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LA-6661-MS

Informal Report

UC-20

Issued: January 1977

**PLASMX: Multigroup Ionization and Charge Exchange
Cross-Section Code for Neutral Hydrogen Transport
in Plasmas**

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Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161
Price: Printed Copy \$4.00 Microfiche \$3.00

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PLASMX:
MULTIGROUP IONIZATION AND CHARGE EXCHANGE CROSS-SECTION CODE
FOR NEUTRAL HYDROGEN TRANSPORT IN PLASMAS

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ABSTRACT

NOTICE

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1. Program Identification: **PLASMX**
2. Computer for Which Program is Designed: **CDC-7600, CDC-6600**
3. Description of Function: **PLASMX** generates effective multigroup macroscopic cross sections for discrete-ordinates calculations of neutral hydrogen atom transport in Tokamak systems. If the user so desires, effective microscopic cross sections can be generated at the midpoint energies of the multigroup bin structure.
4. Restrictions: Variable dimensioning presently restricts the number of energy groups to 22, the number of spatial regions to 10, and the number of Legendre polynomial moments to 7 (P_6). Changes for user applications are easily effected, however.
5. Running Times: A two-group, two-region, P_3 calculation requires approximately 30 s on a CDC-7600. An 11-group, 10-region P_3 calculation requires approximately 30 min.
6. Unusual Features: **None.**
7. Machine Requirements: Two system input/output units and two output disks or tapes.
8. Related Programs: **PLASMX** generates multigroup cross sections on one of the output files in a standard DTF-IV format suitable for one- and two-dimensional cylindrical discrete-ordinates transport codes, such as **ONETRAN**, **TWOTRAN**.
9. Material Available: Source deck (1 683 cards), test problem, and this report available from author (BRW).

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I. INTRODUCTION

Neutral gas penetration problems are of considerable interest in the analysis of CTR systems. Although the interaction physics of neutral gas atoms is different from that of neutrons, discrete ordinates, multigroup, neutron transport codes can be used to make neutral gas transport calculations if certain simplifying assumptions are made.¹ The PLASMX code has been written to provide multigroup cross sections for neutral hydrogen atom transport calculations in Tokamak-type CTR plasmas. These cross sections are written to tape in a format specifically tailored to the LASL neutron transport codes,² but they can be written in any specific format.

II. THE TOKAMAK MODEL

The actual three-dimensional tokamak geometry is toroidal. Our cylindrical two-dimensional model assumes a cut across the circular cross section of the torus.

As shown in Fig. 1, the plasma column has an outer radius, RC , and the confinement wall has an inner radius, RW . The plasma is assumed to be composed of an equal number of protons and electrons (charge-neutral), and both the particle densities and temperatures are assumed to vary quadratically with radius. The specific dependences are as follows.

$$\rho_e(r) = \rho_p(r) = 0.5\rho_{\max} [1 - (r/RC)^2] \quad , \quad (1)$$

where

$$\begin{aligned} \rho_e(r) &= \text{the electron particle density,} \\ \rho_p(r) &= \text{the proton particle density,} \\ \rho_{\max} &= \text{the maximum total particle density;} \end{aligned}$$

and

$$T_e(r) = T_{e\max} [1.0 - (r/RW)^2], \quad (2)$$

where

$T_e(r)$ = the electron temperature,

$T_{e_{\max}}$ = the maximum electron temperature;

and

$$T_p(r) = T_{p_{\max}} [1.0 - (r/RW)^2] , \quad (3)$$

where

$T_p(r)$ = the proton temperature and

$T_{p_{\max}}$ = the maximum proton temperature.

The electron and proton velocity distribution functions are assumed to be Maxwellian.

$$N_e(r,V) = \frac{\exp[-m_e V^2/2kT_e(r)]}{\int_0^{t_{\max}} \exp[-m_e V^2/2kT_e(r)]} , \quad (4)$$

where

$N_e(r,V)$ = the electron velocity distribution function,

m_e = the electron mass, and

$t_{\max}$ = the maximum energy in the hydrogen atom group structure;

$$N_p(r,V) = \frac{\exp[-m_p V^2/2kT_p(r)]}{\int_0^{t_{\max}} \exp[-m_p V^2/2kT_p(r)]} , \quad (5)$$

where

$N_p(r,V)$ = the proton velocity distribution function and

m_p = the proton mass.

The actual tokamak distribution function is composed of a relatively small drift velocity superposed on a Maxwellian distribution. However, for reasons discussed in Sec. III, this drift velocity is neglected.

III. MICROSCOPIC CROSS SECTIONS

Analytic expressions chosen for the microscopic ionization and charge-exchange cross sections are given by Gryzinski and Riviere.³

The cross section for ionization of hydrogen atoms by electrons is

$$\sigma_{\text{ion}}^e = 3.52 \times 10^{-16} g(x) \text{ cm}^2, \quad (6)$$

where

$$g(x) = \frac{1}{x} \left(\frac{x-1}{x+1} \right)^{3/2} \left[1 + \frac{2}{3} \left(1 - \frac{1}{2x} \right) \ln(2.7 + \sqrt{x-1}) \right], \quad (7)$$

and x is the dimensionless ratio of the relative electron energy and the hydrogen ionization energy, $(1/2 m_e v_r^2) / (13.605 \text{ eV})$.

The cross section for ionization of hydrogen atoms by protons is given by the following expression.

$$\sigma_{\text{ion}}^p = \begin{cases} 10^{-0.871} 2(\log_{10} E)^2 + 8.156(\log_{10} E) - 34.833 \text{ cm}^2 & E \leq 150 \text{ keV} \\ 3.6 \times 10^{-12} \frac{1}{E} \log_{10}(0.1666E) \text{ cm}^2 & E > 150 \text{ keV}, \end{cases} \quad (8)$$

where E is the relative proton energy in eV, $(1/2 m_p v_r^2)$.

The cross section for charge-exchange is expressed as follows.

$$\sigma_{\text{exch}} = \frac{0.6937 \times 10^{-14} (1 - 0.155 \log E)^2}{1 + 0.1112 \times 10^{-14} E^{3.3}} \text{ cm}^2, \quad (9)$$

where E is the relative proton energy in eV, $(1/2 m_p v_r^2)$.

Functional dependencies of cross sections on energy can be seen in Figs. 2, 3, and 4.

Fig. 1.
Tokamak cross section.

Fig. 2.
Electron ionization cross sections.

Fig. 3.
Proton ionization cross sections.

Fig. 4.
Proton charge exchange cross sections.

IV. THE BOLTZMANN EQUATION

Transport codes solve the following form of the Boltzmann transport equation.

$$\vec{\Omega} \cdot \nabla \phi(\vec{r}, \vec{\Omega}, E) + \Sigma_T(\vec{r}, E) \phi(\vec{r}, \vec{\Omega}, E) = \iint_S \Sigma_S(\vec{r}, \vec{\Omega}' \cdot \vec{\Omega}, E' \rightarrow E) \phi(\vec{r}, \vec{\Omega}', E') d\vec{\Omega}' dE' + S(\vec{r}, \vec{\Omega}, E), \quad (10)$$

where

- $\phi(\vec{r}, \vec{\Omega}, E)$ = the particle flux differential in direction and energy,
- $\Sigma_T(\vec{r}, E)$ = the total effective macroscopic interaction cross section,
- $\Sigma_S(\vec{r}, \vec{\Omega}' \cdot \vec{\Omega}, E' \rightarrow E)$ = the effective macroscopic differential scattering cross section, and
- $S(\vec{r}, \vec{\Omega}, E)$ = the inhomogeneous source term differential in direction and energy.

This equation is generally used in neutron transport, but it can also be used in neutral atom transport because the atomic ionization and charge-exchange interactions are analogous to the neutron absorption and scattering interactions, respectively. Because the average speed of the incident neutral atoms is generally not considerably larger than the average speed of the plasma particles, the calculation of the effective cross sections involves an integration over the phase-space distribution function of the plasma particles. This fact is clearly reflected by the following form of the Boltzmann transport equation.

$$\begin{aligned} & \vec{v} \cdot \nabla n(\vec{r}, \vec{v}) + \int_{\vec{v}} n(\vec{r}, \vec{v}) N(\vec{r}, \vec{v}) \cdot \nabla (|\vec{v} - \vec{v}'|) |\vec{v} - \vec{v}'| d\vec{v}' \\ &= \int_{\vec{v}} \int_{\vec{v}'} n(\vec{r}, \vec{v}') N(\vec{r}, \vec{v}) \Sigma_S(\vec{r}, \vec{v}' \rightarrow \vec{v}, \vec{v}) |\vec{v} - \vec{v}'| d\vec{v} d\vec{v}' + S(\vec{r}, \vec{v}), \end{aligned} \quad (11)$$

where

- $n(\vec{r}, \vec{v})$ = the neutral particle density differential in velocity,

- $N(\vec{r}, \vec{v})$ = the target particle density differential in velocity,
 $\sigma_T(|\vec{v}-\vec{v}'|)$ = the total microscopic interaction cross section as a function of the relative speed between primary and target particles,
 $\sigma_S(\vec{r}, \vec{v}' \rightarrow \vec{v}, \vec{v})$ = the microscopic differential scattering cross section as a function of the target particle velocity, and
 $S(\vec{r}, \vec{v})$ = the inhomogeneous source term differential in velocity.

A static (no target recoil) model leads to the following expression for the microscopic differential scattering cross section.

$$\sigma_S(\vec{v}' \rightarrow \vec{v}, v) = \sigma_{\text{exch}}(|\vec{v}-\vec{v}'|) \delta(\vec{v}-\vec{v}'). \quad (12)$$

Substituting this expression into Eq. (11), we obtain the following result.

$$\begin{aligned}
 \vec{v} \cdot \vec{\nabla} n(\vec{r}, \vec{v}) + \int_{\vec{v}} n(\vec{r}, \vec{v}') N(\vec{r}, \vec{v}) \sigma_T(|\vec{v}-\vec{v}'|) d\vec{v}' \\
 + \int_{\vec{v}'} n(\vec{r}, \vec{v}') N(\vec{r}, \vec{v}) \sigma_{\text{exch}}(|\vec{v}-\vec{v}'|) |\vec{v}-\vec{v}'| d\vec{v}' + S(\vec{r}, \vec{v}) = 0.
 \end{aligned} \quad (13)$$

By comparing equivalent terms in Eqs. (10) and (13) it can be seen that the following expressions result for the effective macroscopic cross sections.

$$\begin{aligned}
 \Sigma_T(\vec{r}, \vec{v}) &= \int_{\vec{v}} \frac{N(\vec{r}, \vec{v}') \sigma_T(|\vec{v}-\vec{v}'|) |\vec{v}-\vec{v}'|}{v} d\vec{v}', \\
 \Sigma_S(\vec{r}, \vec{v}' \rightarrow \vec{v}) &= \frac{N(\vec{r}, \vec{v}') \sigma_{\text{exch}}(|\vec{v}-\vec{v}'|) |\vec{v}-\vec{v}'|}{v'}.
 \end{aligned} \quad (14)$$

It is important to note that if the plasma phase-space distribution function is not isotropic in direction, the cross sections will take the following form in the notation of Eq. (10).

$$\Sigma_T(\vec{r}, \vec{v}) \sim \Sigma_T(\vec{r}, \vec{\Omega}, E) ,$$

$$\Sigma_S(\vec{r}, \vec{v}' \rightarrow \vec{v}) \sim \Sigma_S(\vec{r}, \vec{\Omega}', \vec{\Omega}, E' \rightarrow E) . \quad (15)$$

That is to say that the total effective interaction cross section will depend upon the primary particle direction, and the effective differential scattering cross section will depend on both the direction of the incident primary particle and the outgoing direction of the scattered particle after collision. Current multigroup discrete-ordinates transport codes do not accept cross sections with such directional dependence. Thus, the plasma phase-space distribution function is here assumed to be isotropic in direction. Fortunately, this should not result in too gross an approximation as the distribution function for a Tokamak system generally consists of a relatively small drift velocity superposed on a characteristic Maxwellian distribution.

V. MULTIGROUP MACROSCOPIC EFFECTIVE CROSS SECTIONS

Definitions:

NEG	= the number of energy groups (same for all particles),
$\{E_i\}_{i=1}^{NEG+1}$	= the energy group boundaries in increasing order,
$\{v_i^e\}_{i=1}^{NEG+1}$	= the corresponding electron velocity group boundaries,
$\{v_i^p\}_{i=1}^{NEG+1}$	= the corresponding proton velocity group boundaries,
NLPM	= the number of Legendre moments in the differential scattering cross-section expansions,
NSR	= the number of spatial (temperature) regions,
$\{R_i\}_{i=1}^{NSR}$	= the spatial region boundaries in ascending order,

- $\Sigma_a(I,J)$ = the multigroup effective macroscopic absorption cross section corresponding to the I^{th} spatial region and the J^{th} energy group.
- $\Sigma_s(I,J)$ = the multigroup effective macroscopic scattering cross section corresponding to the I^{th} spatial region and the J^{th} energy group,
- $\Sigma_{sL}(I,J,K,M)$ = the M^{th} Legendre moment of the effective differential macroscopic scattering cross section corresponding to a transfer from energy group J to energy group K in the I^{th} spatial region,
- $w(v)$ = the weighting function used in averaging the cross section within each incident particle energy group. By user option, $w(v) = 1.0$ or $w(v) = v$.
- m_e = the electron mass,
- m_p = the proton mass,
- $T_e(r)$ = the electron temperature function,
- $T_p(r)$ = the proton temperature function,
- $\rho_e(r)$ = the electron particle density function,
- $\rho_p(r)$ = the proton particle density function,
- $N_e(r,v)$ = the electron velocity distribution function
 $= \exp[-m_e v^2 / 2kT_e(r)]$,
- $N_p(r,v)$ = the proton velocity distribution function
 $= \exp[-m_p v^2 / 2kT_p(r)]$,
- v_1 = the target particle speed,
- v_2 = the primary particle speed,
- μ = the cosine of the angle between a primary and target particle,

v_r = the relative speed between a primary and target particle,

$$= \sqrt{v_1^2 + v_2^2 - 2v_1v_2\mu},$$

$\sigma_{ion}^e(v_r)$ = the microscopic cross section for ionization of hydrogen atoms by electrons,

$\sigma_{ion}^p(v_r)$ = the microscopic cross section for ionization of hydrogen atoms by protons,

$\sigma_{exch}(v_r)$ = the microscopic cross section for hydrogen-proton charge exchange,

$P_\ell(\mu)$ = the ℓ 'th Legendre polynomial.

Actual multigroup integrals are given below. The variables v, V are dummy, $v_r = |\vec{v} - \vec{V}|$ and proton group velocity boundaries are implicit in all integral limits except in T1 and T2 where electron group velocity boundaries are required for V_1 to V_{NEG+1} .

$$\Sigma_a(I, J) = T1/T2 + T3/T4, \quad (16)$$

where

$$T1 = \int_{R_I}^{R_{I+1}} \int_{-1}^{+1} \int_{v_J}^{v_{J+1}} \int_{V_1}^{V_{NEG+1}} w(v) \rho_e(r) N_e(r, V) \sigma_{ion}^e(v_r) \frac{v_r}{v} dv dv d\mu dr,$$

$$T2 = 2.0 \int_{R_I}^{R_{I+1}} \int_{v_J}^{v_{J+1}} \int_{V_1}^{V_{NEG+1}} w(v) \rho_e(r) N_e(r, V) dv dv dr,$$

$$T3 = \int_{R_I}^{R_{I+1}} \int_{-1}^{+1} \int_{v_J}^{v_{J+1}} \int_{V_1}^{V_{NEG+1}} w(v) \rho_p(r) N_p(r, V) \sigma_{ion}^p(v_r) \frac{v_r}{v} dv dv d\mu dr,$$

$$T4 = 2.0 \int_{R_I}^{R_{I+1}} \int_{V_J}^{V_{J+1}} \int_{V_1}^{V_{NEG+1}} w(v) \rho_p(r) N_p(r, V) dv dv dr, \quad (17)$$

and

$$\Sigma_S(I, J) = T5/T6, \quad (18)$$

where

$$T5 = \int_{R_I}^{R_{I+1}} \int_{-1}^{+1} \int_{V_J}^{V_{J+1}} \int_{V_1}^{V_{NEG+1}} w(v) \rho_p(r) N_p(r, V) \sigma_{\text{exch}}(v_r) \frac{v_r}{v} dv dv dr, \quad (19)$$

$$T6 = 2.0 \int_{R_I}^{R_{I+1}} \int_{V_J}^{V_{J+1}} \int_{V_1}^{V_{NEG+1}} w(v) \rho_p(r) N_p(r, V) dv dv dr,$$

and

$$\Sigma_S(I, J, K, M) = T7/T8, \quad (20)$$

where

$$T7 = \int_{R_I}^{R_{I+1}} \int_{-1}^{+1} \int_{V_J}^{V_{J+1}} \int_{V_K}^{V_{K+1}} w(v) \rho_p(r) N_p(r, V) \sigma_{\text{exch}}(v_r) \frac{v_r}{v} P_{M-1}(\mu) dv dv dr, \quad (21)$$

$$T8 = 2.0 \int_{R_I}^{R_{I+1}} \int_{V_J}^{V_{J+1}} \int_{V_K}^{V_{K+1}} w(v) \rho_p(r) N_p(r, V) dv dv dr.$$

Since the integrations are performed numerically, the zeroth order scattering moments have to be normalized after evaluation such that

$$\sum_{K=1}^{NEG} \Sigma_{SD}(I,J,K,l) = \Sigma_S(I,J). \quad (22)$$

This normalization simply insures the sum of the upscatter and downscatter cross sections within each group are equal to the total scattering cross section for the group. The higher order moments are also multiplied by the zero'th order normalization factor to maintain the same relative ratio between the coefficients of the expansion.

V. CROSS-SECTION WEIGHTING

The group-averaged cross section σ_g for an energy group bounded by energies E_1 and E_2 is expressed as follows.

$$\sigma_g = \frac{\int_{E_1}^{E_2} \phi(E) \sigma(E) dE}{\int_{E_1}^{E_2} \phi(E) dE}, \quad (23)$$

where $\phi(E)$ is the particle flux differential in energy and $\sigma(E)$ is the point cross section that is being averaged. As is easily seen from the equation, the particle flux serves as a weighting function in the averaging process. There are two options for the functional form of $\phi(E)$ in PLASMK:

- 1) $\phi(E) \sim \text{constant},$
- 2) $\phi(E) \sim \sqrt{\frac{2E}{m}} = v(E).$

The first option is referred to as uniform weighting, while the second option is referred to as velocity weighting. Since $\phi(E) = N(E)v(E)$, where $N(E)$ is the particle density, velocity weighting is equivalent to a constant particle density.

As can be seen in Sec. IV, the integrands in the expressions for the effective multigroup macroscopic cross sections are inversely proportional to the incident particle velocity. If uniform weighting is used, the inverse velocity term remains, but if velocity weighting is used, the inverse velocity term is cancelled out. This cancellation results in a significantly lower computational cost for the evaluation of the effective multigroup macroscopic cross sections. Thus, lacking any prior knowledge of the accuracy of either weighting option, the velocity weighting option is recommended.

VI. POINT MICROSCOPIC EFFECTIVE CROSS SECTIONS

PLASMX can be used to calculate point microscopic effective cross sections as well as multigroup macroscopic effective cross sections. The effective microscopic cross sections are referred to as point cross sections because they are evaluated at a specific incident hydrogen atom energy and a specific plasma temperature. For instance, let σ be the microscopic cross section for some interaction of interest. Then the effective microscopic cross section for the interaction can be expressed as follows.

$$\sigma_{\text{eff}}(\vec{v}) = \frac{\int_{\vec{V}} N(\vec{V}) \sigma(|\vec{V}-\vec{v}|) \frac{|\vec{V}-\vec{v}|}{v} d\vec{V}}{\int_{\vec{V}} N(\vec{V}) d\vec{V}}, \quad (24)$$

where

$N(\vec{V})$ = the plasma phase space distribution function, and

$\vec{v}$ = the velocity of the incident particle.

Microscopic cross sections are generated for three interactions: ionization of hydrogen by electrons, ionization of hydrogen by protons, and charge exchange between hydrogen and protons. The incident hydrogen energies are those of the energy groups boundaries, and the plasma temperatures are those at the midpoint of each spatial region.

The point microscopic cross sections are not directly usable in transport calculations, but they provide useful information on the behavior of the macroscopic cross sections as a function of incident hydrogen atom energy and plasma temperature. The computational cost of calculating point microscopic cross sections is exceptionally small relative to the cost of calculating macroscopic cross sections. Any additional running time incurred through the generation of point microscopic cross sections is negligible.

VII. NUMERICAL INTEGRATION TECHNIQUES

For general one-dimensional applications, adaptive integration routines have been proven to be the most efficient. However, for multidimensional applications, no single technique has been shown to be clearly superior. A reasonable approach was taken in PLASMX by coupling several equivalent one-dimensional adaptive integration routines to perform the multidimensional cross-section integrations. This technique is well known and can be easily demonstrated for a two-dimensional integration.

Let $f(x,y)$ be the function to be integrated between fixed limits. Then

$$\int_{y_1}^{y_2} \int_{x_1}^{x_2} f(x,y) dx dy = \int_{y_1}^{y_2} F(y) dy, \quad (25)$$

where

$$F(y) = \int_{x_1}^{x_2} f(x,y) dx. \quad (26)$$

One routine is used to integrate the one-dimensional function $F(y)$. When this routine calls for a value of F at a quadrature point, y_0 , another equivalent routine integrates the one-dimensional function $f(x,y_0)$ over x to provide that value.

The $SIMP^4$ routine is the basic one-dimensional integration routine used in PLASMX. It uses a Simpson's rule (three-point Newton-Coates) quadrature in conjunction with an adaptive algorithm. The most distinguishing feature of the code is the use of an L1 relative error norm. Under this norm, the relative error, $RELERR$, is defined as follows.

$$RELERR = \frac{\int f(x) dx - ANS}{\int |f(x)| dx}, \quad (27)$$

where ANS is the numerical approximation to the integral of $f(x)$. If $f(x)$ is

positive definite over the range of integration, the L1 relative error is equivalent to the standard relative error. However, if $f(x)$ is oscillatory, the use of the L1 norm results in a less stringent absolute error requirement. This is particularly useful in the evaluation of higher order Legendre polynomial moments.

The size of a moment relative to the zeroth order moment is a measure of the importance of that moment to the differential cross-section expansion. With the use of the L1 relative error norm, the zeroth order moments, or integral cross sections, are calculated subject to the standard relative error norm. However, the smaller, less important moments are calculated subject to an absolute error requirement that is less stringent than that resulting from the use of the standard norm. Thus, in a somewhat limited sense, the computational effort expended in the calculation of a moment is proportional to the importance of that moment.

If a standard relative error requirement ϵ is specified for each of the coupled one-dimensional integrations, the expression for an upper bound ϵ^n on the relative error of the complete multidimensional integral takes the following form:

$$\epsilon^n = (1 + \epsilon)^n - 1, \quad (28)$$

where n is the dimensionality of the integral. For $\epsilon \ll 1$,

$$(1 + \epsilon)^n - 1 \approx n\epsilon. \quad (29)$$

If the PLASM user specifies a relative error tolerance TOL for the cross-section integrations, each one-dimensional integration is performed subject to a relative error tolerance of ϵ , where

$$\epsilon = \text{TOL}/n. \quad (30)$$

Experience has shown this approach to be highly conservative. Error cancellation usually occurs between dimensions such that the true relative error is on the order of ϵ rather than TOL.

VIII. INPUT INSTRUCTIONS

CARD 1 Format (8A10)

TITLE - user-desired title

CARD 2 Format (6I10)

NEG - number of energy groups
NSR - number of spatial (temperature) regions
NLPM - number (not order) of Legendre polynomial moments
IEGN - 1/2/3
 1/read energy group boundaries/
 2/read minimum and maximum energies and generate NEG
 groups with uniform logarithmic spacing/
 3/same as 2 with uniform linear spacing/
IMCRO - 0/1/2
 0/multigroup macroscopic cross sections only/
 1/point microscopic cross sections only/
 2/both
INGHT - 1/2
 1/velocity weighting within each energy group/
 2/uniform weighting within each energy group/

CARD 3 Format (5E12.5)

ETEMP - maximum electron plasma temperature in eV
PTEMP - maximum proton plasma temperature in eV
DENMAX - maximum plasma density (electron + proton) in particles/cm³
RCOL - plasma column radius in cm
RWALL - confinement wall inner radius in cm

CARD 4

Format (6E12.5)

If IEGN = 1,

EGRID(I) - energy group boundaries in ascending order in eV; more than one
I=1, NEG+1 card may be necessary

If IEGN=2,3,

EMIN,EMAX - the minimum and maximum energy group boundaries in eV

CARD 5

Format (E12.5)

TOL - integral relative error tolerance

CARD 6

Format (6E12.5)

RGRID(I) - spatial region boundaries in ascending order in cm; RGRID(1) must
be zero and RGRID(NEG+1) must be equal to RCOL; more than one card
I=1, NSR+1 may be necessary

IX. OUTPUT

Three output files are written by PLASMX: Tape 6, Tape 7, and Tape 8.

Tape 6 is the standard printer output. The following information is
printed:

1. values for all input variables,
2. the energy group boundaries,
3. the corresponding electron velocity group boundaries,
4. the corresponding proton velocity group boundaries, and
5. point microscopic cross sections, if they are specified in input.

The macroscopic cross sections do not appear in the printed output. However, they may be copied from Tape 7 to the output file with control cards if the user so desires.

Tape 7 is written in card image format and is suitable to be copied to the punch file. It is intended to provide the user with an output file which contains the macroscopic cross sections and all of the information necessary to interpret them.

The following information appears on the file:

1. values for all input variables,

2. the energy group boundaries identified as the EGRID array,
3. the corresponding electron and proton velocity group boundaries identified as the VGRID array, where the first half of the values are the electron velocities, and the remaining half of the values are the proton velocities,
4. the macroscopic absorption and scattering cross sections as a function of spatial interval and the energy groups of the incident hydrogen atoms, and
5. the Legendre moments in ascending order as each possible energy group transfers as a function of spatial interval and the energy group of the incident hydrogen atoms.

It should be noted that the internal notation of PLASMX is used on Tape 7 in referring to the energy groups. Under this notation, group 1 is the group of lowest energies. This is contrary to the standard multigroup notation.

Tape 8 contains the macroscopic cross sections in standard IASL input format. It may be copied to the punch file with control cards if the user so desires.

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APPENDIX A

COMMON BLOCK VARIABLE DEFINITIONS

1. Unlabeled Common:

NEG	- Number of energy groups
NLDM	- Number (not order) of Legendre moments to be calculated
NSR	- Number of spatial (temperature) regions
TOL	- Integral relative error tolerance
IEGN	- Energy group structure trigger:

IEGN=1, energy group boundaries are read in
 IEGN=2, minimum and maximum energies are read in and NEG groups are generated with uniform logarithmic spacing
 IEGN=3, same as IEGN=2 with uniform linear spacing

IMCRO - Cross-section calculation trigger:
 IMCRO=0, only macroscopic cross sections calculated
 IMCRO=1, only microscopic cross sections calculated
 IMCRO=2, both macroscopic and microscopic cross sections generated

EGRID(I) - The energy group boundaries in ascending order
 VGRID(1,I) - The corresponding electron velocity group boundaries
 VGRID(2,I) - The corresponding proton velocity group boundaries
 XA(I,J) - The macroscopic absorption (ionization) cross section for spatial interval I and energy group J
 XS(I,J) - The macroscopic scattering (charge-exchange) cross section for spatial interval I and energy group J
 XDS(I) - The one-dimensional array within which the Legendre moments of the transfer matrix are stored. The function subroutine IX computes addresses for the XDS array such that XDS(IX(I,J,K,M)) is the Mth Legendre moment corresponding to the spatial interval I for a transfer from energy group J to energy group K
 XNCFS(I,J) - An array of factors used in the normalization of the scalar proton cross-section integrals
 XNCDFS(I,J) - An array of factors used in the normalization of the Legendre moments integrals
 DV(I,J) - An array of factors used in the normalization of all macroscopic cross-section integrals
 RGRID(I) - The spatial interval boundaries in ascending order.

2. Labeled Common:

K - The factor for converting electron volts to ergs
 ME - The electron mass in grams
 MP - The proton mass in grams
 ID,JD,KD,LD - Constants used in computing addresses for the XDS array
 MM - The value of the index M when XDS(IX(I,J,M,L)) is being calculated
 LPL - The value of the index L when XDS(IX(I,J,M,L)) is being calculated
 IWGHT - If IWGHT=1, velocity weighting is used in the multigroup cross-section averaging; if IWGHT=2, a constant weighting function is used

ETEMP	- The maximum electron plasma temperature
PTEMP	- The maximum proton plasma temperature
DEFMAX	- The maximum plasma (electrons + protons) density
RCOL	- The plasma column radius
RWALL	- The confinement wall radius.

APPENDIX B

SAMPLE PROBLEM AND ZONING

The input and output follow for a three-group, three-spatial-region problem with one Legendre moment (P_0) in the differential cross-section expansion. Uniform logarithmic spacing is used for the energy group structure with minimum and maximum energies of 1.0 eV and 4 641.5 eV, respectively. Microscopic cross sections are generated and velocity weighting is used in averaging the cross sections. The maximum electron plasma temperature is 800 eV and the maximum proton plasma temperature is 250 eV. The maximum plasma density is 6.0×10^{13} particles/cm³. The plasma column radius is 23.0 cm and the confinement wall inner radius is 25.0 cm. All integrations are performed subject to an LL relative error tolerance of 0.05. The spatial region boundaries are 0.0 cm, 16.0 cm, 21.0 cm, and 23.0 cm, respectively.

One method of zoning a plasma consists in finding boundaries of zones of equal relative temperature change. For a plasma of N zones, with $n \leq N$, we have for constant K in zone n ,

$$\frac{T_{n+1} - T_n}{T_{n+1} + T_n} = K$$

$$\frac{T_{n+1}}{T_n} = \left(\frac{1+K}{1-K} \right). \quad (B-1)$$

Iterating on T_0 , it follows that

$$\frac{T_n}{T_O} = \left(\frac{1+K}{1-K} \right)^n = Q^n . \quad (B-2)$$

Choosing both T_N and T_O , we can solve for Q , for any N ,

$$\frac{T_N}{T_O} = Q^N$$

$$Q = \left(\frac{T_N}{T_O} \right)^{\frac{1}{N}} . \quad (B-3)$$

As example, take $N = 10$ and $T_{10}/T_O = 6.510\ 416\ 667$, so

$$\left(\frac{T_n}{T_O} \right) = Q^n \quad n = 0, 1, 2, \dots, N . \quad (B-4)$$

and, therefore,

$$\begin{aligned} T_O &= 0.153\ 6 T_{10} \\ T_1 &= 0.185\ 2 T_{10} \\ T_2 &= 0.223\ 4 T_{10} \\ T_3 &= 0.269\ 4 T_{10} \\ T_4 &= 0.325\ 0 T_{10} \\ T_5 &= 0.391\ 9 T_{10} \\ T_6 &= 0.472\ 66 T_{10} \\ T_7 &= 0.570\ 1 T_{10} \\ T_8 &= 0.687\ 5 T_{10} \\ T_9 &= 0.829\ 2 T_{10} \\ T_{10} &= 1.0 T_{10} . \end{aligned}$$

We now use the T/T_{10} ratio to determine the appropriate r mesh,

$$T_n/T_{10} = [1 - (r_n/25)^2]$$

$$(r_n/25)^2 = 1 - T_n/T_{10}$$

$r_n = 25 \sqrt{1 - T_n/T_{10}} \text{ cm}$,
so that

$$r_0 = 23.0$$

$$r_1 = 22.57$$

$$r_2 = 22.03$$

$$r_3 = 21.37$$

$$r_4 = 20.54$$

$$r_5 = 19.5$$

$$r_6 = 18.15$$

$$r_7 = 16.39$$

$$r_8 = 13.98$$

$$r_9 = 10.33$$

$$r_{10} = 0.0 \quad ,$$

or in terms of T/T_0 and r for the plasma under consideration,

r	T/T_0
0	1.0
2	0.993 6
4	0.974 4
6	0.942
8	0.897 6
10	0.840 0
12	0.769 6
14	0.686 4
16	0.590 4
18	0.481 6
20	0.36
22	0.225 6
24	0.078 4
25	0.0

Taking the rigorous approach:

$$T = T_0 [1 - (r/25)^2]$$

$$T \left| \begin{matrix} r_{n+1} \\ r_n \end{matrix} \right| = \frac{T_o}{r_{n+1} - r_n} \int_{r_n}^{r_{n+1}} (1 - r^2/625) dr = \frac{T_o}{r_{n+1} - r_n} \left| \begin{matrix} r_{n+1} \\ r_n \end{matrix} \right| r - \frac{r^3}{1875} .$$

$$\bar{T}_{n+1} = \frac{T_o}{r_{n+1} - r_n} \left[(r_{n+1} - r_n) + \frac{r_n^3 - r_{n+1}^3}{1875} \right]$$

$$\begin{aligned} |T_{n+1} - T_n| &= T_o [1 - (r_n/25)^2] - T_o [1 - (r_{n+1}/25)^2] \\ &= \frac{T_o}{625} (r_{n+1}^2 - r_n^2) . \end{aligned} \quad (B-6)$$

We want to find K such that

$$\frac{|T_{n+1} - T_n|}{\bar{T}_{n+1}} = K , \quad r_0 = 0, \quad r_{10} = 23.0 . \quad (B-7)$$

Substituting, one finds

$$\begin{aligned} \frac{|T_{n+1} - T_n|}{\bar{T}_{n+1}} &= \frac{T_o (r_{n+1}^2 - r_n^2)}{625} \left(\frac{r_{n+1} - r_n}{T_o} \right) \left[(r_{n+1} - r_n) + \frac{r_n^3 - r_{n+1}^3}{1875} \right]^{-1} \\ &= \frac{(r_{n+1}^2 - r_n^2) (r_{n+1} - r_n)}{625} \frac{(1875)}{(1875) (r_{n+1} - r_n) + (r_n^3 - r_{n+1}^3)} . \end{aligned}$$

$$K = \frac{3(r_{n+1}^2 - r_n^2) (r_{n+1} - r_n)}{(1875) (r_{n+1} - r_n) + (r_n^3 - r_{n+1}^3)} . \quad (B-8)$$

This system must obviously be solved by iteration. Results are:

$$r_0 = 0.0$$

$$r_1 = 10.46$$

$$r_2 = 14.054$$

$$r_3 = 16.445$$

$$r_4 = 18.189$$

$$r_5 = 19.517$$

$$r_6 = 20.554$$

$$r_7 = 21.376$$

$$r_8 = 22.035$$

$$r_9 = 22.567$$

$$r_{10} = 23.000$$

The exact relationships between T/T_0 and r from Eq. (B-8) are depicted in Fig. B-1.

Fig. B-1.
Regions of equal weighted relative temperature change.

SAMPLE INPUT

```

***THREE GROUP, THREE REGION, P0 SAMPLE PROBLEM***
      3      3      1      3      2      1
      .800000E+03 .250000E+03 .600000E+14 .230000E+02 .250000E+02
      .100000E+01 .464160E+04
      .500000E-01
      .000000E+00 .160000E+02 .210000E+02 .230000E+02

```

SAMPLE OUTPUT

```

***THREE GROUP, THREE REGION, P0 SAMPLE PROBLEM***

```

NUMBER OF ENERGY GROUPS= 3

NUMBER OF SPATIAL REGIONS= 3

NUMBER OF LEGENDRE POLYNOMIAL MOMENTS= 1

IGEN= 3

IMCRO= 2

VELOCITY WEIGHTING USED WITHIN EACH ENERGY GROUP

MAXIMUM ELECTRON TEMPERATURE (EV)= .80000E+03

MAXIMUM PROTON TEMPERATURE (EV)= .25000E+03

MAXIMUM PLASMA DENSITY (PARTICLES/CM*3)= .60000E+14

PLASMA COLUMN RADIUS (CM)= .23000E+02

CONFINEMENT WALL RADIUS (CM)= .25000E+02

INTEGRAL ERROR TOLERANCE= .50000E-01

THE ENERGY GROUP BOUNDRIES FOLLOW (EV)

.10000E+01 .16681E+02 .27826E+03 .46416E+04

THE CORRESPONDING ELECTRON VELOCITY GROUP BOUNDRIES FOLLOW (CM/SEC)

.59304E+08 .24221E+09 .98926E+09 .40404E+10

THE CORRESPONDING PROTON VELOCITY GROUP BOUNDRIES FOLLOW (CM/SEC)

.13851E+07 .56572E+07 .23105E+08 .94367E+08

THE SPATIAL REGION BOUNDRIES FOLLOW (CM)

0. .16000E+02 .21000E+02 .23000E+02

----- POINT MICROSCOPIC CROSS-SECTIONS (CM**2) -----

TARGET ELECTRON TEMPERATURE (EV)=	.71808E+03	TARGET PROTON TEMPERATURE (EV)=	.22440E+03
INCIDENT ENERGY (EV)	ELECTRON IONIZATION	PROTON IONIZATION	PROTON CHARGE EXCHANGE
.10000E+01	.66362E-15	.26402E-17	.43606E-13
.16681E+02	.16175E-15	.75287E-18	.10806E-13
.27826E+03	.35097E-16	.87813E-18	.31021E-14
.46416E+04	.51344E-17	.28945E-16	.12944E-14

TARGET ELECTRON TEMPERATURE (EV)=	.36192E+03	TARGET PROTON TEMPERATURE (EV)=	.11310E+03
INCIDENT ENERGY (EV)	ELECTRON IONIZATION	PROTON IONIZATION	PROTON CHARGE EXCHANGE
.10000E+01	.70224E-15	.22260E-18	.35495E-13
.16681E+02	.17093E-15	.75185E-19	.90060E-14
.27826E+03	.39106E-16	.24259E-18	.28899E-14
.46416E+04	.51694E-17	.25946E-16	.12927E-14

TARGET ELECTRON TEMPERATURE (EV)=	.18048E+03	TARGET PROTON TEMPERATURE (EV)=	.54400E+02
INCIDENT ENERGY (EV)		PROTON IONIZATION	PROTON CHARGE EXCHANGE
.10000E+01	.74558E-15	.13220E-19	.29303E-13
.16681E+02	.18238E-15	.62255E-20	.75172E-14
.27824E+03	.42130E-16	.79558E-19	.27912E-14
.66414E+04	.51835E-17	.24418E-16	.12918E-14

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*****THREE GROUP, THREE REGION, 20 SAMPLE PROBLEM*****
 NUMBER OF ENERGY GROUPS

NUMBER OF SPATIAL REGIONS

NUMBER OF LEGENDRE POLYNOMIAL MOMENTS

VELOCITY WEIGHTING USED WITHIN EACH ENERGY GROUP

MAXIMUM ELECTRON TEMPERATURE (EV)

.800000000E+03

MAXIMUM PROTON TEMPERATURE (EV)

.2500000000E+03

MAXIMUM PLASMA DENSITY (PARTICLES/CM³)

.8000000000E+14

PLASMA COLUMN RADII'S (CM)

.2300000000E+02

CONFINEMENT WALL RADIUS (CM)

.2500000000E+02

INTEGRAL ERROR TOLERANCE

.500000000E-11

GRID ARRAY (EV)

.100000000E+01

.14681875E+02

.2782563865E+03

.4641400000E+04

VGNID ARRAY (CM/SEC)			
.5930442032E+00	.2422135029E+09	.9892501473E+09	.4040367983E+10
.1305121971E+07	.5657170960E+07	.2310524557E+08	.9430737486E+08
HGNID ARRAY (CM) 0.			
		.1400002000E+02	.2100000000E+02
ZONE NUMBER 1			
TOTAL MACROSCOPIC ABSORPTION CROSS-SECTIONS			
.50699148E+00	.4138913838E-01	.1531181724E-01	
TOTAL MACROSCOPIC SCATTERING CROSS-SECTIONS			
.7999974203E+00	.1067452280E+00	.4024472597E-01	
LEGENDRE SCATTERING MOMENTS			
PMOM GROUP 1	TO GROUP	1	
.2773305856E-02	TO GROUP	2	
PMOM GROUP 1	TO GROUP	3	
.1799619446E+00	TO GROUP	1	
PMOM GROUP 1	TO GROUP	2	
.2172021698E+00	TO GROUP	3	
PMOM GROUP 2	TO GROUP	1	
.1256889060E-02	TO GROUP	2	
PMOM GROUP 2	TO GROUP	3	
.5068549617E-01	TO GROUP	1	
PMOM GROUP 2	TO GROUP	2	
.5480284276E-01	TO GROUP	3	
PMOM GROUP 3	TO GROUP	1	
.4413267216E-03	TO GROUP	2	
PMOM GROUP 3	TO GROUP	3	
.2140417306E-01	TO GROUP	1	
PMOM GROUP 3	TO GROUP	2	
.1219522619E-01	TO GROUP	3	
ZONE NUMBER 2			
TOTAL MACROSCOPIC ABSORPTION CROSS-SECTIONS			
.1298020117E+00	.2178219279E-01	.7895604076E-02	
TOTAL MACROSCOPIC SCATTERING CROSS-SECTIONS			
.1612603792E+00	.4531111417E-01	.1866975999E-01	
LEGENDRE SCATTERING MOMENTS			
PMOM GROUP 1	TO GROUP	1	
.2877498745E-02	TO GROUP	2	
PMOM GROUP 1	TO GROUP	3	
.1134368183E+00	TO GROUP	1	
	TO GROUP	2	
	TO GROUP	3	

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P 0 CROSS-SECTIONS FOR MATERIAL 1
 .15312E-01 0. .55557E-01 .21726E+00 .54803E-01 .18199E-01
 0. 0. .61389E-01 0. .16813E+00 0.
 .17996E+00 .50685E-01 .21404E-01 0. .25070E+00 0.
 .65070E+00 0. 0. .27733E-02 .12569E-02 .64133E-03
 P 0 CROSS-SECTIONS FOR MATERIAL 2
 .78956E-02 0. .26565E-01 .44946E-01 .11399E-01 .39338E-02
 0. 0. .31782E-01 0. .77093E-01 0.
 .11344E+00 .32607E-01 .14070E-01 0. .12980E+00 0.
 .29106E+00 0. 0. .28775E-02 .13046E-02 .66581E-03
 P 0 CROSS-SECTIONS FOR MATERIAL 3
 .21858E-02 0. .69991E-02 .18588E-02 .47444E-03 .16883E-03
 0. 0. .88180E-02 0. .19529E-01 0.
 .31240E-01 .94163E-02 .42266E-02 0. .36014E-01 0.
 .70918E-01 0. 0. .18051E-02 .82018E-03 .41780E-03

COPYSF .END OF INFORMATION