T**1.5
SIGVEI=9.56E-06*DEXP(-ENI)/DENOM
RETURN
END

```

```

FUNCTION SIGVED(N2,N1,T)
C   Routine computes the collisional de-excitation
c   rate via the Principle of Detailed Balance.
c   Parameters:
C   N2 - EXCITED STATE  $i_{N1}$ 
C   N1 - DE-EXCITED STATE
C   T - ELECTRON TEMPERATURE (eV)
C
implicit real*8(a-h,o-z)
ENM=13.598*(1/(N1*N1)-1/(N2*N2))
T1=T+ENM
SIGVED=SIGVEE(N1,N2,T1)*T1*N1*N1/(T*N2*N2)
RETURN
END

```

```

FUNCTION SIGVEE(M,N,T)

```

```

c   Function computes the electron excitation rate
c   for neutral hydrogen from state at principle
c   quantum number m to principle quantum number n due
c   to a Maxwellian electron temperature distribution.
c   Parameters:
C     M - INITIAL QUANTUM STATE
C     N - FINAL QUANTUM STATE
C     T - ELECTRON TEMPERATURE
C     THE FIRST 9 COEFFICIENTS ARE THE 1S -> 2P
C     THE SECOND 9 COEFFICIENTS ARE THE 1 -> 3
C     THE THIRD 9 COEFFICIENTS ARE THE 1S -> 2S
C     THE FINAL SET IS THE 2 -> 3
C
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION A(0:8,2:3,2)
DATA A/-28.14949375869,10.09828023274,-4.771961915818,
11.467805963618,-0.2979799374553,3.861631407174D-02,
2-3.05168578077D-03,1.33547272099D-04,-2.47608839250D-06,
3-29.70637658833,7.919010878178,-2.324345724144,
40.3395454031585,-2.461414798949D-02,6.936731760702D-04,
50.0,0.0,0.0,
6-28.33259375256,9.587356325603,-4.833579851041,
71.41586337352,-2.537887918825D-01,2.800713977946D-02,
8-1.87140817257D-03,6.98666831841E-05,-1.1237585042E-06,
9-15.19633266088,2.4210211292538,-1.033796621854,
A0.1974466783434,-1.769417818291D-02,5.85374678691D-04,
B0.0,0.0,0.0/
IF((M.LT.2.01).AND.(N.LT.3.01))THEN
c   For the lower transitions use the fits based on
C   JANE ✓, PPL-TM-368
C   VALID ONLY FOR ENERGIES LESS THAN 10 keV
TLOG=DLOG(T)
SUM=0.0
DO 10 I=8,1,-1
10  SUM=TLOG*(A(I,N,M)+SUM)
SUM=SUM+A(0,N,M)
SIGVEE=DEXP(SUM)
IF((M.LT.1.01).AND.(N.LT.2.01))THEN
C   ADD CONTRIBUTION OF 1S -> 2S TO 1S -> 2P
SUM=0.0
DO 20 I=8,1,-1
20  SUM=TLOG*(A(I,2,2)+SUM)
SUM=SUM+A(0,2,2)
SIGVEE=SIGVEE+DEXP(SUM)
END IF
ELSE
c   For all other transitions use the results of
C   VRIENS & SMEETS
ENI=13.589/(N*N*T)
EMI=13.589/(M*M*T)
ENM=EMI-ENI
SIGVEE=5.19E-06*ENI**1.5*DEXP(-ENM)/(T*EMI**2.33)
END IF
RETURN
END

```


B Proton Reaction Rate Code *prate.f*

```

c   Program generates three ASCII files for the proton
c   impact ionization, charge exchange, and excitation
c   of a neutral hydrogen beam. The files contain reaction
c   rates rates (cm3 s-1) for an isotropic, Maxwellian
c   proton distribution and a mono-directional, mono-
c   energetic hydrogen beam. These rates readily scale
c   to impurity reactions with normalized temperature T/AZ
c   and energies E/AZ and a scale factor of Z-3/2.
c
c   Parameters:
c   nsize -i number of temperature and beam grid locations
c   nord  -i number of principle quantum states for
c           hydrogen to compute rates for.
c
c   Compilation:
c   Requires linking with a library to compute Gaussian
c   and Laguerre quadrature. The user will be prompted
c   for other relevant data.
C
implicit real*8(a-h,o-z)
PARAMETER (NSIZE=10,NORD=15)
CHARACTER *64 FILEE,FILEI,FILEC
C
c   get input data for program run
CALL INPUT(NMORE,FILEE,FILEI,FILEC)
c   generate rates
CALL PRATE(NMORE)
C   DUMP DATA
CALL OUTI(FILEI)
CALL OUTC(FILEC)
CALL OUTE(FILEE)
END

SUBROUTINE OUTI(FILE)
C   ROUTINE DUMPS ION IMPACT IONIZATION ARRAY
C   PARAMETERS:
C   FILE - NAME OF OUTPUT FILE
C
implicit real*8(a-h,o-z)
CHARACTER *64 FILE
PARAMETER (NSIZE=10,NORD=15)
DIMENSION IDIMSIZ(3)
COMMON/RRATE/SVIE(NSIZE,NSIZE,NORD,NORD),
1 SVII(NSIZE,NSIZE,NORD),SVIC(NSIZE,NSIZE,NORD)
COMMON/PARAM/AP,AB,TPOINT(NSIZE),EPOINT(NSIZE),
1 IROW(NORD),NEGRID,NIMAX,NTGRID
NTGRID=NSIZE
NIMAX=NORD
C
C   SET ARRAY SIZES FOR IONIZATION FILE DUMP
IDIMSIZ(1)=NTGRID
IDIMSIZ(2)=NEGRID
IDIMSIZ(3)=NIMAX
irank=3
zero=0.0d+00
open(3,file=file,status='new')
write(3,*)irank
do 10 i=1,irank
10  write(3,*)idimsiz(i)
C
do 20 i=1,idimsiz(1)
20  write(3,999)tpoint(i)

```

```

do 30 i=1,idimsiz(2)
30  write(3,999)epoint(i)
do 40 i=1,idimsiz(3)
40  write(3,*)i
do 70 i=1,idimsiz(1)
do 60 j=1,idimsiz(2)
do 50 k=1,idimsiz(3)
50  write(3,999)SVII(i,j,k)
60  continue
70  continue
999 format(d12.5)
RETURN
END

```

```

SUBROUTINE OUTC(FILE)
C  ROUTINE DUMPS CHARGE EXCGANGE ARRAY
C  PARAMETERS:
C  FILE - NAME OF OUTPUT FILE
C  _____
implicit real*8(a-h,o-z)
CHARACTER *64 FILE
PARAMETER (NSIZE=10,NORD=15)
DIMENSION IDIMSIZ(3)
COMMON/RRATE/SVIE(NSIZE,NSIZE,NORD,NORD),
1  SVII(NSIZE,NSIZE,NORD),SVIC(NSIZE,NSIZE,NORD)
COMMON/PARAM/AP,AB,TPOINT(NSIZE),EPOINT(NSIZE),
1  IROW(NORD),NEGRID,NIMAX,NTGRID
NTGRID=NSIZE
NIMAX=NORD
C  _____
C  SET ARRAY SIZES FOR IONIZATION FILE DUMP
IDIMSIZ(1)=NTGRID
IDIMSIZ(2)=NEGRID
IDIMSIZ(3)=NIMAX
C  _____
irank=3
zero=0.0d+00
open(3,file=file,status='new')
write(3,*)irank
do 10 i=1,irank
10  write(3,*)idimsiz(i)
do 20 i=1,idimsiz(1)
20  write(3,999)tpoint(i)
do 30 i=1,idimsiz(2)
30  write(3,999)epoint(i)
do 40 i=1,idimsiz(3)
40  write(3,*)i
do 70 i=1,idimsiz(1)
do 60 j=1,idimsiz(2)
do 50 k=1,idimsiz(3)
50  write(3,999)SVIC(i,j,k)
60  continue
70  continue
999 format(d12.5)
RETURN
END

```

```

SUBROUTINE OUTE(FILE)
C  ROUTINE DUMPS ION IMPACT EXCITATION ARRAY
C  PARAMETERS:
C  FILE - NAME OF OUTPUT FILE
C  _____
implicit real*8(a-h,o-z)

```

```

      CHARACTER *64 FILE
      PARAMETER (NSIZE=10,NORD=15)
      DIMENSION IDIMSIZ(4)
      COMMON/RRATE/SVIE(NSIZE,NSIZE,NORD,NORD),
1       SVII(NSIZE,NSIZE,NORD),SVIC(NSIZE,NSIZE,NORD)
      COMMON/PARAM/AP,AB,TPOINT(NSIZE),EPOINT(NSIZE),
1       IROW(NORD),NEGRID,NIMAX,NTGRID
      NTGRID=NSIZE
      NIMAX=NORD
C
C   SET ARRAY SIZES FOR IONIZATION FILE DUMP
      IDIMSIZ(1)=NTGRID
      IDIMSIZ(2)=NEGRID
      IDIMSIZ(3)=NIMAX
      IDIMSIZ(4)=NIMAX
C
      irank=4
      zero=0.0d+00
      open(3,file=file,status='new')
      write(3,*)irank
      do 10 i=1,irank
10      write(3,*)idimsiz(i)
C
      do 20 i=1,idimsiz(1)
20      write(3,999)tpoint(i)
      do 30 i=1,idimsiz(2)
30      write(3,999)epoint(i)
      do 40 i=1,idimsiz(3)
40      write(3,*)i
      do 45 i=1,idimsiz(4)
45      write(3,*)i
      do 70 i=1,idimsiz(1)
      do 60 j=1,idimsiz(2)
      do 50 k=1,idimsiz(3)
      do 49 l=1,idimsiz(4)
49      write(3,999)SVIE(i,j,k,l)
50      continue
60      continue
70      continue
999  format(d12.5)
      RETURN
      END

      SUBROUTINE INPUT(NMORE,FILEE,FILEI,FILEC)
C   ROUTINE INPUTS RELEVANT PROGRAM INFORMATION
C   PARAMETERS:
C       NIMAX - NUMBER OF EXCITATION GROUPS
C       NMORE - NUMBER OF ENHANCEMENT GROUPS
C       TMIN  - MINIMUM PLASMA TEMPERATURE
C       TMAX  - MAXIMUM PLASMA TEMPERATURE
C       NTGRID - NUMBER OF LOG SPACED POINTS
C       TPOINT - ARRAY OF LOG SPACED TEMPERATURES
C
      imp='it real*8(a-h,o-z)
      CHARACTER *64 FILEE,FILEI,FILEC
      PARAMETER (NSIZE=10,NORD=15)
      COMMON/QUAD/NGMAX,NLMAX,XG(20),WG(20),XL(40),WL(40)
      COMMON/PARAM/AP,AB,TPOINT(NSIZE),EPOINT(NSIZE),
1       IROW(NORD),NEGRID,NIMAX,NTGRID
      dimension endpts(2),bg(20),bl(40)
      WRITE(*,*)'INPUT THE MAXIMUM NUMBER OF STATES'
      READ(5,*)NIMAX
      if(nimax.ne.nord)then
        write(6,*)'Feature unavailable, setting variable'

```

```

        write(6,*)'equal to nord.'
        nimax=nord
    end if
    DO 5 I=1,NIMAX
5   IROW(I)=1
    WRITE(*,*)'INPUT THE NUMBER OF ENHANCEMENT STATES'
    READ(5,*)NMORE
C
    WRITE(*,*)'INPUT THE MINIMUM TEMPERATURE (eV)'
    READ(5,*)TMIN
    WRITE(*,*)'INPUT THE MAXIMUM TEMPERATURE (eV)'
    READ(5,*)TMAX
    WRITE(*,*)'INPUT THE NUMBER OF LOG SPACED TEMPS'
    READ(5,*)NTGRID
    WRITE(*,*)'INPUT THE PLASMA ATOMIC NUMBER'
    READ(5,*)AP
    AMULT=DEXP( (DLOG(TMAX)-DLOG(TMIN)) /(NTGRID-1))
    TPOINT(1)=TMIN
    DO 10 I=2,NTGRID
10  TPOINT(I)=TPOINT(I-1)*AMULT
C
    WRITE(*,*)'INPUT THE MINIMUM BEAM ENERGY (eV)'
    READ(5,*)EMIN
    WRITE(*,*)'INPUT THE MAXIMUM BEAM ENERGY (eV)'
    READ(5,*)EMAX
    WRITE(*,*)'INPUT THE NUMBER OF LOG SPACED BEAMS'
    READ(5,*)NEGRID
    WRITE(*,*)'INPUT THE BEAM ATOMIC NUMBER'
    READ(5,*)AB
    AMULT=DEXP( (DLOG(EMAX)-DLOG(EMIN)) /(NEGRID-1))
    EPOINT(1)=EMIN
    DO 20 I=2,NEGRID
20  EPOINT(I)=EPOINT(I-1)*AMULT
C
C   INTEGRATION COEFFICIENTS & WEIGHTS
    WRITE(*,*)'INPUT GAUSSIAN INTEGRATION'
    READ(5,*)NGMAX
    call gaussq(1,ngmax,0.0,0.0,0,0,endpts,bg,xg,wg)
    WRITE(*,*)'INPUT LAGUERRE INTEGRATION ORDER'
    READ(5,*)NLMAX
    call gaussq(6,nlmax,0.0,0.0,0,0,endpts,bl,xl,wl)
C
    WRITE(*,*)'READ OUTPUT FILENAME FOR EXCITATION'
    READ(*,9999)FILEE
    WRITE(*,*)'READ OUTPUT FILENAME FOR IONIZATION'
    READ(*,9999)FILEI
    WRITE(*,*)'READ OUTPUT FILENAME FOR CHARGE EXCHANGE'
    READ(*,9999)FILEC
    RETURN
9999 FORMAT(A64)
END

```

```

SUBROUTINE PRATE(NMORE)
C   ROUTINE COMPUTES THE REACTION RATE MATRIX FOR
C   NEUTRAL HYDROGEN IMPACTING ON A HYDROGEN PLASMA
C   THOMAS A GIANAKON 7-16-90
C   PARAMETERS:
C   TEMP - ION TEMP FOR ISOTROPIC MAXWELLIAN (eV)
C   AP - ATOMIC MASS OF PLASMA PARTICLE (AMU)
C   EB - BEAM ENERGY (eV)
C   AB - ATOMIC MASS OF BEAM PARTICLE (AMU)
C   Q(N,M) - REACTION RATE MATRIX
C   NIMAX - MAXIMUM EXCITATION STATE
C   NGMAX - GAUSSIAN INTEGRATION ORDER

```

```

C      NLMAX - LAGUERRE INTEGRATION ORDER
c-----
      implicit real*8(a-h,o-z)
      PARAMETER (NORD=15,NSIZE=10)
      COMMON/QUAD/NGMAX,NLMAX,XG(20),WG(20),XL(40),WL(40)
      COMMON/RRATE/SVIE(NSIZE,NSIZE,NORD,NORD),
1      SVII(NSIZE,NSIZE,NORD),SVIC(NSIZE,NSIZE,NORD)
      COMMON/PARAM/AP,AB,TPOINT(NSIZE),EPOINT(NSIZE),
1      IROW(NORD),NEGRID,NIMAX,NTGRID
      DIMENSION QI(NORD,NORD),QION(NORD),QCX(NORD)
C-----
      DO 60 ITEMP=1,NTGRID
      DO 59 IBEAM=1,NEGRID
      DO 58 N=1,NIMAX
      DO 57 M=1,NIMAX
57      SVIE(ITEMP,IBEAM,M,N)=0.0
      SVII(ITEMP,IBEAM,N)=0.0
58      SVIC(ITEMP,IBEAM,N)=0.0
59      CONTINUE
60      CONTINUE
C-----
C      COMPUTE REACTION RATE OVER PLASMA TEMPERATURES
      DO 2000 ITEMP=1,NTGRID
      TOVM=TPOINT(ITEMP)/AP
C      COMPUTE REACTION RATE OVER BEAM ENERGIES
      DO 1000 IBEAM=1,NEGRID
      EBOVM=EPOINT(IBEAM)/AB
C      PERFORM ENERGY INTEGRATION
      DO 300 K=1,NLMAX
      EPOVM=TOVM*XL(K)
      ETERM=2.0*(EBOVM*EPOVM)**0.5
C-----
C      ZERO THE INNER REACTION RATE MATRIX
      DO 65 N=1,NIMAX
      DO 55 M=1,NIMAX
55      QI(M,N)=0.0
      QION(N)=0.0
      QCX(N)=0.0
65      CONTINUE
C-----
C      PERFORM ANGULAR INTEGRATION
      DO 200 I=1,NGMAX
C      CALCULATE EFFECTIVE COLLISION ENERGY PER AMU
      OF PLASMA PARTICLE
      EFFCE=EPOVM+EBOVM-ETERM*XG(I)
      VTERM=EFFCE**0.5
      TERM=WG(I)*VTERM
C      CALCULATE THE EXCITATION REACTION RATES
      DO 160 M=1,NIMAX-1
      DO 150 N=M+1,NIMAX
150      QI(M,N)=QI(M,N)+TERM*SIGPNM(N,M,EFFCE)
160      CONTINUE
C      CALCULATE THE DE-EXCITATION RATES
      DO 180 M=2,NIMAX
      DO 170 N=1,M-1
170      QI(M,N)=QI(M,N)+TERM*SIGPMN(M,N,EFFCE,AP)
180      CONTINUE
C-----
C      CALCULATE THE EXCITATION TO STATES GREATER
c      THAN the maximum table value AND add to
C      IONIZATION AND THE CHARGE EXCHANGE
      DO 190 M=1,NIMAX
      SUML=0.0
      DO 185 JN=NIMAX+1,NIMAX+NMORE
185      SUML=SUML+SIGPNM(JN,M,EFFCE)

```

```

      QION(M)=QION(M)+TERM*SIGPI(M,EFFCE)
      QCX(M)=QCX(M)+TERM*SIGPC(M,EFFCE)
      QI(M,M)=QI(M,M)+TERM*SUML
190  C
200  C
210  C
      TERM=WL(K)*(XL(K))**.5
      DO 220 M=1,NIMAX
      DO 210 N=1,NIMAX
210  SVIE(ITEMP,IBEAM,M,N)=SVIE(ITEMP,IBEAM,M,N)+
      1      QI(M,N)*TERM
      SVII(ITEMP,IBEAM,M)=SVII(ITEMP,IBEAM,M)+
      1      QION(M)*TERM
      SVIC(ITEMP,IBEAM,M)=SVIC(ITEMP,IBEAM,M)+
      1      QCX(M)*TERM
220  C
300  C
      CONTINUE
      C
      DO 240 M=1,NIMAX
      DO 230 N=1,NIMAX
230  SVIE(ITEMP,IBEAM,M,N)=SVIE(ITEMP,IBEAM,M,N)*7.80864d+05
      SVII(ITEMP,IBEAM,M)=SVII(ITEMP,IBEAM,M)*7.80864d+05
      SVIC(ITEMP,IBEAM,M)=SVIC(ITEMP,IBEAM,M)*7.80864d+05
240  C
      CONTINUE
1000 C
2000 C
      RETURN
      END

```

```

      FUNCTION SIGPMN(N2,N1,ESUBN,AP)
      C  PROTON IMPACT DE-EXCIATION CROSS-SECTION
      C  OF EXCITED H VIA DETAILED BALANCE
      C  THOMAS A GIANAKON 6-28-90
      C  PARAMETERS:
      C  N2 - EXCITED STATE
      C  N1 - EXCITED/GROUND STATE BELOW N2
      C  E - EFFECTIVE COLLISION ENERGY (eV)
      C
      implicit real*8(a-h,o-z)
      ENM=13.598*(1./(N1*N1)-1./(N2*N2))/AP
      ESUBM=ESUBN+ENM
      SIGPMN=SIGPNM(N2,N1,ESUBM)*ESUBM*N1/(ESUBN*N2*N2)
      RETURN
      END

```

```

      FUNCTION SIGPNM(N,M,E)
      C  PROGRAM COMPUTES THE IMPACT EXCITATION
      C  CROSS-SECTION FOR PROTONS ON NEUTRAL HYDROGEN
      C  PARAMETERS:
      C  M -i INITIAL STATE
      C  N -i FINAL STATE
      C  E -i RELATIVE COLLISION ENERGY (eV/AMU)
      C
      implicit real*8(a-h,o-z)
      DIMENSION AB(4,2:6)
      DATA AB/36.86,41.69,2.167,0.4166,5.912,40.34,3.706,0.8260
      1,2.093,35.17,1.922,0.7666,1.266,27.48,1.364,0.2007
      2,0.8348,29.50,2.933,0.08883/
      IF(M.LT.1.01)THEN
      C  USE THE JANEV FITS FOR GROUND STATE EXCITATIONS
      C  PPL-TM-368
      EN=E*1.E-3

```

```

      IF(N.LT.5.01)THEN
        SIGPNM=AB(1,N)*DEXP(-AB(2,N)/EN)/EN*DLOG(AB(3,N)+
1      AB(4,N)*EN)*1E-16
      ELSE
        SIGPE=AB(1,5)*DEXP(-AB(2,5)/EN)/EN*DLOG(AB(3,5)+
1      AB(4,5)*EN)*1E-16
        SIGPNM=SIGPE*(6./N)**3
      END IF
    ELSE
C      USE THE LODGE FORMULATION FOR ALL NON-GROUND
C      STATE EXCIATIONS LODGE ALSO REASONABLY REPRODUCES
C      THE GROUND STATE EXCIATIONS
      EBAR=4.00546E-05*E
      S=N-M
      A=2.666678/S*(N/(S*M))**3*(0.184-0.04/S**0.666667)*
1      (1.-0.2*S/(M*N))**(1.+2.*S)
      D=DEXP(-1./(N*M*EBAR*EBAR))
      U=N-2./N
      RL=1.+0.53*EBAR*EBAR*M*U/(1.+0.4*EBAR)
      RL=DLOG(RL)
      F=(1.-0.3*S*D/(N*N))**(1.+2.*S)
      G=0.5*(EBAR*M*M/(N-1./N))**3
      XTERM=(2.-M*M/(N*N))**0.5
      U=EBAR*M*M
      XPLUS=2./(U*(XTERM+1))
      XMINUS=2./(U*(XTERM-1))
      Y=1./(1.-DLOG(18.*S)/(4.*S))
      C2P=XPLUS*XPLUS*DLOG(1.+2.*XPLUS/3.)/(2.*Y+1.5*XPLUS)
      C2M=XMINUS*XMINUS*DLOG(1.+2.*XMINUS/3.)/(2.*Y+1.5*XMINUS)
      H=C2M-C2P
C      THIS IS NOT THE SAME AS THE LODGE FORM
C      LODGE HAS D MULTIPLYING ONLY A*RL
C      THIS CHANGE PROVIDES A BETTER SHAPE AT LOW ENERGIES
      TERM=(A*RL+F*G*H)*D
      SIGPNM=TERM*M**4.*8.79745E-17/EBAR
    END IF
  RETURN
END

FUNCTION SIGPI(N,E)
C  ROUTINE COMPUTES THE ionization CROSS SECTION
C  FOR PROTONS IMPACTING ON NEUTRAL HYDROGEN.
C  THOMAS A. GIANAKON 8-17-92
C  PARAMETERS:
C  N - INITIAL QUANTUM STATE
C  E - EFFECTIVE COLLISION ENERGY (eV/AMU)
C  REF. JANEV PPL-TM-368 for ground state n=1
c  Higher excited states, scale the ground-state
c  based on the loss cross-section
C
  implicit real*8(a-h,o-z)
  u=dble(n*n)
  ebarp=E*u
  ebar=1.0d+00/ebarp
c  compute ground state ionization
  sigpi=1.76d-16*(1.6160*dbeta(1.0999d+04*ebar)+
1  0.24827*dbeta(6.98240e+03*ebar))
  if(sigpi.lt.0) sigpi=0.0d+00
c  compute excited state ionization by scaling from
c  the ground-state to the excited states as per
c  the loss cross-section, see routine sigpc
  sigpi=sigpi*u*(1-dexp(-ebarp*0.10799E-03))/
1  (1-dexp(-E*0.10799E-03))
  RETURN

```

END

```

FUNCTION SIGPC(N,E)
c Routine computes the charge exchange cross-section
c for protons impacting on neutral hydrogen by
c computing the electron loss cross-section and
c subtracting the ionization cross-section.
C THOMAS A. GIANAKON 2-23-92
C PARAMETERS:
C N - INITIAL QUANTUM STATE
C E - EFFECTIVE COLLISION ENERGY (eV/AMU)
C
implicit real*8(a-h,o-z)
U=N*N
c compute the loss cross-section
sigpl=1.467E-11*U*(1.-DEXP(-U*E*0.10799E-03))/E
c compute the charge exchange cross-section
SIGPC=sigpl-sigpi(n,e)
if(sigpc.lt.0)sigpc=0.0d+00
RETURN
END

```

```

function dbeta(x)
c Routine computes the function D'beta used in
c the ionization cross-section
c Reference Janev and Presnyakov (1980)
c
implicit real*8(a-h,o-z)
dimension dfcn(17)
data dfcn/0.057,0.094,0.139,0.187,0.264,0.350,0.401
1 ,0.387,0.318,0.243,0.186,0.146,0.110,0.0853
2 ,0.0624,0.0442,0.028/
data ten025/1.778279d+00/
if(x.lt.1.0d-03)then
dbeta=4.00d+00*x*dlog(1.4d+00/x)
elseif(x.gt.10.d+00)then
dbeta=0.5d+00*x*dexp(-(2.0d+00*x)**0.5d+00)
else
x0=1.d+00/x
n=5+4*dlog10(x0)
xn=ten025**(n-5)
dbeta=dfcn(n)+(x0-xn)*(dfcn(n)-dfcn(n+1))
1 /(xn*(1.0d+00-ten025))
end if
return
end

```


C Radiative Decay Rate Code *rrate.f*

```

c   Program generates an ASCII file for the radiant
c   decay of neutral hydrogen atom
c   Parameter:
c     nord -i Number of principle quantum states
C-----
      implicit real*8(a-h,o-z)
      PARAMETER (NORD=10)
      CHARACTER *64 FILER
      COMMON/RAD/QRAD(NORD,NORD),nimax
C-----
      WRITE(*,*)'INPUT THE MAXIMUM NUMBER OF STATES'
      READ(5,*)NIMAX
      WRITE(*,*)'INPUT FILENAME FOR RADIANT DECAY'
      READ(*,9999)FILER
C-----
      IF(NIMAX.NE.1)THEN
C       COMPUTE THE RADIATIVE DECAY
        DO 50 N=2,NIMAX
          DO 45 M=1,N-1
45      QRAD(N,M)=RADIAT(M,N)
50      CONTINUE
        END IF
C-----
C       DUMP DATA
      CALL OUTR(FILER)
9999  FORMAT(A)
      END

      SUBROUTINE OUTR(FILE)
C       ROUTINE DUMPS ELECTRON IONIZATION ARRAY IN HDF FORMAT
C       PARAMETERS:
C       FILE - OUTPUT FILE
C-----
      implicit real*8(a-h,o-z)
c     integer*4 ret
      CHARACTER *64 FILE
      PARAMETER (NORD=10)
      COMMON/RAD/QRAD(NORD,NORD),nimax
      DIMENSION IDIMSIZ(2)
      NIMAX=NORD
C-----
C     SET ARRAY SIZES FOR IONIZATION FILE DUMP
      irank=2
      IDIMSIZ(1)=NIMAX
      IDIMSIZ(2)=NIMAX
C-----
      open(3,file=file,status='new')
      write(3,*)irank
      do 10 i=1,irank
10      write(3,*)idimsiz(i)
      do 11 i=1,idimsiz(1)
11      write(3,*)i
      do 12 i=1,idimsiz(2)
12      write(3,*)i
      do 30 i=1,idimsiz(1)
        do 20 j=1,idimsiz(2)
20      write(3,9999)qrad(i,j)
30      continue
999  format(D12.5)
      RETURN
      END

```

```

      FUNCTION RADIAT(M,N)
C     ROUTINE COMPUTES THE RADIATIVE TRANSITION PROBABILITY
C     REF NBS & JOHNSON
C     THOMAS A GIANAKON  6-29-90
C     PARAMETERS:
C       M - DE-EXCITED STATE
C       N - EXCITED STATE (I.E., TRANSITION FROM N-2M)
C -----
      implicit real*8(a-h,o-z)
      FK=1.0/(N*N)
      FI=1.0/(M*M)
      X=1.-FK*M*M
C -----
C     COMPUTE GAUNT FACTOR
      IF(M.LT.1.01)THEN
        G0=1.1330
        G1=-0.4059
        G2=0.07014
      ELSEIF(M.GT.2.99)THEN
        RN=1./M
        G0=0.9935+RN*(0.2328-0.1296*RN)
        G1=-RN*(0.6282+RN*(-0.5598+RN*0.5299))
        G2=RN*RN*(0.3887+RN*(-1.181+1.470*RN))
      ELSE
        G0=1.0785
        G1=-0.2319
        G2=0.02947
      END IF
      G=G0+(G1+G2/X)/X
C -----
      FNM=1.960281*M*G/(N*X)**3
      RADIAT=80.2862E+08*FNM*(FI-FK)**2*FK*(M*M)
      RETURN
      END

```

D Beam Deposition Code *exc_dep.f*

```

subroutine exc_dep(rtol,atol,zon'dist,state'int,ierr)
c  routine takes zonal temperature and density
c  for each plasma species of interest and computes
c  ionization and charge exchange rates for each plasma
c  species. Calculation is based on excited states of the
c  neutral beam. The reaction rates are returned in the
c  common block /fmicx/ and are normalized to a comparable
c  ground state calculation.
c  the following common blocks must be initialized prior
c  to a call to this routine
C  (see the include file exc_dep.lis)
c  /gquad/ - contains gaussian quadrature and weights
c  /trate/ - reaction rate tables - a call to QREAD
c  /tspec/ - parameters which describe the zone plasma
c  species, beam characteristics and
c  calculational control parameters
c
c  parameters:
c  rtol - relative tolerance of equation solver (input)
c  atol - absolute tolerance of equation solver (input)
c  zon'dist - distance (cm) of beam across zone (input)
c  state'int() - on input initial intensities of beam states
c  - on output intensities of states at zon'dist
c  ierr - return error code
c  ierr = 0 ; succesful calculation
c  ierr ; -200 ; leading value gives lside error
c  see the subroutine lside
c  -200 ; ierr ; 200; table extrapolation problems
c  see the subroutine MRATE
c
include 'exc_dep.lis'
dimension xg'loc(0:nquad+1),wg'loc(0:nquad+1)
dimension quad'state(0:nquad+1,nord),zone'sum(nord)
dimension state'int(nord)
dimension gsii(numspc),gscx(numspc)
dimension rwork(lrw),iwork(liw)
external exc_fcn
c
c  set Lorentz ionization limit
c  dumb=7.d+00*(3.0d+00/b'perp)**0.25d+00*
1  (5.d+04/eb)**0.125d+00
nlmax=int(dumb)
if(nlmax.gt.nimax)nlmax=nimax
if(nlmax.lt.1)nlmax=1
c
c  set zone quadrature locations and weights
delta=0.5*zon'dist
xg'loc(0)=0.0
do 10 i=1,ngmax
wg'loc(i)=delta*wgquad(i)
10 xg'loc(i)=(1.0d+00+xgquad(i))*delta
xg'loc(ngmax+1)=zon'dist
C
c  compute reaction rate matrices for each species
call mrate(ierr)
if(ierr.ne.0)return
c  mix reaction rate matrices into total reaction rate
call qrate(sigma'gs,v0'beam)
c
c  compute total number of particles initially in beam
beam'dens=0.0d+00
do 4 n=1,nlmax
4 beam'dens=beam'dens+ state'int(n)

```

```

c   populations above Lorentz limit are ionized and
c   appear as an ionization value in fmi(0)
fmi(0)=0
do 5 n=nlmax+1,nimax
c   and treat Lorentz ionization limit as species 0
fmi(0)=fmi(0)+state'int(n)
c   add beam density above Lorentz limit to gs calc
beam'dens=beam'dens+state'int(n)
5   state'int(n)=0.0d+00
c
C   -----
C   integrate differential equation across zone
itol=1
itask=1
iopt=1
c   iwork(6) number of internal calls within lsode
iwork(6)=nimax*1000
mf=10
x0=0.0d+00
do 20 i=1,ngmax+1
    istate=1
    x1=xg'loc(i)
    call lsode(exc'fcn,nlmax,state'int,x0,x1,itol,rtol,
1        atol,itask,istate,iopt,rwork,lrw,iwork,
2        liw,jac,mf)
    if(istate.lt.0)then
        ierr=10*istate
c       when istate = -1 excessive work
c       more than nimax*1000 internal calls
c       but lsode doesn't integrate to its current endpoint
c       typically occurs only for large number of states
        if(istate.lt.-1)then
c           true error with lsode
            ierr=100*istate
            return
        end if
c       loop to integrate to endpoint on istate=-1
c       this slows down the calculation by several orders
        ierr=ierr+iwork(11)
70    istate=2
        call lsode(exc'fcn,nlmax,state'int,x0,x1,itol,rtol,
1        atol,itask,istate,iopt,rwork,lrw,iwork,
2        liw,jac,mf)
        if(istate.lt.0)goto 70
    end if
c   assign values of state intensities to quadrature array
do 15 n=1,nlmax
15    quad'state(i,n)=state'int(n)
c   states above Lorentz limit are set to zero
do 16 n=nlmax+1,nimax
16    quad'state(i,n)=0.0d+00
20    continue
c   perform zone quadrature for each state
do 30 n=1,nimax
    zone'sum(n)=0.0
    do 25 i=1,ngmax
25        zone'sum(n)=zone'sum(n)+quad'state(i,n)*wg'loc(i)
30    continue
C   -----
c   compute zonal deposition based on ground state
term=dexp(-sigma'gs*zon'dist)
val=beam'dens*(1.d+00-term)/(sigma'gs*v0'beam)
do 142 i=1,nspec
    fmi(i)=0.0
    ffcx(i)=0.0
    gsii(i)=qi(i,1)*val

```

```

142  gscx(i)=qc(i,1)*val
C
c   compute zonal deposition based on excited states
c   but normalize result to previous ground state calc
c   sumcx=0.0
c   sumii=ffii(0)
do 245 i=1,nspec
  if(nspec'tab(i).eq.1)then
    do 242 m=1,nlmax
      sumii=sumii+(qi(i,m)+qe(i,m,m))*zone'sum(m)
c   include excitation above lorentz limit in ioniza
      exc'ion=0.0d+00
do 241 j=nlmax+1,nimax
  241   exc'ion=exc'ion+qe(i,m,j)
  242   fii(i)=fii(i)+(qi(i,m)+qe(i,m,m)+exc'ion)*zone'sum(m)
      fii(i)=fii(i)/(gsii(i)*v0'beam)
      ffcx(i)=0.0
    else
      do 243 m=1,nimax
c       sumii=sumii+(qi(i,m)+qe(i,m,m))*zone'sum(m)
c       sumcx=sumcx+qc(i,m)*zone'sum(m)
c       fii(i)=fii(i)+(qe(i,m,m)+qi(i,m))*zone'sum(m)
  243   ffcx(i)=ffcx(i)+qc(i,m)*zone'sum(m)
      fii(i)=fii(i)/(gsii(i)*v0'beam)
      ffcx(i)=ffcx(i)/(gscx(i)*v0'beam)
    end if
  245 continue
c   sumcx=sumcx/v0'beam
c   sumii=sumii/v0'beam
c   sumshi=0.0
c   do 270 n=1,nimax
c270   sumshi=sumshi+state'int(n)
C
c   write(6,*)sumii,sumcx,sumshi
c   particle balance checker
c   write(6,*)beam'dens-(sumii+sumcx+sumshi)
  return
end

SUBROUTINE exc'fcn(ndumb,T,Y,F)
C
C   ROUTINE CALLED BY DIFFEQ SOLVER WHICH EVALUATES
C   A NEW SET OF FIRST DERIVATIVES F(M) AT LOCATION T BASED
C   ON THE EXCITED STATE populations Y(M)
C
include 'exc'dep.lis'
dimension y(ndumb),f(ndumb)
C
C   COMPUTE TEMP AND DENSITY AT SPOT T AND UPDATE REACTION
C   RATE ARRAYS IF NECESSARY
C   COMPUTE FIRST DERIVATIVES
DO 20 N=1,ndumb
  SUM=0.0
  DO 10 NP=1,ndumb
  10   SUM=SUM+QTOT(NP,N)*Y(NP)
      F(N)=SUM
  20 CONTINUE
  RETURN
END

SUBROUTINE MRATE(ierr)
C
C   ROUTINE EVALUATES THE REACTION RATE ARRAY FOR EACH
C   SPECIES FOR THE PROSCRIBED TEMPERATURE AND DENSITY

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C THOMAS A GIANAKON 8-2-90
C PARAMETERS:
c ierr - error return parameter
c      = 0 successful run
c      = +10*k, extrapolation above beams for species k
c      = -10*k, extrapolation below beams for species k
c      = +k, extrapolation above temps for species k
c      = -k, extrapolation below temps for species k
C NSPEC - NUMBER OF SPECIES
C NIMAX - NUMBER OF NEUTRAL BEAM EXCITED STATES
C EB - BEAM ENERGY (eV/amu)
C QC(,) - CHARGE EXCHANGE REACTION RATE*DENSITY
C QI(,) - IONIZATION REACTION RATE*DENSITY
C QE(,,) - EXCITATION REACTION RATE*DENSITY
C
C include 'exc' dep.lis'
C
c ierr=0
c do 100 k=1,nspec
c if(nspec'tab(k).eq.1)then
C TREAT ELECTRONS SEPERATELY SINCE NO BEAM DEPENDENCE.
C IBEAM=1
c i=nspec'tab(k)
c ITEMP=1+(IDIMSIZ(i,1)-1)*
1 (DLOG(TSPEC(k))-DLOG(TPOINT(1,1)))
1 /(DLOG(TPOINT(i,IDIMSIZ(i,1)))-DLOG(TPOINT(1,1)))
C TRAP FOR TEMPERATURES OUTSIDE THE TABLE, EXTRAPOLATION
IF(ITEMP.LT.1)THEN
ITEMP=1
ierr=-k
return
END IF
IF(ITEMP.GE.IDIMSIZ(i,1))THEN
ITEMP=IDIMSIZ(i,1)-1
ierr=k
return
END IF
C
C TERMT=(DLOG(TSPEC(k))-DLOG(TPOINT(I,ITEMP)))/(
1 (DLOG(TPOINT(I,ITEMP+1))-DLOG(TPOINT(I,ITEMP)))
DO 29 M=1,NIMAX
DO 28 N=1,NIMAX
C EXCITATION ARRAY
QE(k,M,N)=DSPEC(k)*(SVE(I,ITEMP,IBEAM,M,N)+TERMT*
1 (SVE(I,ITEMP+1,IBEAM,M,N)-SVE(I,ITEMP,IBEAM,M,N)))
28 CONTINUE
C IONIZATION ARRAY
QI(k,M)=DSPEC(k)*(SVI(I,ITEMP,IBEAM,M)+TERMT*
1 (SVI(I,ITEMP+1,IBEAM,M)-SVI(I,ITEMP,IBEAM,M)))
C CHARGE EXCHANGE ARRAY FOR ELECTRONS IS SET TO ZERO
QC(k,M)=0.0
29 CONTINUE
C
c else
c non-electron species or species with beam dependence
c i=nspec'tab(k)
C
C COMPUTE THE LOCATION ALONG THE BEAM AXIS table
C IBEAM=1+(IDIMSIZ(1,2)-1)
1 *(DLOG(EB'pframe(k)/zspec(k))-DLOG(EPOINT(1,2)))
1 /(DLOG(EPOINT(1,IDIMSIZ(1,2)))-DLOG(EPOINT(1,2)))
C TRAP FOR BEAMS OUTSIDE THE TABLE, EXTRAPOLATION
IF(IBEAM.LT.1)THEN
IBEAM=1
ierr=-k*10

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```

        return
    END IF
    IF(IBEAM.GE.IDIMSIZ(1,2))THEN
        IBEAM=IDIMSIZ(1,2)-1
        ierr=k*10
        return
    END IF
C
C      COMPUTE THE LOCATION ALONG THE TEMPERATURE AXIS
ITEMP=1+(IDIMSIZ(1,1)-1)*
1      (DLOG(TSPEC(k)/zspec(k))-DLOG(TPOINT(1,1)))
2      /(DLOG(TPOINT(1,IDIMSIZ(1,1)))-DLOG(TPOINT(1,1)))
IF(ITEMP.LT.1)THEN
    ITEMP=1
    ierr=-k
    return
END IF
IF(ITEMP.GE.IDIMSIZ(1,1))THEN
    ITEMP=IDIMSIZ(1,1)-1
    ierr=+k
    return
END IF
C
C      COMPUTE INTERPOLATION FACTORS
TERMT=(DLOG(TSPEC(k)/zspec(k))-DLOG(TPOINT(1,ITEMP)))/
1      (DLOG(TPOINT(1,ITEMP+1))-DLOG(TPOINT(1,ITEMP)))
TERMB=(DLOG(EB'pframe(k)/zspec(k))-DLOG(EPOINT(1,IBEAM)))/
1      (DLOG(EPOINT(1,IBEAM+1))-DLOG(EPOINT(1,IBEAM)))
C      INTERPOLATE IN TABLE
DO 20 M=1,NIMAX
    DO 10 N=1,NIMAX
C      CALCULATE THE EXCITATION ARRAY
FY0=SVE(1,ITEMP,IBEAM,M,N)+TERMT*
1      (SVE(1,ITEMP+1,IBEAM,M,N)-SVE(1,ITEMP,IBEAM,M,N))
FY1=SVE(1,ITEMP,IBEAM+1,M,N)+TERMT*
1      (SVE(1,ITEMP+1,IBEAM+1,M,N)-SVE(1,ITEMP,IBEAM+1,M,N))
QE(k,M,N)=(FY0+TERMB*(FY1-FY0))
1      *DSPEC(k)*zspec(k)**1.5d+00
10    CONTINUE
C      CALCULATE THE IONIZATION ARRAY
FY0=SVI(1,ITEMP,IBEAM,M)+TERMT*
1      (SVI(1,ITEMP+1,IBEAM,M)-SVI(1,ITEMP,IBEAM,M))
FY1=SVI(1,ITEMP,IBEAM+1,M)+TERMT*
1      (SVI(1,ITEMP+1,IBEAM+1,M)-SVI(1,ITEMP,IBEAM+1,M))
QI(k,M)=(FY0+TERMB*(FY1-FY0))*DSPEC(k)
1      *(zspec(k)**1.5d+00)
C      CALCULATE THE CHARGE EXCHANGE ARRAY
FY0=SVC(1,ITEMP,IBEAM,M)+TERMT*
1      (SVC(1,ITEMP+1,IBEAM,M)-SVC(1,ITEMP,IBEAM,M))
FY1=SVC(1,ITEMP,IBEAM+1,M)+TERMT*
1      (SVC(1,ITEMP+1,IBEAM+1,M)-SVC(1,ITEMP,IBEAM+1,M))
QC(k,M)=(FY0+TERMB*(FY1-FY0))*DSPEC(k)
1      *zspec(k)**1.5d+00
20    CONTINUE
    end if
100  CONTINUE
    RETURN
    END

SUBROUTINE QRATE(sigma'gs,v00)
C      ROUTINE COMPUTES THE REACTION RATE MATRIX AS A SUM OF
C      CONTRIBUTIONS FROM ELECTRON,PROTON,HEAVY ION IMPACT
C      AND RADIATIVE DECAY.
C      THOMAS A. GIANAKON 8-2-90

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C   PARAMETERS:
C   NSPEC  - NUMBER OF SPECIES
C   NIMAX  - NUMBER OF NEUTRAL BEAM STATES
C   QC(,)  - CHARGE EXCHANGE REACTION RATE*DENSITY
C   QI(,)  - IONIZATION REACTION RATE*DENSITY
C   QE(,,) - EXCITATION REACTION RATE*DENSITY
C   QRAD(,) - RADIANT PROBABILITY
C   QTOT(,) - MATRIX FOR USE BY DIF EQ SOLVER
C -----
C   include 'exc'dep.lis'
C -----
C   ZERO THE TOTAL REACTION RATE MATRIX
C   DO 50 M=1,NIMAX
C     DO 40 N=1,NIMAX
40    QTOT(M,N)=0.0d+00
50    CONTINUE
C -----
C   ADD THE CONTRIBUTION TO THE TOTAL REACTION RATE
C   FROM EACH OF THE SPECIES -
C   NOTE: QE HAS ALREADY BEEN MULTIPLIED BY THE DENSITY
C   OF EACH SPECIES.
C   sigma'gs=0.0d+00
C   DO 130 I=1,NSPEC
C     sigma'gs=sigma'gs+qi(i,1)+qc(i,1)
C     DO 120 M=1,NIMAX
C       DO 110 N=1,NIMAX
110      QTOT(M,N)=QTOT(M,N)+QE(I,M,N)
120      QTOT(M,M)=QTOT(M,M)+QI(I,M)+QC(I,M)
130    CONTINUE
C -----
C   ADD THE CONTRIBUTION FROM RADIATIVE DECAY
C   DO 250 N=1,NIMAX
C     DO 240 M=1,NIMAX
240      QTOT(N,M)=QTOT(N,M)+QRAD(N,M)
250    CONTINUE
C -----
C   DEFINE DIAGONAL AS THE SUM OF ALL LOSS CHANNELS FOR A STATE
C   DO 350 N=1,NIMAX
C     SUM=0.
C     DO 340 M=1,NIMAX
340      SUM=SUM+QTOT(N,M)
C     QTOT(N,N)=-SUM
350    CONTINUE
C -----
C   DIVIDE THE REACTION RATE BY lab VELOCITY of the neutral
C   V00=1.384d+06*EB**0.5
C   V0=1./V00
C   sigma'gs=sigma'gs*v0
C   DO 450 N=1,NIMAX
C     DO 440 M=1,NIMAX
440      QTOT(N,M)=QTOT(N,M)*V0
450    CONTINUE
C -----
C   RETURN
C   END

SUBROUTINE QREAD(FILER,FILEI,FILEC,FILEE)
C   ROUTINE RETRIEVES REACTION RATE ARRAYS FROM FILES
C   -SOME IMPROVEMENTS COULD BE MADE TO THIS ROUTINE
C   TO ALLOW GREATER FLEXIBILITY IN THE SIZE OF THE
C   READ IN ARRAYS, PRESENTLY THE SIZE OF THE
C   ARRAYS MUST MATCH THOSE OF THE REACTION RATE
C   GENERATING ROUTINES (PRATE,ZRATE,ERATE,RRATE).
C   NORD and nsize MUST ALSO BE consistent.

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C   THOMAS A GIANAKON   8-2-90
C   PARAMETERS:
C   FILER   - RADIATIVE DECAY FILE
C   FILEI(1) - IMPACT IONIZATION INPUT FILE OF SPECIES 1
C   FILEC(1) - CHARGE EXCHANGE INPUT FILE OF SPECIES 1
C   FILEE(1) - CHARGE EXCHANGE INPUT FILE OF SPECIES 1
C
C   include 'exc'dep.lis'
C
C   CHARACTER *64 FILEI(NUMSPC),FILEC(NUMSPC),FILEE(NUMSPC)
1   ,FILER
C   DIMENSION IDIMI(3),IDIM(4)
C
C   INCREMENT THROUGH EACH table of PLASMA SPECIES
C   DO 1000 ISPEC=1,n'tab
C
C   RETRIEVE IONIZATION FILE
C   open(3,file=FILEI(ISPEC),status='old')
C   read(3,*)iprank
C   read(3,*)IDIMI(1)
C   read(3,*)IDIMI(2)
C   read(3,*)IDIMI(3)
C   IDIMSIZ(ISPEC,1)=IDIMI(1)
C   IDIMSIZ(ISPEC,2)=IDIMI(2)
C   NIMAX=IDIMI(3)
C   DO 10 ITGRID=1,IDIMI(1)
10  read(3,999)tpoint(ispec,itgrid)
C   DO 20 IBGRID=1,IDIMI(2)
20  read(3,999)epoint(ispec,ibgrid)
C   do 25 i=1,nimax
25  read(3,*)idumb
C   DO 50 ITGRID=1,NSIZE
C   DO 40 IBGRID=1,NSIZE
C   DO 30 N=1,NORD
30  read(3,999)SVI(ISPEC,ITGRID,IBGRID,N)
40  CONTINUE
50  CONTINUE
C   close(3)
C
C   GET CX FILE EXCEPT SKIP ELECTRONS
C   IF(ISPEC.ne.1)THEN
C   open(3,file=FILEC(ISPEC),status='old')
C   read(3,*)iprank
C   read(3,*)IDIMI(1)
C   read(3,*)IDIMI(2)
C   read(3,*)IDIMI(3)
C   DO 110 ITGRID=1,IDIMI(1)
110  read(3,999)tpoint(ispec,itgrid)
C   DO 120 IBGRID=1,IDIMI(2)
120  read(3,999)epoint(ispec,ibgrid)
C   do 125 n=1,idimi(3)
125  read(3,*)idumb
C   DO 150 ITGRID=1,IDIMI(1)
C   DO 140 IBGRID=1,IDIMI(2)
C   DO 130 N=1,IDIMI(3)
130  read(3,999)SVC(ISPEC,ITGRID,IBGRID,N)
140  CONTINUE
150  CONTINUE
C   close(3)
C   else
C   DO 151 ITGRID=1,IDIMI(1)
C   DO 141 IBGRID=1,IDIMI(2)
C   DO 131 N=1,IDIMI(3)
131  SVC(ISPEC,ITGRID,IBGRID,N)=0.0d+00
141  CONTINUE

```

```

151     CONTINUE
      END IF
C
C     GET EXCITATION FILE
      open(3,file=FILEE(ISPEC),status='old')
      read(3,*)iprank
      read(3,*)IDIM(1)
      read(3,*)IDIM(2)
      read(3,*)IDIM(3)
      read(3,*)IDIM(4)
      DO 210 ITGRID=1,IDIM(1)
210   read(3,999)tpoint(ispec,itgrid)
      DO 220 IBGRID=1,IDIM(2)
220   read(3,999)epoint(ispec,ibgrid)
      do 221 n=1,IDIM(3)
221   read(3,*)idumb
      do 222 n=1,IDIM(4)
222   read(3,*)idumb
      DO 250 ITGRID=1,IDIM(1)
      DO 240 IBGRID=1,IDIM(2)
      DO 230 N=1,IDIM(3)
      DO 225 M=1,IDIM(4)
225   read(3,999)SVE(ISPEC,ITGRID,IBGRID,N,M)
230   CONTINUE
240   CONTINUE
250   CONTINUE
      close(3)
C
1000 CONTINUE
C     GET RADIANT DECAY FILE
      open(3,file=FILER,status='old')
      read(3,*)iprank
      read(3,*)IDIM(1)
      read(3,*)IDIM(2)
      do 321 i=1,nimax
321   read(3,*)idumb
      do 322 i=1,nimax
322   read(3,*)idumb
      DO 330 N=1,IDIM(1)
      DO 325 M=1,IDIM(2)
325   read(3,999)QRAD(N,M)
330   CONTINUE
      close(3)
999   format(d12.5)
      RETURN
      END

```

E Beam Deposition Common Block

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C  PARAMETERS:
C  NSIZE - SETS THE NUMBER OF TEMPERATURE AND BEAM
C  ENERGY ARRAYS USED IN THE REACTION RATES
C  AS RETRIEVED FROM AN ascii FILE
C  NORD - MAXIMUM NUMBER OF EXCITED STATES
C  NUMSPC - MAXIMUM NUMBER OF SPECIES
C  IW - SIZE OF WORKING ARRAY PASSED TO DIFEQ SOLVER
C  IZONEMAX- MAXIMUM NUMBER OF ZONES
C  NQUAD - MAXIMUM QUADRATURE ORDER FOR ZONE INTEGRATION
C  IINTG - MAXIMUM NUMBER OF ORDINATE LOCATIONS
C  USED IN CONJUNCTION WITH ZONAL INTEGRATION
C
C  implicit real*8(a-h,o-z)
C  PARAMETER (NSIZE=10,NORD=15,NUMSPC=4)
C  PARAMETER (lrw=NORD*(NORD+9)+22,liw=20+nord)
C  PARAMETER (lrw=20+16*NORD,liw=20)
C  PARAMETER (IZONEMAX=25)
C  PARAMETER (NQUAD=10,IINTG=1+IZONEMAX*NQUAD)
C
C  COMMON BLOCKS:
C
C  /gquad/: - common block for storage of gaussian quadrature
C  points and weights on the interval (-1,1)
C  xgquad()- quadrature locations
C  wgquad()- quadrature weights
C  common/gquad/xgquad(nquad),wgquad(nquad)
C
C  /tRRATE/: - reaction rate tables
C  IDIMSIZ(1,1) - NUMBER OF TEMPERATURE POINTS IN
C  LINEAR INTERPOLATION TABLE OF
C  THE REACTION RATE OF SPECIES I
C  IDIMSIZ(1,2) - NUMBER OF BEAM POINTS
C  TPOINT(1,J) - TEMPERATURE (eV/amu) ASSOCIATED WITH
C  SPECIES I AT REACTION RATE J
C  EPOINT(1,K) - BEAM ENERGY (eV/amu)
C  SVE(1,J,K,M,N) - EXCITATION/DEXCITATION/ENHANCEMENT
C  REACTION RATE (CM3 S-1) FOR M -> N
C  SVI(1,J,K,M) - IONIZATION REACTION RATE
C  SVC(1,J,K,L) - CHARGE EXCHANGE REACTION RATE
C
C  COMMON/tRRATE/TPOINT(NUMSPC,NSIZE),EPOINT(NUMSPC,NSIZE),
C  1 SVE(NUMSPC,NSIZE,NSIZE,NORD),
C  2 SVI(NUMSPC,NSIZE,NSIZE,NORD),SVC(NUMSPC,NSIZE,NSIZE,NORD),
C  3 IDIMSIZ(NUMSPC,2)
C
C  /tSPECI/: - zone temperature and density parameters
C  b'perp - Magnetic Field perpendicular to beam (T)
C  eb - beam energy in lab frame (eV/amu)
C  ZSPEC(1) - Z NUMBER OF SPECIES I ()
C  ASPEC(1) - ATOMIC NUMBER OF SPECIES I (amu)
C  DSPEC(1) - DENSITY OF SPECIES I (# cm-3)
C  TSPEC(1) - SPECIES I TEMP (eV) for electron species
C  (eV/amu) otherwise
C  NSPEC - ACTUAL NUMBER OF SPECIES (INPUT SCALAR)
C  ngmax - zone quadrature order
C  NIMAX - NUMBER OF EXCITED STATES IN CALCULATION
C  n'tab - number of reaction rate tables
C  eb'pframe - ENERGY OF BEAM in plasma frame (eV/amu)
C  nspec'tab(k) table value associated with species k
C
C  COMMON/SPECI/b'perp,eb,ZSPEC(NUMSPC),ASPEC(NUMSPC),
C  1 dspec(NUMSPC),TSPEC(NUMSPC),eb'pframe(NUMSPC),NSPEC,
C  2 ngmax,nimax,n'tab,nspec'tab(numspc)

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C -----
C /QRATE0/: - Zone reaction rates interpolated from table
C   QC(I,M) - CHARGE EXCHANGE REACTION RATE FOR SPECIES I
C             FROM EXCITED STATE M (WORKING ARRAY)
C   QI(I,M) - IONIZATION REACTION RATE
C   QE(I,M,N)- EXCITATION/DEXCITATION/ENHANCEMENT
C             REACTION RATE
C   QRAD(M,N)- RADIANT DEXCITATION PROBABILITY
C   QTOT(M,N)- ARRAY USED IN DIFEQ SOLVER, COMPRISED OF AN
C             APPROPRIATE SUM OVER ALL SPECIES
C -----
COMMON/QRATE0/QC(NUMSPC,NORD),QI(NUMSPC,NORD),
1  QE(NUMSPC,NORD,NORD),QRAD(NORD,NORD),QTOT(NORD,NORD)
C -----
C /fficx/: - normalized reaction rates
C   ffi(numspc) - ratio of impact ionization for excited
C               states to ground state for a species
C   ffi(0) - any beam intensity above Lorentz limit
C           entering zone is ionized and the sum
C           is stored in this array
C   ffcx(numspc) - ratio of charge exchange for excited
C               states to ground state for a species
C common/fficx/ffi(0:numspc),ffcx(numspc)

```

END

**DATE
FILMED**

12 / 1 / 92