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MASTER

TOPICAL REPORT

TRANSPORT PHENOMENA IN A PLASMA DIODE

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BY Jack H Kahnfamh
DATE 6/5/72

M. Clark and J. Keck

September 1971

Thermo Electron Corporation
85 First Avenue
Waltham, Massachusetts 02154

Prepared for

U. S. Atomic Energy Commission
Space Nuclear Systems Division
Contract AT(11-1)-3056

Lester K. Price, AEC Project Manager

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INTRODUCTION

The results derived from the theoretical study of the plasma serve to guide the development of the thermionic converter and form a foundation for both converter diagnostics and the evaluation of techniques which improve the performance To maintain continued progress in converter development, there must be a continuous interchange between theory and the experimental data obtained from the converter

Most of the present plasma theories have considered the interelectrode space as being separable into three regions: an emitter sheath, a neutral plasma, and a collector sheath By assigning different physical phenomena to the sheath and plasma regions, it has been possible to derive solutions which satisfy the emitter and collector boundary conditions and which give such information as particle concentrations, energy flux and electron temperature as a function of position in the interelectrode space Comparisons of the predictions of these analyses with experimental results have verified the correctness of some of the predictions Thus, the presence of a region of strong ionization near the emitter, an inverse dependence of output voltage on spacing-pressure product, and a near diffusion-dominated plasma seem to correlate well at wider spacings However, neither the existence of an optimum spacing nor the discrepancy between the measured collector work function and the apparent collector work function under power conditions is consistent with the present understanding These phenomena are important for converter optimization.

Extension of the present approaches to the theory requires a more careful look at the underlying assumptions In the plasma, both quasi-neutrality (deviations from neutrality are small compared to the charged particle density) and quasi-equilibrium (each group of particles is in local equilibrium) are assumed. The sheathes are assumed to be collisionless and a few Debye lengths in width, an assumption which has not been verified. Furthermore, the potential distribution in the sheaths can be monotonic or non-monotonic, with significantly different impacts on the plasma boundary conditions. There have not been any criteria for the formation of a monotonic or non-monotonic sheath. Since the plasma theories can be made to fit experimental data with either monotonic or non-monotonic sheath assumptions, it is not possible to determine which assumption is correct without a more fundamental approach to the sheath and plasma problems.

For the interelectrode spacings greater than optimum values, the computer methods have furnished reasonable descriptions of the particle densities and related quantities. However, when these methods are combined with reactor calculations, the costs in computer time and program complexity become too great for practical use. In addition, because of the numeric nature of the results, it is difficult to gain insight into the physical phenomena and their interrelations. Part I of this report presents a technique which, while providing relatively simple analytic forms for the solutions, preserves the features observed in the computer analyses. The results provide a reasonably simple method for calculating dependence of the converter J-V characteristics on various parameters and with further development could be used for design calculations.

In the plasma, as the pressure spacing product is reduced and the various particle mean-free paths approach the dimensions of the plasma width, the quasi-equilibrium condition may no longer be valid In additive converters, which characteristically operate at low cesium pressures, such conditions can occur at spacings of practical interest The analysis must then include the transition region between the sheath and the quasi-neutral plasma. At smaller spacings, there may be no quasi-neutral region at all Within the transition region, the collision processes must be added to the analysis and new boundary conditions determined from the behavior of the particles. These solutions may then be used to determine the extent of the validity of the quasi-equilibrium solutions. Part II of this report is devoted to the analysis of the sheath and transition regions of the converter. The simple collisionless sheath approximation is examined; it proved to be incapable of satisfying all the required boundary conditions With collisions occurring within the sheath, the actual shape of the particle and potential distributions must be known to define the plasma boundary conditions properly. This is particularly true in the case of non-monotonic potential distributions where the height of the barrier is determined by the sheath phenomena. By using an integral method to find solutions for the Boltzmann equation, it was possible to obtain rapid convergence without encountering severe instabilities The study, although only partially completed, was able to show particle and speed distributions through the sheath. The physical interpretation of the equations developed does give some insight into the sheath phenomena, but the actual solutions must be obtained from numerical integration.

The overall objective of the more complex plasma theories must be to give insight into converter behavior and to allow its performance to be extrapolated into the area for which there are no empirical data available This insight will permit the development of more efficient and useful diagnostic techniques and the evaluation of the influence of design changes on the overall converter performance. It is difficult to gain insight from many of the mathematical treatments of the converter, but any simplification necessarily requires neglecting at least one particular converter phenomenon An important application of the complete analysis will be the evaluation of the significance of particular phenomena in various portions of the J-V characteristic and under differing converter conditions.

I. THEORY OF THE IGNITED MODE IN THERMIONIC ENERGY CONVERTERS

A INTRODUCTION

An approximate analytic technique for solving the transport equations describing the diffusion region of a thermionic energy converter has been developed. The method involves assuming a parametric form for the electron production term. The transport equations are then integrated and the parameters adjusted to give the best fit to the equation. The method is considerably more accurate than previous analytic techniques and very much simpler and more flexible than numerical integration of the equations.

A preliminary description of the technique was reported in Reference 1, and is repeated in Section B. This analysis included a number of simplifying assumptions, the most important of which were: (1) The electron temperature gradient was constant across the converter, and (2) The electronic heat conduction to the collector was negligible. While these assumptions can be justified for converters operating near the maximum power point, subsequent analysis has shown that they are restricted to a very narrow range along the I-V characteristic and that a more careful treatment of the electron energy transport is required. We have therefore developed an improved treatment which includes integration of the electron energy equation. Although this complicates the analysis somewhat, it leads to a substantial improvement in the results and is still very much simpler than the currently available numerical methods of integrating the full set of transport equations. Unfortunately, there has been insufficient time to complete this work under the current contract; however, a brief description of the progress to date is included in Section C

B. AN APPROXIMATE ANALYTIC TECHNIQUE FOR DETERMINING THE OPERATING CHARACTERISTICS OF THERMIONIC CONVERTERS IN THE IGNITED MODE

1. Introduction

The problem of determining the arc drop in the plasma of a thermionic energy converter operating in the ignited mode has been treated by many authors.[2] The basic equations governing the transport phenomena in the diffusion region of the plasma have been derived by Wilkins and Gyftopoulos[3] and appropriate boundary conditions which apply across the sheaths have been set forth by Wilkins and McCandless.[4]

The solution of these equations has proved to be exceedingly difficult, however. The analytic techniques[5] which have been presented previously employ numerous simplifying approximations which in general limit them to pressure-spacing products pd considerably greater than those of practical interest for power converters. On the other hand, the numerical "shooting" techniques[6] which have been developed are subject to severe instabilities which make them exceedingly difficult and expensive to carry out. Moreover, numerical solutions give very little insight into the relative importance of the various physical phenomena and parameters which determine converter performance. Finally, none of the existing treatments, either analytic or numerical, has predicted the experimentally observed optimum value of the pd product at which the arc drop across the plasma for fixed current is a minimum.

In this section we present an approximate analytic method for solving the converter plasma equations which is very much simpler than the numerical "shooting" techniques and considerably more accurate than previous analytic treatments. It is based on assuming a parametric form for the net electron production in the converter. The transport equations may then be integrated to obtain the electron concentration, temperature, and potential energy distributions. These may in turn be used to calculate the corresponding net electron production from the ionization equation. Finally, the parameters in the assumed form are adjusted to make the assumed and calculated production agree as closely as possible. The success of the technique is determined by accuracy of the fit obtained. Systematic improvement of the results can be made by introducing progressively more complicated functional forms for the assumed production.

The basic equations and boundary conditions used in our analysis are presented in section 2. The method of solution and the mathematical results are given in section 3. The key element in the solution is a transcendental equation. A graphical method of solving this equation and some illustrative results are given in section 4. Finally section 5 briefly summarizes our conclusions.

2. Mathematical Model

a. Transport Equations

We shall consider a one dimensional three component plasma consisting of ion (i), electron (e), and neutrals (n). We assume low degrees of ionization so that

$$n_e = n_i << n_n , \tag{2.1}$$

where n_σ is the concentration of species σ, and equality of ion and neutral temperatures so that

$$\theta_i = \theta_n \tag{2.2}$$

where $\theta_\sigma = kT_\sigma$. For such a plasma, the equation of state is

$$p = n_e (\theta_e + \theta_n) + n_n \theta_n \approx n_n \theta_n \tag{2.3}$$

and the transport equations are[3]

$$\frac{d\Gamma_e}{dx} = \frac{d\Gamma_i}{dx} = S, \tag{2.4}$$

$$\frac{\Gamma_e}{\mu_e} = -\frac{dp_e}{dx} - n_e \frac{d\psi}{dx}, \tag{2.5}$$

$$\frac{\Gamma_i}{\mu_i} = -\frac{dp_i}{dx} + n_e \frac{d\psi}{dx} \tag{2.6}$$

$$Q_e = \Gamma_e \left(\frac{5}{2} \theta_e + \psi \right) - 2 n_e \mu_e \theta_e \frac{d\theta_e}{dx} \tag{2.7}$$

$$Q_n = - 2 n_n \mu_n \theta_n \frac{d\theta_e}{dx}, \tag{2.8}$$

where Γ_α, Q_α, p_α and μ_α are the particle flux, energy flux, pressure and mobility of species α, S is the net ionization rate, and ψ is the potential energy of an electron. The mobilities are related to the collision cross-sections $\sigma_{\alpha\beta}$ for species α and β by

$$\mu_{en}^{-1} = m_e \bar{c}_e (\sigma_{en} n_n + \sigma_{ei} n_e), \tag{2.9}$$

$$\mu_{in}^{-1} = \sqrt{2}\, m_n \bar{c}_n \sigma_{in} n_n, \tag{2.10}$$

$$\mu_{nn}^{-1} = \sqrt{2}\, m_n \bar{c}_n \sigma_{nn} n_n, \tag{2.11}$$

where m_α is the mass and

$$\bar{c}_\alpha = (8\,\theta_\alpha/\pi m_\alpha)^{1/2} \tag{2.12}$$

is the mean thermal speed of species α. Note that in the above equations we have omitted the thermal diffusion terms and the forces arising from the transfer of directed momentum from electrons to ions. We have also assumed that the energy flux carried by ions is negligible compared to that carried by neutrals.

If we further assume that radiation losses and energy transfer from electrons to heavy particles are small, then we have for neutrals

$$d\,Q_n/dx = 0 \tag{2.13}$$

and for electrons

$$d\,Q_e/dx = -\,V_i S, \tag{2.14}$$

where V_i is the ionization potential.

For collisional ionization and threebody recombination the net ionization rate is

$$S = \beta_r\, n_e\, (n_s^2 - n_e^2) \tag{2.15}$$

where

$$\beta_r\ (\mathrm{cm}^6/\mathrm{sec}) \approx 4 \times 10^{-27}\, [\theta_e\ (\mathrm{eV})]^{-9/2} \tag{2.16}$$

is the threebody recombination rate constant[7] and

$$n_s = n_n^{1/2} \left(\frac{m_e\,\theta_e}{2\pi\ \hbar^2}\right)^{3/4} e^{-V_i/2\theta_e} \tag{2.17}$$

is the Saha electron concentration. Over a reasonable range about a reference temperature θ^*, n_s can be well approximated by

$$n_s \approx n^* e^{-V^*/\theta_e}, \tag{2.18}$$

where

$$n^* = n_n^{1/2} \left(\frac{2.72\, m_e\, \theta^*}{2\pi\, \hbar^2} \right)^{3/4} \tag{2.19}$$

and

$$V^* = \frac{1}{2} V_i + \frac{3}{4} \theta^* \tag{2.20}$$

b. Boundary Conditions

We assume a motive diagram of the type shown in Figure I-1. Under these conditions the emitter boundary conditions are[4]

$$\Gamma_{eo} = \Gamma_E - \left(R_{eo} - \frac{1}{2} \Gamma_{eo} \right) e^{-V_E/\theta_{eo}}, \tag{2.21}$$

$$\Gamma_{io} = -2\, R_{io}, \tag{2.22}$$

$$Q_{eo} = \Gamma_E (2\theta_E + V_E) - (\Gamma_E - \Gamma_{eo})(2\theta_{eo} + V_E), \tag{2.23}$$

and the collector boundary conditions are

$$\Gamma_{ed} = (R_{ed} + \frac{1}{2} \Gamma_{ed})\, e^{-V_C/\theta_{ed}}, \tag{2.24}$$

$$\Gamma_{id} = 2\, R_{id}, \tag{2.25}$$

$$Q_{ed} = \Gamma_{ed} (2\theta_{ed} + V_C + \psi_d), \tag{2.26}$$

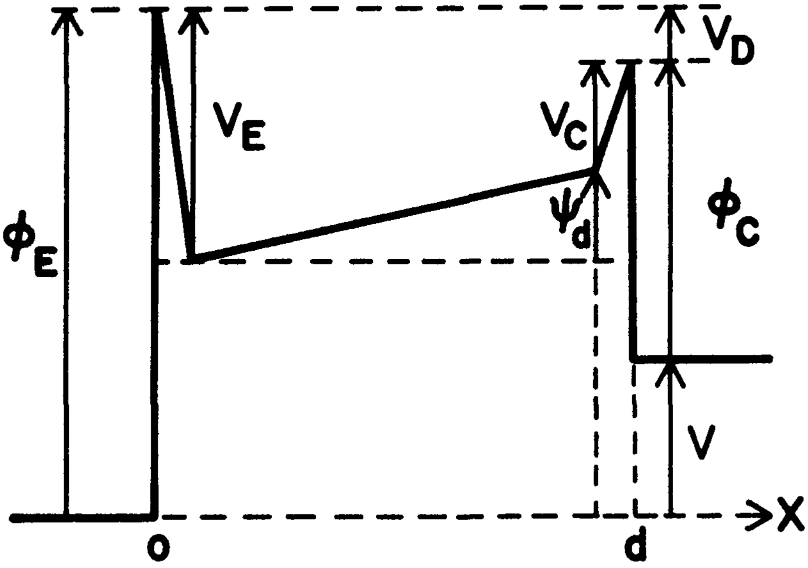


Figure I-1. Schematic Illustration of Motive Diagram Assumed in the Analysis.

where Γ_E is the emitter saturation current and

$$R_\alpha = n_\alpha \bar{c}_\alpha /4 \qquad (2.27)$$

is the random current for species α. Note that we have assumed back emission from the collector is negligible

The arc drop obtained from inspection of Figure I-1 is

$$V_D = V_o - V = V_E - V_C - \psi_d \qquad (2.28)$$

where

$$V_o = \phi_E - \phi_C \qquad (2.29)$$

is the contact potential.

3. Method of Solution

a Temperature Distribution for Neutrals

We shall begin by considering the temperatures of the neutrals since this determines both the ion temperature and the neutral particle density which will be needed later. Substituting (2.3), (2.11), and (2.12) into (2.8) and integrating we find for constant σ_{nn}

$$\theta_n = \theta_E [1 - \eta(1 - \epsilon_{CE}^{3/2})]^{2/3} , \qquad (3.1)$$

where

$$\eta = x/d \qquad (3.2)$$

is a dimensionless distance and

$$\epsilon_{CE} = \theta_C/\theta_E \qquad (3.3)$$

is the ratio of collector and emitter temperatures.

The corresponding heat flux carried by the neutrals is

$$Q_n = \frac{\pi}{6\sqrt{2}} \left(\frac{\theta_E}{\sigma_{nn} d} \right) \left(\frac{8\,\theta_E}{\pi m_n} \right)^{1/2} \left(1 - \epsilon_{CE}^{\;3/2}\right) . \tag{3.4}$$

b. Electron Density Distribution

To obtain an approximate analytic solution for the electron concentration, we assume that the net electron production S given by (2.15) can be approximated by a function of the form

$$S^* = A \tanh \left(\frac{\eta + a}{b} \right) \operatorname{sech}^2 \left(\frac{\eta + a}{b} \right) \tag{3.5}$$

where A, a, and b are parameters which will be adjusted later to give the best fit of S and S*. Obviously, this choice of S* is by no means unique and more complicated functional forms could be used which might give better results. The reasons for choosing this particular form for our initial investigation are 1) it has a shape which is physically reasonable, 2) it approximates quite well the forms obtained in previous numerical investigations, and 3) it is relatively simple and convenient to integrate. It should be emphasized, however, that the success of this or any other form for S* can only be determined a posterior by assessing the accuracy of the fit to S.

Substituting S* for S in (2.4) and integrating we obtain

$$\Gamma_i = \Gamma_e - \Gamma$$

$$= \Gamma_{id} + \frac{1}{2} Abd \left[\tanh^2 \left(\frac{\eta + a}{b} \right) - \tanh^2 \left(\frac{1 + a}{b} \right) \right] \tag{3.6}$$

where $\Gamma = J/e$ is the converter current divided by the electronic charge. Adding (2.5) and (2.6) and using (2.9), (2.10), (2.12), (2.25), (2.27) and (3.2) gives

$$\frac{d\overline{P}}{d\eta} + d_{ei}\,\overline{P} = -d_{in}(\overline{\Gamma}_i + \epsilon_{ei}), \tag{3.7}$$

where

$$\overline{P} = n_e(\theta_e + \theta_i)/n_{ed}\,(\theta_{ed} + \theta_C), \tag{3.8}$$

$$\overline{\Gamma}_i = \Gamma_i/\Gamma_{id}\,, \tag{3.9}$$

$$d_{ei} = \frac{8\Gamma_{ed}\,\sigma_{ei}\,d\theta_e}{\pi\bar{c}_e\,(\theta_e + \theta_i)}\,, \tag{3.10}$$

$$d_{in} = \frac{4\,\sigma_{in}\,pd}{\pi(\theta_{ed} + \theta_C)}\left(\frac{2\,\theta_C}{\theta_i}\right)^{1/2}, \tag{3.11}$$

$$\epsilon_{ei} = \frac{\Gamma_{ed}\,\sigma_{en}}{R_{ed}\,\sigma_{in}}\left(\frac{\theta_{ed}\,\theta_e}{8\theta_C\,\theta_i}\right)^{1/2}, \tag{3.12}$$

and we used the approximation $\Gamma_e \approx \Gamma_{ed}$. Note d_{ei} and d_{in} are essentially the converter spacing divided by the electron-ion and ion-neutral mean free paths respectively while ϵ_{ei} is the ratio of the ion-neutral to electron-neutral mean free paths.

Before attempting to integrate (3.7) it is useful to estimate the magnitude of the coefficients d_{ei}, d_{in} and ϵ_{ei}. Using the cross-sections[8] summarized in Table I-1 and the reference conditions $T_{eo} \sim T_{ed} \sim 1.5\,T_E \sim 4.0\,T_C \sim 2800\,°K$ and $\Gamma \sim R_{ed}$ we find

TABLE I-1

SUMMARY OF CROSS SECTIONS[8]

$$\sigma_{in} \approx 1200\ \text{A}^2$$

$$\sigma_{en} \approx 400\ \text{A}^2$$

$$\sigma_{nn} \approx 100\ \text{A}^2$$

$$\sigma_{ei} = \left(\frac{\pi^2}{16}\right)\left(\frac{e^2}{kT_e}\right)^2 \ln \Lambda_e \sim 10^4\ \text{A}^2$$

$$d_{ei} \approx Jd\ (\text{mil a/cm}^2)/700, \qquad (3.13)$$

$$d_{in} \approx 1.1\ pd\ (\text{mil torr}), \qquad (3.14)$$

and

$$\epsilon_{ei} \approx 1/3\ , \qquad (3.15)$$

where we have assumed $\theta_i \approx \sqrt{\theta_E\ \theta_C}$.

It can be seen from (3.13) that for Jd << 700 mil a/cm^2, which is the range of interest for most practical converters, the term proportional to d_{ei} in (3.7) will be small. It can also be seen from (3.15) that the dependence on ϵ_{ei} is relatively weak. Thus, since the temperature dependence of σ_{in} is also relatively weak, it is a good first approximation to drop the term proportional to d_{ei} and assume d_{in} and ϵ_{ei} are constant. (3.7) can then easily be integrated to give

$$\overline{P} = 1 + \overline{d}\left\{\left[1 + B\,\mathrm{sech}^2\left(\frac{1+a}{b}\right)\right]\left(\frac{1-\eta}{1+a}\right) - B\left(\frac{b}{1+a}\right)\left[\tanh\left(\frac{1+a}{b}\right) - \tan h\left(\frac{\eta+a}{b}\right)\right]\right\}, \qquad (3.16)$$

where

$$\overline{d} = (1 + a)\ (1 + \epsilon_{ei})\ d_{in} \qquad (3.17)$$

and

$$B = A\,b\,d/2\ \Gamma_{id}\ (1 + \epsilon_{ei}). \qquad (3.18)$$

We can now obtain an expression for the electron production in terms of $\overline{P}$ by substituting (3.8) into (2.15). This gives

$$S = (2\Gamma_{id}/d)\, d_r\, \overline{P}(\overline{P}_S^{\,2} - \overline{P}^{\,2}) \tag{3.19}$$

where

$$\overline{P}_S = n_s\,(\theta_e + \theta_i)/n_{ed}\,(\theta_{ed} + \theta_C) \tag{3.20}$$

and

$$d_r = \frac{\beta_r\, n_{ed}^2\, d}{\overline{c}_{id}} \left(\frac{\theta_{ed} + \theta_C}{\theta_e + \theta_i} \right)^3 . \tag{3.21}$$

Note d_r is essentially the converter spacing divided by the mean free path for ion recombination at the collector.

To determine the parameters B, a, and b we require that S given by (3.19) fit S* given by (3.5) as closely as possible. A simple (but not necessarily the best) method of doing this is to match S and S* at the extrapolated end point η = -a and at the point of maximum electron production $\eta = \eta_1$. Matching at the extrapolated end point requires S(-a) = S* (-a) = 0 which gives

$$1 + \overline{d}\ [1 + B\,\mathrm{sech}^2\left(\frac{1+a}{b}\right) - B\left(\frac{b}{1+a}\right)\tanh\left(\frac{1+a}{b}\right) = 0\ . \tag{3.22}$$

Matching the positions of the maximum electron production requires $(dS/d\eta)_1 = (dS^*/d\eta)_1 = 0$ which gives

$$\left[(\overline{P}_S^{\,2} - 3\,\overline{P}^{\,2})\,\frac{d\overline{P}}{d\eta} + 2\,\overline{P}\,\overline{P}_S\,\frac{d\overline{P}_S}{d\eta}\right]_1 = 0 \tag{3.23}$$

and

$$(\eta_1 + a)/b = \delta_1 = \coth^{-1}\sqrt{3} \tag{3.24}$$

where the subscript 1 denotes quantities evaluated at $\eta = \eta_1$. Note that in differentiating (3.19) we have neglected the temperature dependence of d_r in comparison with that of $\overline{P}_S$. Finally, matching the values of S and S* at the $\eta = \eta_1$ gives

$$2\,B\,(1 + \epsilon_{ei})/b\,3\sqrt{3} = d_{r1}\,\overline{P}_1\,(\overline{P}_{S1}^{\,2} - \overline{P}_1^{\,2}) \qquad (3.25)$$

where we have used (3.18) and (3.24).

The three equations (3.22), (3.23), and (3.25) are sufficient to determine the unknown parameters B, a, and b. An additional equation which can be used to determine $\overline{P}_{S1}$ can be obtained by substituting the boundary conditions (2.22) and (2.25) into (3.6) and using (2.12), (2.27), (3.8), (3.9), and (3.18). This gives

$$\begin{aligned}\overline{\Gamma}_{io} &= -\,\overline{P}_o\,(\theta_{ed} + \theta_C)/(\theta_{eo} + \theta_E)\,\sqrt{\epsilon_{CE}} \\ &= 1 + B\,(1 + \epsilon_{ei})\left[\tanh^2\left(\frac{a}{b}\right) - \tanh^2\left|\frac{1+a}{b}\right|\right].\end{aligned} \qquad (3.26)$$

To solve this set of equations, it is convenient to introduce the variable

$$(\eta + a)/b = \delta\,. \qquad (3.27)$$

We then obtain from (3.16) and (3.22)

$$B = (\overline{d} + 1)\,\delta_d\,\coth\delta_d/\overline{d}\,(1 - C) \qquad (3.28)$$

and

$$\overline{P} = (\overline{d}/\delta_d)\,(B\tanh\delta - D\delta), \qquad (3.29)$$

where

$$\delta_d = (1 + a)/b, \qquad (3.30)$$

$$C = 2\,\delta_d/\sinh 2\,\delta_d \qquad (3.31)$$

and

$$\begin{aligned} D &= 1 + B \operatorname{sech}^2 \delta_d \\ &= (\bar{d} + C)/\bar{d}(1 - C) \ . \end{aligned} \tag{3.32}$$

Combining (3.29) with (3.17) and (3.25) and using (3.28) and (3.30) - (3.32) we obtain

$$\left(\frac{\bar{P}_S}{\bar{P}}\right)_1^2 = 1 + \frac{2 E^2}{\epsilon_r \bar{d}^2 (\bar{d} + 1)^2} \tag{3.33}$$

where

$$E = \frac{(1 - C)\delta_d}{\coth \delta_d} \left[1 - 1.14 \frac{D}{B}\right]^{-3/2} \tag{3.34}$$

and

$$\begin{aligned} \epsilon_r &= d_{rl}/d_{in} (1 + \epsilon_{ei})^2 \\ &= \frac{\pi \beta_{rl} n_{ed}^2 (\theta_{ed} + \theta_C)(\theta_{ed} \theta_i)^{1/2}}{4\sqrt{2}\, \sigma_{in} \bar{c}_{ed}\, p\, \theta_C (1 + \epsilon_{ei})^2} \left(\frac{m_n}{m_e}\right)^{1/2} \left(\frac{\theta_{ed} + \theta_C}{\theta_{el} + \theta_{il}}\right)^3 . \end{aligned} \tag{3.35}$$

Note ϵ_r is essentially the ratio of the ion neutral mean free path to the ion recombination length at the collector. For the reference conditions $T_{eo} \sim T_{ed} \sim 1.5\ T_E \sim 4.0\ T_C \sim 2800\,^\circ\mathrm{K}$ and $\Gamma \sim (n_e \bar{c}_e/4)_d$

$$\epsilon_r \approx 3 \times 10^{-7}\ J^2\ (a^2/cm^4)/p\ (torr) \tag{3.36}$$

so that for typical operating conditions ϵ_r is very small. Substituting (3.33) into (3..23) gives

$$\Delta\chi = -(d \ln \overline{P}_S/d\eta)_1$$

$$= \left(\frac{E^2 - \epsilon_r \, \overline{d}^2 \, (\overline{d} + 1)^2}{E^2 + \frac{1}{2} \, \epsilon_r \, \overline{d}^2 \, (\overline{d} + 1)^2} \right) F \tag{3.37}$$

where

$$F = \frac{1}{2} \, (d \ln \overline{P}/d\eta)_1$$

$$= \frac{\delta_d - 3 \, (\overline{d} + C)/2 \, (\overline{d} + 1) \coth \delta_d}{\sqrt{3} \, (1 + a) \, (1 - 1.14 \, D/B)} \; . \tag{3.38}$$

To obtain the extrapolated end point a, we first observe that for $\eta = 0$, (3.28) gives

$$\overline{P}_o = (\overline{d}/\delta_d) \, (B \tanh \delta_o - D \, \delta_o) \tag{3.39}$$

where from (3.27)

$$a = b\delta_o = \delta_o/(\delta_d - \delta_o). \tag{3.40}$$

We next anticipate that for most conditions of interest δ_o coth δ - 1 << δ_d coth δ_d - 1 so that

$$\overline{P}_o \approx (\overline{d}/\delta_d) \, (B - D) \tanh \delta_o \; . \tag{3.41}$$

Substituting (3.41) into (3.26) and using (3.30) and (3.40) we obtain

$$B(1 + \epsilon_{ei}) \tanh^2 \delta_o + G \tanh \delta_o - H = 0 \tag{3.42}$$

which may be solved to give

$$\tanh \delta_o = \frac{G}{2B \, (1 + \epsilon_{ei})} \left[\left(1 + \frac{4B \, (1 + \epsilon_{ei}) \, H}{G^2} \right)^{1/2} - 1 \right] \tag{3.43}$$

where

$$G = \left(\frac{\theta_{ed} + \theta_C}{\theta_{eo} + \theta_E}\right)\frac{\bar{d}\,(B - D)}{\sqrt{\epsilon}_{CE}\,\delta_d} \tag{3.44}$$

and

$$H = B\,(1 + \epsilon_{ei})\,\tanh^2 \delta_d - 1 \,. \tag{3.45}$$

For $G^2 >> 4B\,(1 + \epsilon_{ei})\,H$, which corresponds to $\delta_d << (\bar{d} + 1)/2\, \sqrt{\epsilon}_{CE}\,(1 + \epsilon_{ei})$,

$$\delta_o \approx H/G \tag{3.46}$$

and

$$\bar{P}_o \approx \sqrt{\epsilon}_{CE}\,(\theta_{eo} + \theta_E/\theta_{ed} + \theta_C)\,H, \tag{3.47}$$

while for $G^2 << 4B\,(1 + \epsilon_{ei})H$, corresponding to $\delta_d >> (\bar{d} + 1)/2\sqrt{\epsilon}_{CE}\,(1 + \epsilon_{ei})$,

$$\delta_o \approx \frac{1}{2}\ln\,(4H/G) \tag{3.48}$$

and

$$\bar{P}_o \approx \bar{d} + 1 \,. \tag{3.49}$$

Using (3.28), (3.31) and (3.32) it can be seen from (3.46) and (3.48) that for $d > 1$ the approximation $\delta_o \coth \delta_o - 1 << \delta_d \coth \delta_d - 1$ used to obtain (3.42) is valid for all δ_d.

This completes the determination of the parameters necessary to specify the electron concentration and we may now use our results to calculate the electron potential energy and electron temperature distributions.

c. Electron Potential Energy

To obtain an equation for the electron potential energy we use (2.5) and the equation $p_i = p_e \theta_i/\theta_e$ to eliminate dp_i/dx from (2.6). Then using (2.9), (2.10), (2.12), (2.25), (2.27), (3.2), (3.8), (3.9), (3.11), and (3.12) and the approximation $\mu_i \ll \mu_e$ we find

$$\frac{d\psi}{d\eta} = \frac{d_{in}}{\overline{P}} \left[\overline{\Gamma}_i \theta_e - \epsilon_{ei} \theta_i \right] + \theta_e \frac{d}{d\eta} \ln \left[1 + \frac{\theta_i}{\theta_e} \right]. \qquad (3.50)$$

We then substitute (3.27), (3.30) and (3.45) into (3.6) to obtain

$$\overline{\Gamma}_i = -H + B(1 + \epsilon_{ei}) \tanh^2 \delta . \qquad (3.51)$$

Using (3.51) and (3.29), (3.50) may now be formally integrated to give

$$\psi_d = \psi_1 + \psi_2 + \psi_3 \qquad (3.52)$$

$$\psi_1 = \int_0^1 \theta_e \left[\frac{d}{d\eta} \ln \left(1 + \frac{\theta_i}{\theta_e} \right) \right] d\eta \approx \theta_C - \theta_E \qquad (3.53)$$

$$\psi_2 = \int_{\delta_o}^{\delta_d} \frac{(\theta_e I - \epsilon_{ei} \theta_i) \tanh^2 \delta \, d\delta}{(1 + \epsilon_{ei}) (B \tanh \delta - D\delta)} \qquad (3.54)$$

and

$$\psi_3 = - \int_{\delta_o}^{\delta_d} \frac{(\theta_e H + \epsilon_{ei} \theta_i) \operatorname{sech}^2 \delta \, d\delta}{(1 + \epsilon_{ei})(B \tanh \delta - D\delta)}, \qquad (3.55)$$

where

$$I = B (1 + \epsilon_{ei}) \operatorname{sech}^2 \delta_d + 1. \qquad (3.56)$$

To evaluate ψ_2 we observe that the integrand is a rapidly increasing function of δ so that the major contribution to the integral comes from the vicinity of the end point δ_d. Thus, it is a good approximation to set $\tanh \delta \approx \tanh \delta_d$ and $\theta_e I - \epsilon_{ei}\,\theta_i \approx \theta_{ed} I - \epsilon_{ei}\,\theta_C$ and using (3.28) we obtain

$$\psi_2 \approx \left(\frac{\theta_{ed} I - \epsilon_{ei}\,\theta_C}{(1 + \epsilon_{ei})D}\right)(\tanh^2 \delta_d) \ln\left(\frac{\bar{d} + 1}{1 - C}\right) \tag{3.57}$$

where we have assumed $\delta_o << \delta_d$.

To evaluate ψ_3 we proceed in a similar manner and observe first the important contribution to the integral in this case comes from the vicinity of the end point δ_o where it is a good approximation to set $\tanh \delta = \delta$ and $\theta_e H + \epsilon_{ei}\,\theta_i \approx \theta_{eo} H + \epsilon_{ei}\,\theta_E$. We thus obtain

$$\psi_3 \approx -\left(\frac{\theta_{eo} H + \epsilon_{ei}\,\theta_E}{(1 + \epsilon_{ei})\,(B - D)}\right) \ln\left(\frac{\tanh \delta_d}{\tanh \delta_o}\right). \tag{3.58}$$

d. Electron Temperature

The electron temperature may now be determined from (2.7) which using (2.9), (2.10), (2.12), (2.25), (2.27), (3.2), (3.8), (3.10), (3.11), and (3.12) can be written

$$\frac{d\theta_e}{d\eta} = \frac{1}{2}\left(1 + \frac{\theta_i}{\theta_e}\right)\left(\frac{\epsilon_{ei}\, d_{in}}{\bar{P}} + d_{ei}\right)\left(\frac{5}{2}\,\theta_e + \psi - \frac{Q_e}{\Gamma_e}\right). \tag{3.59}$$

In principle this equation can be integrated using the same techniques employed in the preceding section. Since this is somewhat complicated, however, we shall not attempt it in the present analysis and instead we shall assume that to a first approximation:

$$d\,\theta_e/d\eta = -\,\Delta\,\theta_e \tag{3.60}$$

where $\Delta\theta_e \approx \theta_{eo} - \theta_{ed}$ is a constant. Then using (3.59), (3.60) and the boundary condition (2.26) we find

$$\ln\left(\frac{R_{ed}}{\Gamma_{ed}}+\frac{1}{2}\right)=\frac{1}{2}+\frac{2\,\Delta\,\theta_e}{(\theta_{ed}+\theta_C)(\epsilon_{ei}\,d_{in}+d_{ei})}\ . \tag{3.61}$$

From (3.12) we see that ϵ_{ei} contains the factor Γ_{ed}/R_{ed} so that (3.61) is an implicit rather than explicit equation for R_{ed}/Γ_{ed}. However, for $2\,\Delta\theta \ll (\theta_{ed}+\theta_C)(\epsilon_{ei}\,d_{in}+d_{ei})$, it is an excellent approximation to evaluate $\epsilon_{ei}\,d_{in}+d_{ei})$, it is an excellent approximation to evaluate ϵ_{ei} at $R_{ed}/\Gamma_{ed} = \exp\left(\frac{1}{2}\right) - \frac{1}{2} = 1.15$.

At this point we note that since $\overline{P}_S$ is a function of θ_e we have in effect three unknowns: θ_{eo}, $\Delta\theta_e$, and δ_d and two equations (3.33) and (3.37) which relate to them. To obtain a third equation which will permit us to solve the set we subtract (2.26) from (2.23) which gives

$$Q_{eo} - Q_{ed} = 2\Gamma_E\,(\theta_E - \theta_{eo}) + (\Gamma_{eo} - \Gamma_{ed})\,(2\theta_{eo} + V_E)$$

$$+\,\Gamma_{ed}\,(2\,\Delta\theta_e + V_E - V_C - \psi_d). \tag{3.62}$$

Integrating (2.4) and (2.14) we find

$$\Gamma_{ed} - \Gamma_{eo} = \Gamma_{id} - \Gamma_{io} \tag{3.63}$$

and

$$Q_{eo} - Q_{ed} = V_i\,(\Gamma_{id} - \Gamma_{io}). \tag{3.64}$$

Substituting (3.63) and (3.64) into (3.62) and using (2.28), (3.6), and (3.9), then gives

$$(V_i + 2\theta_{eo} + V_E)\,\epsilon_m\,(1 - \bar{\Gamma}_{io}) = 2(\Gamma_E/\Gamma_{ed})(\theta_E - \theta_{eo})$$

$$+ 2\,\Delta\theta_e + V_E - V_C - \psi_d\,, \tag{3.65}$$

where from (2.25), (2.27), and (2.12)

$$\epsilon_m = \frac{\Gamma_{id}}{\Gamma_{ed}} = 2\left(\frac{R_{ed}}{\Gamma_{ed}}\right)\left(\frac{m_e\,\theta_C}{m_n\,\theta_{ed}}\right)^{1/2} \approx \frac{1}{500}\,. \tag{3.66}$$

From (2.21) and (2.24) we find

$$V_C = \theta_{ed}\,\ln\left(\frac{R_{ed}}{\Gamma_{ed}} + \frac{1}{2}\right) \tag{3.67}$$

and

$$V_E = \theta_{eo}\,\ln\left(\frac{R_{eo}}{\Gamma_{eo}} - \frac{1}{2}\right)\left(\frac{\Gamma_E}{\Gamma_{eo}} - 1\right)^{-1}\,, \tag{3.68}$$

where from (2.12), (2.25), (2.27), (3.6), (3.9), (3.63) and (3.66) we we have

$$\frac{R_{eo}}{\Gamma_{eo}} = -\,\bar{\Gamma}_{io}\,\sqrt{\epsilon}_{CE}\left(\frac{\theta_{eo}}{\theta_{ed}}\right)^{1/2}\left(\frac{R_{ed}}{\Gamma_{ed}}\right)\left(\frac{\Gamma_{ed}}{\Gamma_{eo}}\right) \tag{3.69}$$

and

$$\frac{\Gamma_{eo}}{\Gamma_{ed}} = 1 - \epsilon_m\,(1 - \bar{\Gamma}_{io}). \tag{3.70}$$

Finally, from (2.18), (2.19), (3.24), (3.28), (3.29), (3.33), (3.24), (3.37) and (3.60) we find

$$\theta_{eo} = \theta_{ed} + \Delta\theta_e = \theta_{el} + \eta_1 \Delta\theta_e \tag{3.71}$$

$$\Delta\theta_e = \theta_{el} \Delta\chi/\chi_1 \tag{3.72}$$

$$\theta_{el} = V^*/\chi_1 \tag{3.73}$$

where

$$\chi_1 = N + \ln\left[\frac{\bar{d}}{\delta_d}\left(1 - 1.14\,\frac{D}{B}\right)^{1/2}\left(1 + \frac{\epsilon_r \bar{d}^2 (\bar{d}+1)^2}{2\,E^2}\right)^{-1}\right] \tag{3.74}$$

and

$$N = \ln\left(\frac{3\,\epsilon_r}{2}\right)^{1/2} \frac{n^* (\theta_{el} + \theta_{il})}{n_{ed}(\theta_{ed} + \theta_C)}$$

$$= \frac{1}{2}\ln\left(\frac{2.72\, m_e \theta^*}{\pi \hbar^2}\right)^{3/2} \left(\frac{m_n \theta_{ed}}{m_e \theta_i}\right)^{1/2} \times$$

$$\frac{3\pi \beta_{r1} (\theta_{ed} + \theta_C)^2}{32\, \sigma_{in} \bar{c}_{ed} (1 + \epsilon_{ei})\, \theta_C (\theta_{el} + \theta_{il})} \tag{3.75}$$

For our reference conditions, $\theta^* \sim \theta_{el} \sim \theta_{ed} \sim 1.5\,\theta_E \sim 4\,\theta_C \sim 2800\,°K$.

$$N \approx 7.8\,. \tag{3.76}$$

We now observe that by means of the equations developed in this section all quantities in (3.65) can be found as functions of Γ_E/Γ_{eo} and δ_d. Thus given Γ_E/Γ_{eo} we can solve (3.65) either graphically or numerically to obtain δ_d which in turn determines all other variables

e. Current-Voltage Characteristics

Using (3.6), (3.66) and (3.70), the ratio of the total current to the emitter electron current is found to be

$$\Gamma/\Gamma_{eo} = (1 - \epsilon_m)/[1 - \epsilon_m (1 - \Gamma_{io})] \qquad (3.77)$$

The arc drop may be determined from (2.28) and (3.65) and is given by

$$\begin{aligned} V_D &= V_E - V_C - \psi_d \\ &= 2\,(\Gamma_E/\Gamma_{eo})(\theta_{eo} - \theta_E) - 2\,\Delta\theta_e \qquad (3.78) \\ &\quad + (V_i + 2\,\theta_{eo} + V_E)\,\epsilon_m\,(1 - \bar{\Gamma}_{io}). \end{aligned}$$

4. Graphical Solution and Illustration Results

To obtain a graphical solution for the equations of the previous section, we substitute (3.67) - (3.73) into (3.65) and solve for $\Delta\chi$. This gives

$$\Delta\chi = \chi_1\,[Q - (\chi_1/\chi_E)P]/(1 + R - \eta_1\,Q) \qquad (3.79)$$

where

$$\begin{aligned} Q = {} & \frac{\Gamma_E}{\Gamma_{eo}} + \frac{1}{2}\ln\left[\left(\frac{\Gamma_E}{\Gamma_{eo}} - 1\right)\left(1 + \frac{\Gamma_{ed}}{2R_{ed}}\right)\left(1 - \frac{\Gamma_{eo}}{2\,R_{eo}}\right)^{-1}\left(1 - \frac{D}{B}\right)^{-1}\right] \\ & - \frac{1}{2}\left(\frac{\epsilon_{ei} - I\,\mathrm{sech}^2\,\delta_d}{D\,(1 + \epsilon_{ei})}\right)\ln\left(\frac{\bar{d} + 1}{1 - C}\right) \qquad (3.80) \\ & - \frac{1}{2}\,\frac{\epsilon_{ei}}{(B - D)\,(1 + \epsilon_{ei})}\ln\left(\frac{\coth\,\delta_o}{\coth\,\delta_d}\right), \end{aligned}$$

$$P = (\Gamma_E/\Gamma_{eo}) - \chi_E \epsilon_m (1 - \bar{\Gamma}_{io}) - \epsilon_{CE} \left(\frac{\epsilon_{ei} \tanh^2 \delta_d}{D (1 + \epsilon_{ei})} \right) \ln \left(\frac{\bar{d} + 1}{1 - C} \right)$$

$$- \frac{\epsilon_{ei}}{(B - D)(1 + \epsilon_{ei})} \ln \left(\frac{\coth \delta_o}{\coth \delta_d} \right), \qquad (3.81)$$

$$R = \frac{1}{2} \left(\frac{1}{1 + \epsilon_{ei}} \right) \ln \left(\frac{\bar{d} + 1}{1 - C} \right), \qquad (3.82)$$

and

$$\chi_E = V^*/\theta_E . \qquad (3.83)$$

In deriving (3.79) - (3.82) we have used (3.26), (3.28) and (3.41) to eliminate Γ_{io} in certain terms. We have also assumed $\Delta\theta_e \ll \theta_{eo} \ll V_i$ and dropped several terms which are small as a consequence.

Equation (3.79) may now be solved simultaneous with (3.37) by plotting them both as a function of δ_d. This is illustrated in Figure I-2 for the case $J_E/J = 2$. The curves identified by the parameters $\sqrt{\epsilon_r}\, \bar{d}$ $(\bar{d} + 1)$ were obtained from (3.37) while those identified by $(\bar{d} + 1)$ were obtained from (3.79). For given ϵ_r and d, the value of δ_d is determined by the intersection of the corresponding pair of curves. The root of interest is the largest one. The other roots correspond to a possible relative minimum in the electron production in the center of the converter and a second maximum in the production near the collector. Due to the form of the production term assumed, the present analysis is limited to cases where the subsidiary maximum and minimum are unimportant. This is the case for a wide range of conditions. Once δ_d is determined, all other variables may be obtained from the equations of the preceding section.

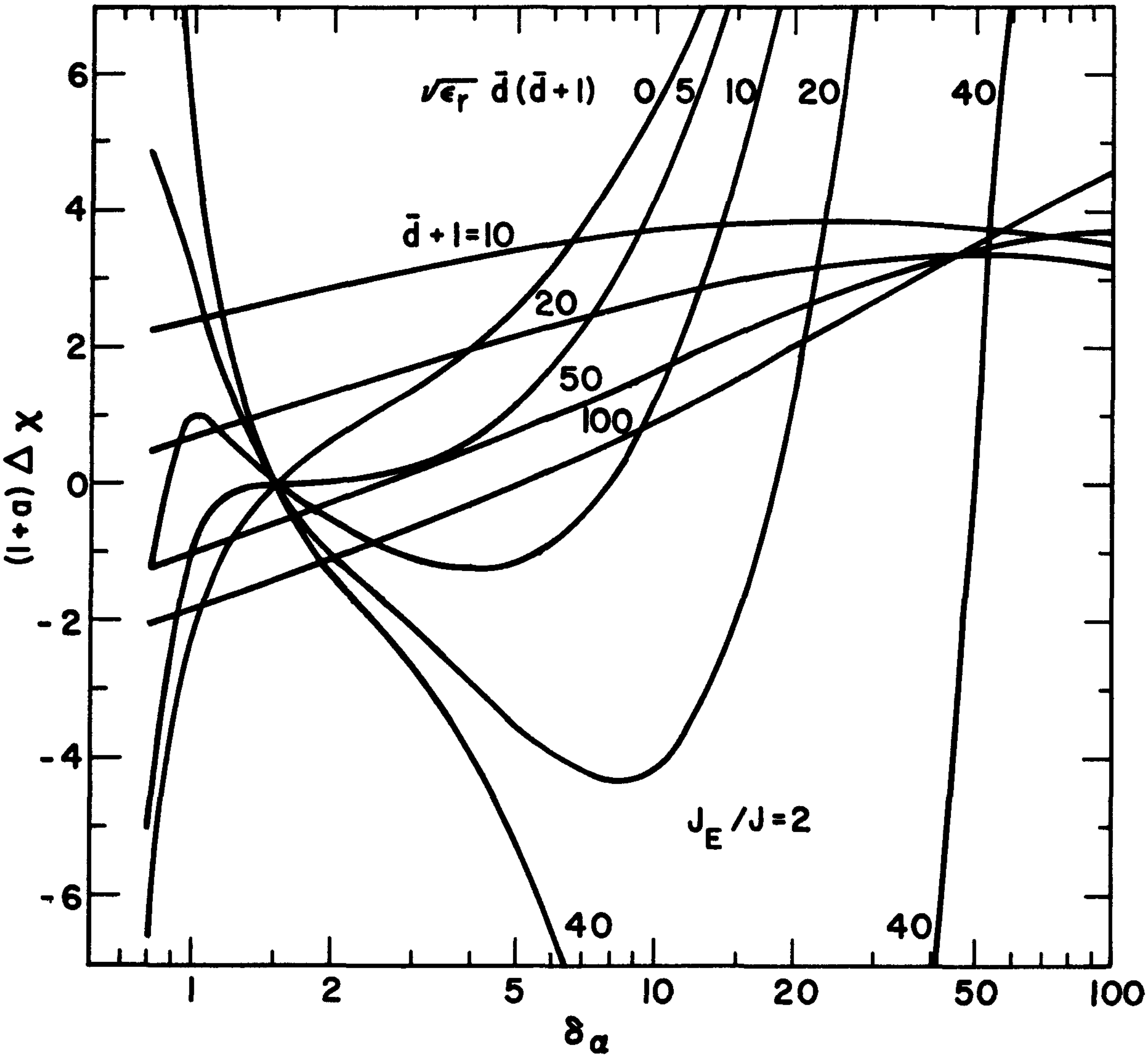
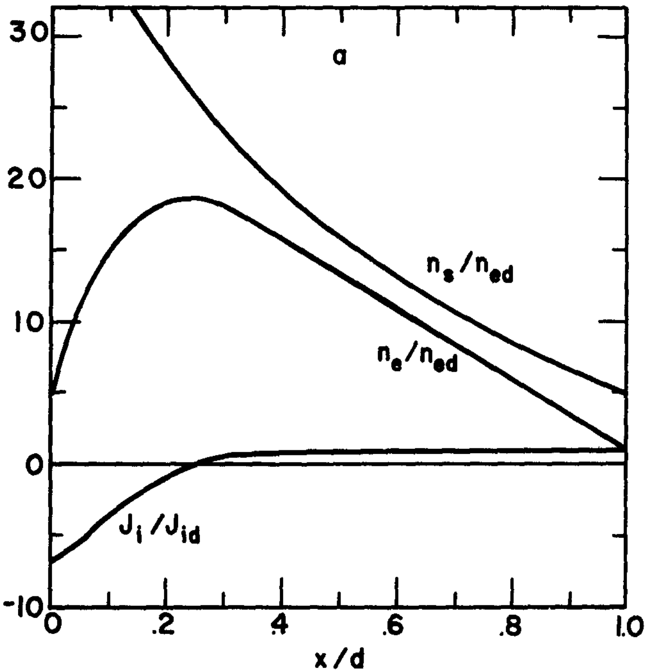


Figure I-2. Illustration of Graphical Solution of Equations (3.37) and (3.79) for $J_E/J = 2$. See text for discussion.

Figure I-3a shows curves for the Saha electron concentration n_S, the actual electron concentration n_e, the ion current J_i as a function of position in the converter for typical operating conditions. All these quantities exhibit the characteristic shapes found in previous numerical solutions[6] of the problem. The two expressions S and S* for the net electron production are compared in Figure I-3b and it can be seen that the fit is very satisfactory.

Figure I-4 shows the electron and ion temperatures as a function of position in the converter for the same conditions as Figure I-3. Note that the electron temperature is a linear function of x/d because the gradient was assumed constant in the analysis. The ion temperature, however, was obtained by integration of the neutral heat flux equation and is not linear due to variations in the thermal conductivity and temperature. The electric field is essentially the product of the ion current density and the electrical resistivity. It rises rapidly in the vicinity of the collector because the low electron density in this region results in a high effective resistivity. A similar effect of opposite sign occurs at the emitter.

The emitter and collector electron temperatures are shown in Figure I-5a as a function of the pd product for $J_E/J = 2$. It can be seen that the emitter electron temperature has a minimum in the neighborhood of pd = 20 and rises for both smaller and larger pd. The physical reason for this is that for small pd electron loss by ambipolar diffusion to the walls is large and consequently the temperature must rise to maintain the ionization required to carry the prescribed current. On the other hand, for large pd a higher electron temperature is required at the emitter to provide the electron concentration gradient necessary



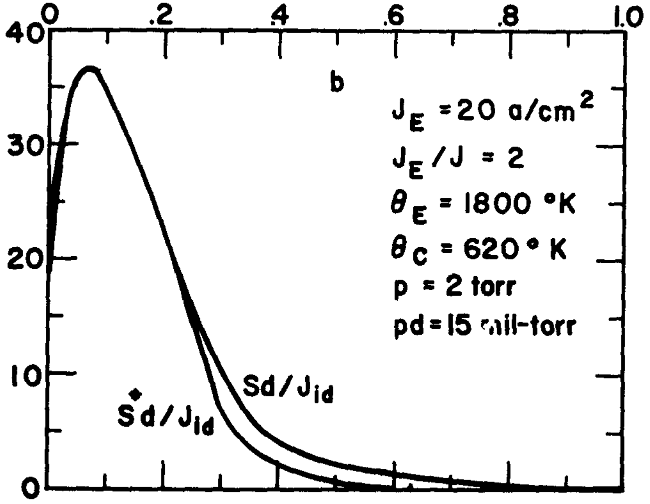


Figure I-3a. Calculated Distributions for Saha Electron Concentration n_s, Electron Concentration n_e, and ion current J_i.

Figure I-3b. Comparison of Assumed and Calculated Expressions for the Net Electron Production. The conditions for (a) and (b) are the same.

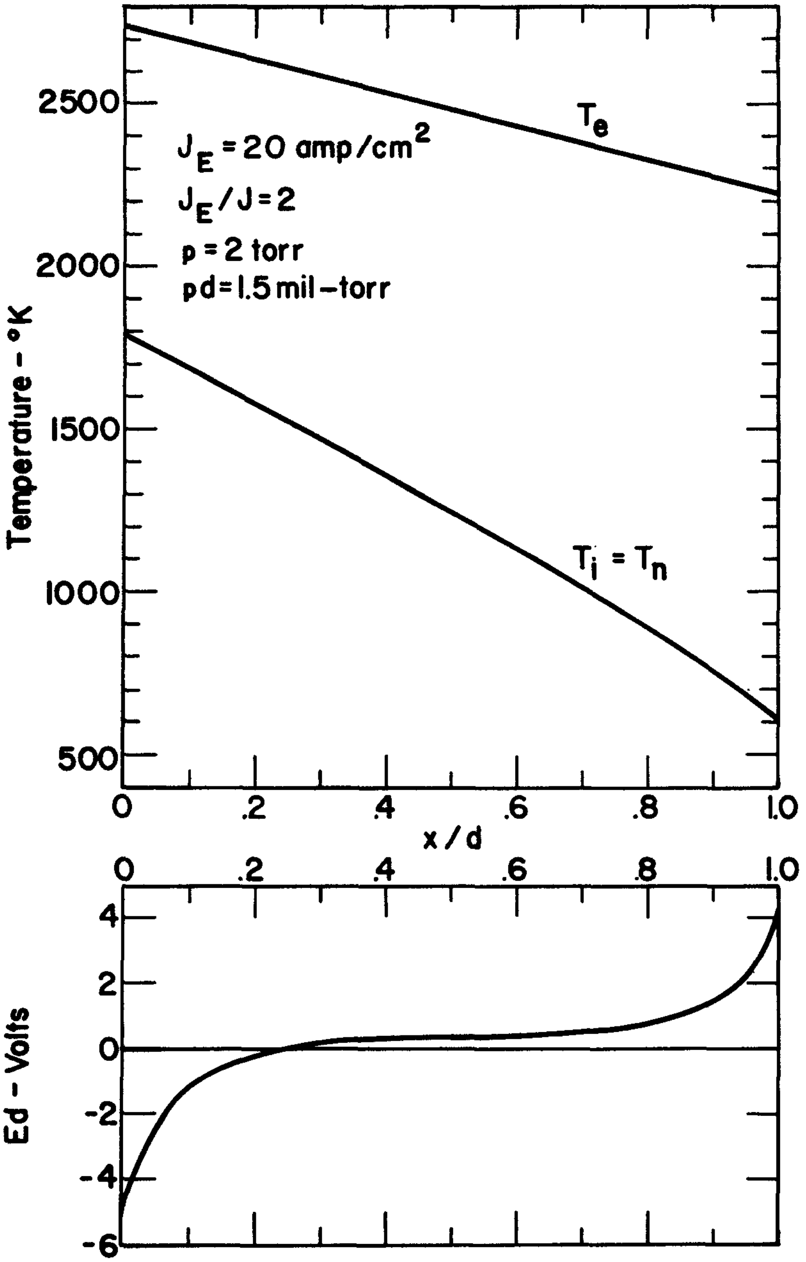


Figure I-4. Calculated Distributions for Electron, Ion and Neutral Temperatures T_e, T_i, and T_n and Electric Field Spacing Product ed. Note T_i was assumed equal to T_n in the analysis.

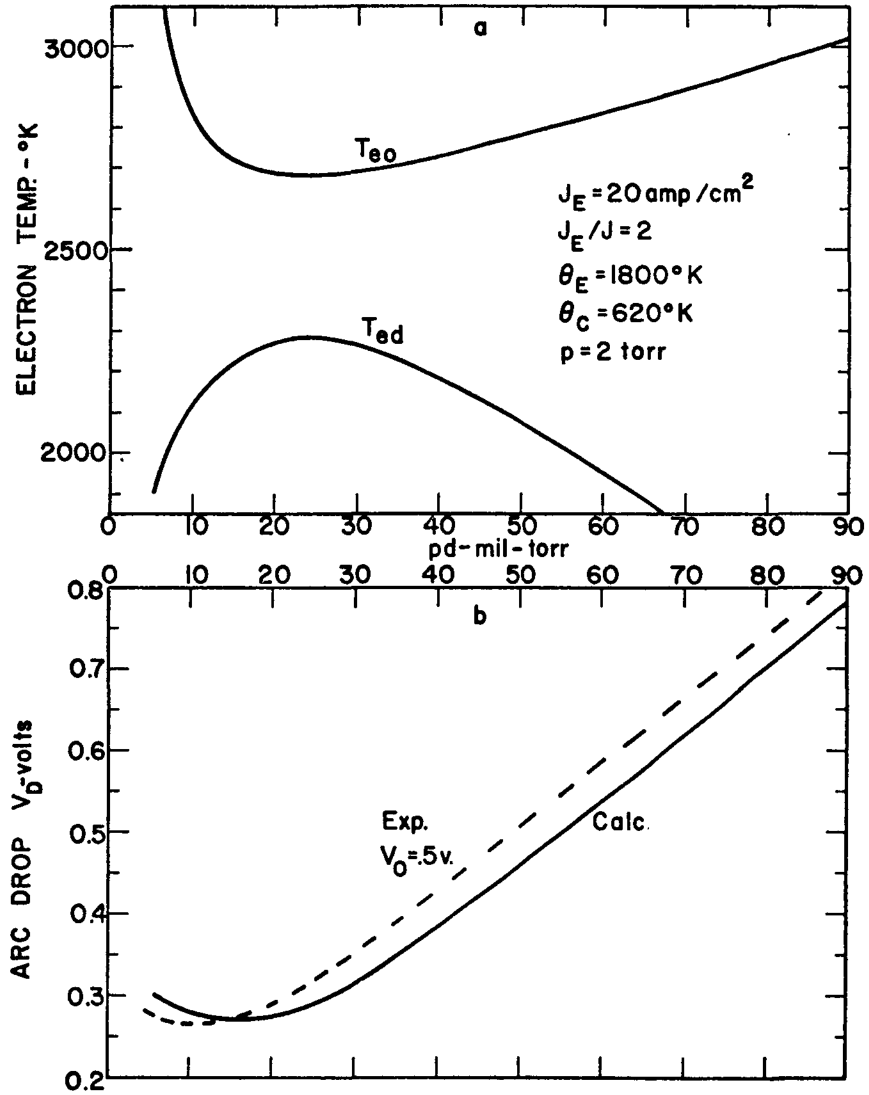


Figure I-5a. Emitter and Collector Temperatures as a Function of pd for Fixed Current.

Figure I-5b. Comparison of Calculated and Measured Arc Drop as a Function of pd for the Same Condition as (a). A contact potential V_0 = 0.5 v was assumed for calculating V_D from the experimental results. Note the existence of an optimum pd in the range 10-20 at which the output voltage is a maximum.

to drive the current through a larger effective resistance. For the same reasons the collector temperatures exhibit a maximum.

The calculated arc drop V_D is compared with experimental results[9] in Figure I-5b for the same conditions as those in Figure I-5a. A value of 0.5 ev was assumed for the contact potential in the experiments. Both the calculated and experimental curves clearly show the existence of an optimum pd at which the arc drop in the converter plasma is a minimum. The calculated value of this minimum based on the cross-sections given in Table I-1 is 0.27 ev which agrees well with recent experimental estimates.[10] The slopes of the calculated and experimental curves at large pd are also in good agreement. This confirms the value of the ion-neutral cross-section which is the most important parameter for determining the slope. This is a result of the fact that the diffusion is ambipolar. Thus, the electron and ions must move together and since the ion-neutral mean free path is smaller than either the electron-neutral or electron-ion mean free paths most of the resistance is due to the ions. As a consequence, accurate values of the ion-neutral mean free path are of considerable importance in determining converter performance.

Calculations of the current-voltage characteristics can be made in the same manner. However, due to a tendency for positive and negative terms to cancel for large and small values of Γ_E/Γ_{eo} they are somewhat more difficult to carry out graphically and are currently being programmed for a numerical computer. In this connection we may note that all the results presented in this paper were obtained by hand computation using a slide rule.

5. Concluding Remarks

On the basis of the analysis presented in this paper we conclude that the approximate analytic technique described can be a very useful tool for the investigation of thermionic energy converters operating in the ignited mode. The method is very much simpler and more efficient than numerical integration and more general and accurate than previous analytic treatments. It gives considerable qualitative insight into the importance and effect of the various physical parameters which determine converter performance and provides the first detailed explanation of an optimum pd product at which the arc drop in the plasma is a minimum. The quantitative comparisons which have been made show reasonable agreement with experiments and with further refinement the method should give results at least as reliable as the input data.

The most questionable approximation made in the present treatment is the assumption of a constant electron temperature gradient. Although this is reasonable for small gradients, its effect is difficult to estimate for large gradients. The approximation can be removed by integrating the energy equation and while this would complicate the analysis somewhat, it should increase the reliability of the results considerably. This is an important improvement which should be made before serious quantitative applications of the method are made.

In addition, the present analysis is limited to the case of monotonic emitter and collector sheaths of the type illustrated in Figure I-1, and the possibility of work function changes due to the Schottky effect at large negative voltages has not been considered. Finally, we have neglected radiation losses and diffusion of excited species in the cascade ionization process. Although the effect of these latter approximations is thought to be small in the range of interest for practical converters, they also need further study.

C IMPROVED TREATMENT OF ELECTRON ENERGY EQUATION

In the analysis presented in the preceding section it was assumed explicitly that the electron temperature gradient could be approximated as a constant in order to avoid the necessity for integrating the electron energy equation. It was also assumed that electronic heat conduction to the collector was negligible in that the term proportional to dT_e/dx in the collector boundary condition could be dropped. Subsequent analysis has shown, however, that while these assumptions are reasonable near the maximum power point on the I-V characteristic, they can be seriously in error at other points. We have therefore improved the treatment by including an approximate but still reasonably accurate integration of energy equation (3.59). To do this we first rewrite (3.59) in the form:

$$\frac{d\theta_e}{d\eta} - \frac{5}{4}\rho\theta_e = -\frac{1}{2}\left(\frac{Q_e}{\Gamma_e} - \psi\right)\rho \qquad (4.1)$$

where

$$\rho = \left(1 + \frac{\theta_i}{\theta_e}\right)\left(\frac{\epsilon_{ei}\, d_{in}}{\bar{P}} + d_{ei}\right) \qquad (4.2)$$

is the effective thermal resistance due to electron neutral and electron ion collisions. Equation (4.1) may now be formally integrated to give

$$\theta_e e^{-5/4K} - \theta_{eo} = -\frac{1}{2}\int_0^{\eta} e^{-5/4K}\left(\frac{Q_e}{\Gamma_e} - \psi\right)\rho\, d\eta' \qquad (4.3)$$

where

$$K = \int_o^{\eta} \rho \, d\eta' \; . \tag{4.4}$$

If we assume $Q_e/\Gamma_e - \psi$ is approximately constant across the converter, then we obtain from (4.3) the result:

$$\theta_e = \theta_{ed} + (\theta_{eo} - \theta_{ed}) \left(1 - e^{-5/4\,(K_d - K)}\right) \Big/ \left(1 - e^{-5/4\,K_d}\right) . \tag{4.5}$$

If we further assume that $(1 + \theta_i/\theta_e)\, \epsilon_{ei}\, d_{in}$ and $(1 + \theta_i/\theta_e)\, d_{ei}$ can be approximated as constants, then (4.4) can be evaluated using the same technique employed to evaluate (3.50). This gives

$$K = \ln \left[\left(\frac{\tanh \delta}{\tanh \delta_o} \right)^{\alpha_1} \left(\frac{B \tanh \delta_d - D\delta_o}{B \tan \delta_d - D\delta} \right)^{\alpha_2} \right] + \left(1 + \frac{\theta_c}{\theta_{ed}} \right) \left(\frac{\delta - \delta_o}{\delta_d - \delta_o} \right) d_{ei} \tag{4.6}$$

where

$$\alpha_1 = \left(1 + \frac{\theta_c}{\theta_{ed}} \right) \frac{\epsilon_{ei}}{(1 + \epsilon_{ei})\,(B - D)} \tag{4.7}$$

and

$$\alpha_2 = \left(1 + \frac{\theta_c}{\theta_{ed}} \right) \frac{\epsilon_{ei} \tanh^2 \delta_d}{(1 + \epsilon_{ei})\, D} \; . \tag{4.8}$$

Substituting (4.5) into (3.59) and imposing the boundary condition (2.26), we obtain

$$V_c = \frac{1}{2}\, \theta_{ed} + \frac{5}{2} \left(\theta_{eo} - \theta_{ed} \right) \Big/ \left(1 - e^{-5/4\, K_d} \right) \tag{4.9}$$

This equation, together with (4.5), provides the relations necessary to replace equations (3.60) and (3.61), which contain the questionable assumptions in analysis of section B. To obtain an improved solution, these two new equations must now be solved simultaneously with (3.33), (3.37), and (3.65). Since this involves the simultaneous solution of two transcendental equations, it is most efficient to use a numerical computer. Unfortunately, the program which has been written to solve the necessary equations has yet not been fully "debugged", so it is not possible to include definitive numerical results. Some preliminary results for the arc drop as a function of pd product are shown in Figure I-6; however, the results are good and are in accord with expectations In particular, the minimum in the neighborhood of pd = 20 is clearly shown.

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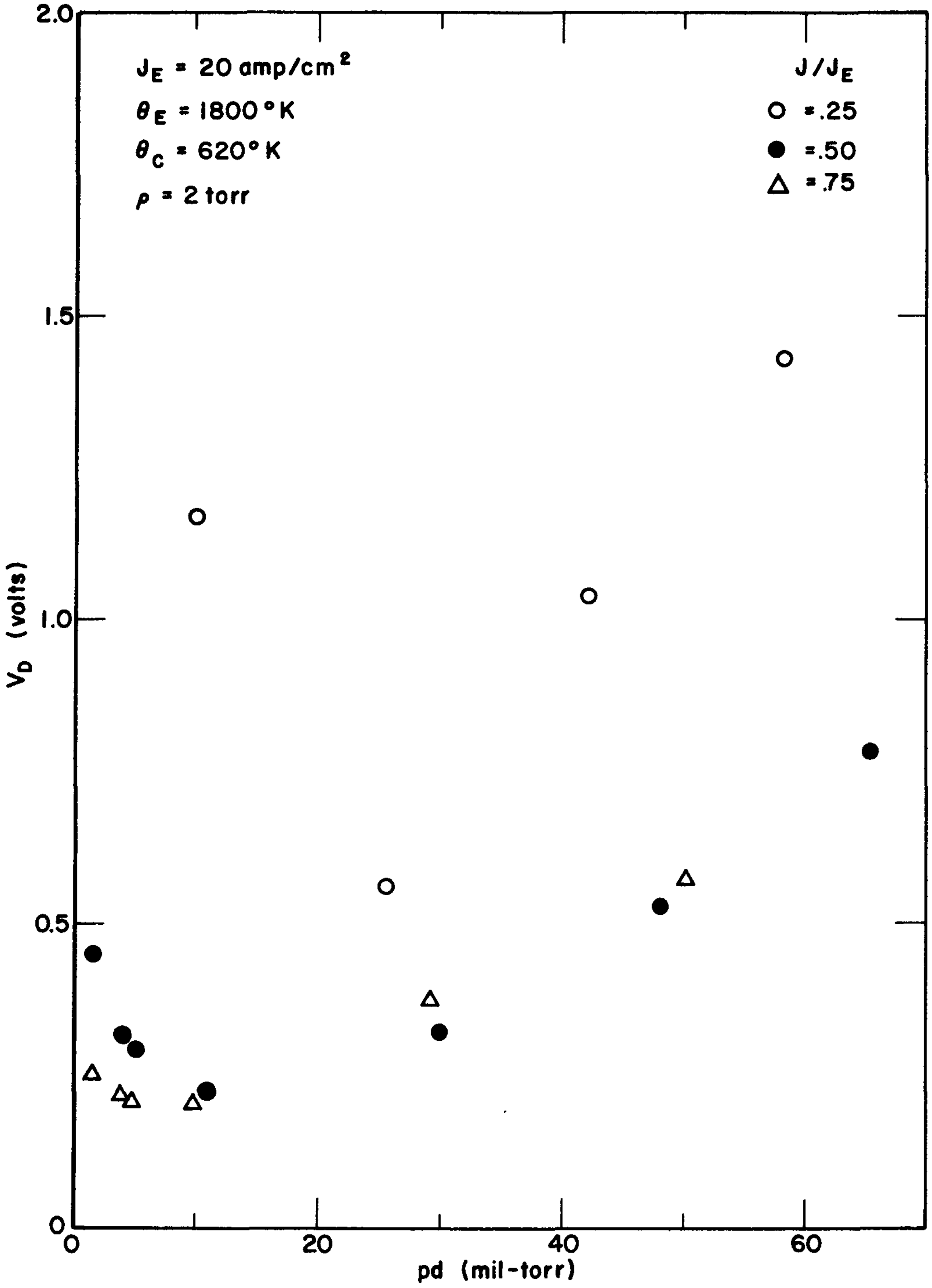

Figure I-6. Arc Drop as a Function of pd.

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II. THEORY OF THE TRANSITION REGIONS OF THERMIONIC ENERGY CONVERTERS

A. SUMMARY

This work is a search for a good method of treating the regions near the electrodes of a thermionic energy converter theoretically. The problem is simple in principle: Poisson's equation is used to relate the potential or electric intensity to the difference in electron and ion densities in the space between the electrodes of the thermionic energy converter. Two Boltzmann equations, one for ions and one for electrons, may be used to relate the relevant particle densities to the potential existing. Then, one merely has to solve the three equations simultaneously together with relevant boundary conditions.

It seemed reasonable to start our search for a method with the simplest available: that of Wang, Lieb, and Pigford.[1] This method is based on the collisionless, one-dimensional Boltzmann equation. We had only to satisfy the boundary conditions of zero electric intensity, and continuity of the potential and densities at the interface with a plasma. Not all boundary conditions could be satisfied simultaneously; it is necessary to consider the anisotropies of the distribution functions in the regions near the electrodes. Next, we considered various improvements based on the magnetohydrodynamic approximation of the Boltzmann equation to the diffusion equations. While the lowest order anisotropies, due to the transport of material, could be encompassed by this method, the resulting equations were nonlinear and required the application of boundary conditions at both ends of the region of integration to achieve a unique, stable solution. The numerical difficulties seemed very difficult to circumvent.

The S_n method was investigated next because it has been very successfully and extensively applied to neutral particle transport and because it had a reputation for being accurate and unconditionally stable - a fact never proved rigorously. The S_n method consists in quantizing the various independent variables in phase space and in approximating the distribution functions by continuous straight line segments between the various subdivisions of each independent variable. Unfortunately, the particle densities computed by this method, especially the electron densities, oscillated, becoming negative in the process. In connection with the investigation of this matter, a proof (the rigor of which has not been investigated) was found that the S_n method applied to problems involving charged particles in an electric field are unconditionally unstable. It was also found that the particular oscillations observed had nothing to do with instabilities, contrary to our initial suspicion, and that conditions could be found to suppress the particular oscillations observed. Because of the prediction of instabilities, we looked into other methods.

During the course of the work on the diffusion method and the S_n methods, it was successively found that the solution for the potential from Poisson's equation could be cast in integral form and later that an integral method could be developed for solving the Boltzmann equations. The integral method for the Boltzmann equations is based on the observation that there are two constants of motion in the problem and that, if these constants of motion are used as independent variables, the density can be a function of only the one independent variable that is not a constant of motion. Also, the resulting, one-dimensional, first order integro-differential equation cast in terms of these variables can be solved by Green's functions technique. A physical interpretation of the integral equations resulting enables us to circumvent any problem arising from a branch point of order 1/2 of the kernel. One can easily see that the densities computed from such a formulation are always positive definite. The integral method is very accurate in view of the extensive averaging over errors, and stable. Convergence of this method was ideal in many cases and extremely good in the other cases when coupled with low-pass filtering. The low-pass filtering suppressed the need to follow ad infinitum the plasma oscillations induced by errors of the numerical method (truncation and round-off) and expedited convergence enormously without suppressing the static phenomena in which we are interested. Low-pass filtering was done in the iteration domain itself, instead of the much more usual conjugate domain, by exploiting the Faltung concept. Much machine time was saved as a result.

The integral method was programmed and coded for a computer. Despite the most inelegant, but easy to debug, way in which the integral method was coded, the program executed with amazing speed and converged extremely well. We had not succeeded in removing all errors from the program by the time the work was terminated: the current of each species was not as constant as we would like; the potential at the plasma did not have zero slope as it must. Otherwise, there are no known errors in the program. Recoding it somewhat more elegantly to exploit calculations already made would greatly speed the execution, probably making each cycle as fast to compute as with a differencing scheme. In view of the paucity of cycles needed by the integral method to converge, it would thus converge much faster indeed than a differential method.

During the course of the work on the S_n method, a method was found that would provide a stable differencing of the Vlasov terms in the Boltzmann equation and that could be extended to several dimensions. While the problem was completely formulated and some of the coding completed, the integral method looked so attractive that the work on the differential method was never completed.

B. INTRODUCTION

For the purposes of this study, a thermionic energy converter is considered to consist of two plane parallel electrodes of infinite extent separated from each other with electrons, cesium atoms and ions inhabiting the intervening space. One of the electrodes, i. e., the cathode,is hotter than the other, i. e., the anode. In practice, the degree of ionization is very small. The geometry is one-dimensional.

The problem is to compute the electron and ion densities, the potential, the current or drift velocity of the ions and electrons, and the temperatures of the ions and electrons as a function of position in the interelectrode space. Knowledge of the directional densities of the electrons and ions, and of the potential in principle enables us to compute any other quantity. The primary goal then is to compute these three quantities. The electrons and ions will have different drift velocities in general, and different temperatures; further, these quantities will be functions of position. Ionization and recombination take place in the region between the electrodes. Radiation losses will be neglected.

The space between the electrodes can be divided into three regions: a cathode sheath adjacent to the cathode, an anode sheath adjacent to the anode, and a plasma between the two sheaths. The plasma is characterized by particle distributions that are nearly isotropic, thermodynamic equilibrium among particles of the same species, and zero electric field. The sheath regions are transition zones between the plasma and the respective electrodes. In these regions. the particle distributions are not isotropic, nor are particles, even of one species, in thermodynamic equilibrium. Further, an electric field exists in each of these regions. The strength of the field is such that recombination and ionization are of secondary importance.

The problem is readily formulated: Poisson's equation is used to relate the electric field or potential to the difference in total ion and total electron densities. The Boltzmann equation relates the particle density of one species of particle to the electric field or potential. There will be a Boltzmann equation for ions and another one for electrons. Because the masses of cesium atoms and ions are nearly equal, the energy distributions of the cesium atoms and ions will be nearly the same where equilibrium exists; i.e., their temperature distributions will be nearly the same. Because of the great disparity in the masses of the electrons and cesium atoms or ions, the electrons will in general have distribution functions rather different from those of the cesium atoms and ions. In other words, where equilibrium exists, at any point, the temperature of the electrons will be different from that of the ions and atoms.

The plasma region has been treated by a number of authors.[2, 3, 4, 5] Diffusion theory has been used in a direct manner despite the instabilities in the method. Boundary conditions, vital to these calculations, are provided by conservation of particles, momentum, and energy across the sheath regions near each electrode. The near isotropy of the distribution functions in the plasma region makes the diffusion theory results meaningful. The absence of an electric field in these regions simplifies the treatment considerably, because the results of Poisson's equation may be incorporated in the statement that the electron and ion densities are equal; in other words, plasma oscillations, which are of very high frequency, are neglected.

The sheath regions between the electrodes and the plasma are much more difficult to treat because of the electric field that exists. In principle, Sockol's 13 moment method[6] could be applied to this problem. With this method it is possible to get currents, stresses, and heat fluxes. Sockol considers the deviation from an equilibrium distribution, so the method can go farther than the Chapman-Enskog method. Further, the method permits each component of a mixture to have its own temperature. The Coulomb interaction is cut off at a Debye length and a rigid sphere model is used for all other interactions. The method does not, however, take collective phenomena into account and is very complicated. Wang, Lieb, and Pigford[1] have treated the sheath regions by the collisionless Boltzmann equation (Vlasov equation) and have restricted their charges to move only along the perpendicular to the plane electrodes. Thus, the effect of the electric field in changing the angular distribution was neglected by these authors. They had problems in simultaneously satisfying the conditions of charge neutrality and zero electric field at some point which could then be taken to be the plasma-sheath interface and in joining their solutions to those of Lieb and Bornhorst[4] for the plasma. In their treatment of the sheath, Rush and Wilkins[7] also used a Vlasov equation like Wang, Lieb, and Pigford, and also neglected the term in the Vlasov equation describing the change in the angular distribution caused by the electric field. The three lowest moments in velocity are used to get conservation equations, half maxwellians being used for the distribution functions. Thus, this theory is equivalent to Yvon's lowest order half-range method. Hansen and Warner[8] treated the plasma and based their work on Nighan's formulation[9, 10, 11] which is based on small departures from equilibrium. Only the lowest order moments of the distribution were used, thereby making their approach equivalent to diffusion theory. They used the so-called shooting technique. Since neither Rush and Wilkins nor Hansen and Warner have actually integrated the densities through the transition region, troubles with the boundary conditions remain unknown.

Reasons for the approximate treatments are easy to find. It is difficult to treat anisotropic transport problems; it is even harder to treat those in which an electric field is present. Nonlinearities of the problem preclude the application of most analytical methods and even some numerical methods, as we shall see. The intercoupling of the charged particles and electric field lead to instabilities of the coupled (nonlinear) equations absent in the individual equations.

Despite these difficulties, it behooves us to try to get a theoretical treatment of the sheath regions. A successful treatment would very probably lead to a much simplified mathematical representation of the region, which is one of several ways of generalizing the results of computer calculations. It could settle the question of whether or not the potential energy of an electron is a monotonic function or is a function having a maximum in the sheath regions. If a maximum exists, it could tell us the height of this maximum. The theory should provide an explanation of the reason that ignition mode theory disagrees with ignition current measurements. Such a theory should explain phenomena taking place at the collector of a thermionic energy converter that are not now explained. The theory would be of assistance in diagnostics: There is now a wealth of information that cannot be associated with either one electrode or the other. A theory would enable us to meaningfully interpolate between data points. Finally, since most of the voltage drop in a thermionic converter is in the sheath regions, it would behoove us to understand these regions better and to have an adequate method of treating them theoretically to determine the effects of various changes in design parameters.

Essentially, in the present work we attempt to take anisotropies, differences in the speed distributions of the electrons and ions, and collisions in the sheath regions into account, thereby getting a method applicable in principle to all three regions of the diode.

Several methods were investigated for treating the sheath region in a thermionic energy converter between either electrode and the plasma. The method of Wang, Lieb, and Pigford, which is based on the one-dimensional, collisionless, Boltzmann equation, was extended slightly to provide a unique, not over- nor under-determined solution by the provision of a boundary condition. The result of this very simple approach indicated that the transition region is decidedly wider than a Debye length computed in the plasma and that the anisotropic distributions inherent in this region must be treated in order to get correct results.

The second method consisted in extending the diffusion equation essentially by considering the next higher order results of hydromagnetic theory so that the next lowest order in the anisotropies could be taken into account. The next lowest order of anisotropies comprised mass flow terms in the momentum and energy conservation equations. Numerical progress with this method was severely limited by the inherent requirement of any diffusion equation. In order that the solution of the problem exist, be unique, not over-determined, stable, nontrivial, Dirichlet or Neumann boundary conditions must be applied at both ends of the region of integration. If the problem had been linear, it would have been possible to effect the numerical integration. However, it is nonlinear and brief numerical examination of the resulting equations with the methods available for nonlinear problems indicated that we would not be so lucky as to escape instabilities, so the method was abandoned after only a little numerical work.

The S_n method has been widely applied to problems involving neutron and gamma ray transport, where it has always exhibited stability and great utility. The S_n method was extended to apply to the Boltzmann equation with an electric field and to apply to all dimensions involved in velocity space and configuration space, instead of just one-dimension in velocity space. The numerical analysis was beset with oscillations of the electron density, thereby giving negative values for this quantity which is inherently positive definite. While the particular oscillations observed probably could have been eliminated by appropriate choice of integration increments, the investigation of these oscillations led to an examination of the stability of the S_n method. No time was spent in determining the rigor of the method used for this stability investigation. To our great surprise, the investigation indicated that the S_n method would be unconditionally unstable when applied to problems having an electric field present, while it would be unconditionally stable if applied to problems having no electric field present, providing one integrates according to the well-known rules for this method. Because at this point the integral method had been developed to the point where it looked very much more promising, we did not try to improve the rigor of our stability investigation or the differencing scheme itself.

In connection with the investigation of the stability of the S_n method, other differencing schemes for the Boltzmann equation were investigated and another was found that is conditionally stable and had been used by others for problems involving plasmas in magnetic fields (but neglecting electrostatic effects that are so important to us in the present problem). However, the integral method remained the most promising, and all work was concentrated on it.

From the inception of this work, it was realized that instabilities of differencing schemes for solving various equations could cause a great amount of trouble. While trying to get the diffusion theory method to work, it was realized that the solution to Poisson's equation could be cast in integral form, and that such a form would be much more accurate and stable than the difference equation scheme then being used. It was also realized that the integral formulation would contain its own boundary conditions, so that an iterative scheme to find the correct potential could be avoided. Consequently, when soon thereafter the anticipated instabilities in the form of negative densities were experienced, the integral method for determining the potential was incorporated into the S_n method.

During the course of the development of the S_n method, it was observed that there were certain constants of motion associated with the transport of the charged particles through the sheath region. (The writer had found constants of motion many years ago for simpler problems involving the Boltzmann equation.) These constants of motion could greatly simplify the form of the Boltzmann equation because, if the independent variables were expressed in terms of the constants of motion, there could be no change of a particle density with respect to some quantity that did not change during the course of motion. Since there are only three independent variables and since two constants of motion had been found, it was evident that the Boltzmann equation must reduce to really only one independent variable. The resulting simplicity would be so great that the Boltzmann equation could be "solved" by casting it into the form of an integral equation by exploiting familiar Green's functions methods. The integral form would then have several advantages: stability, accuracy (because of the extensive averaging over errors), and inherent positive definiteness of the particle density computed. It was further realized that the integral equation had a very simple physical interpretation, i.e., derivation (as all integral formulations seem to), and that this interpretation would enable us to cope with troubles expected from the singularity (comprised of a branch point of order 1/2 in the denominator) of the kernel of the integral equations.

All of the anticipated advantages of the integral method have been borne out in practice.

Convergence of the problem as a whole, in contrast to convergence of just the individual equations, was induced by introduction of low-pass filtering in the real domain. This type of filtering is faster than filtering in the conjugate domain, as is usually done, because there is no need for the double integral transformation required by the Fourier integral theorem. The convergence was very rapid and often ideal. The low-pass filtering suppressed the (plasma) oscillations of the plasma and field, resulting from these two quantities continually trying to re-adjust to each other.

At the time of termination of the project, the integral method had been coded and largely debugged. Among the faults noted was the inconstancy of the electron and ion currents, i. e., lack of particle conservation, to the tolerance desired. Also, the potential function did not develop a zero gradient many mean-free paths away from the nearest electrode and thereby exhibit the presence of a plasma, as it should have. However, this defect may be related to the lack of current constancy.

Total electron and total ion densities were computed, spectral and angular distributions were presented, and electron and ion temperatures were calculated. The present problem was coded so that all quantities are recomputed for each point calculated. Despite this fact, the speed of the method is quite amazing. The integral method could be easily coded as to use all previously calculated information. Very little calculation per iterate would then be involved and the method would then run very fast indeed.

The integral method is discussed throughout all of part C. Some minor improvements in the collisionless sheath method of Wang, Lieb, and Pigford are discussed in the first section of part C; a diffusion theory approach is developed in the second section of part C; the S_n method is applied to our problem in the third section of part C; a stable method of differencing the Boltzmann equation is elaborated in the fourth section of part C.

C. INTEGRAL METHOD

The integral method merely consists of casting the Poisson and Boltzmann equations into integral form and solving these integral forms numerically. There are, of course, two Boltzmann equations, one for electrons and one for ions. The integral form of Poisson's equation results immediately from straightforward integration thereof. The integral formulation of the Boltzmann equations derives from replacement of two of the three original independent variables by two constants of the motion. Since there is then only one independent variable left that actually changes during the course of motion of a particle, the one-dimensional equation is "solved" by Green's function methods (or otherwise, as by integrating factors), thereby casting the Boltzmann equation into integral form. Low-pass filtering in real space, rather than the conjugate space, is introduced to suppress very high frequency oscillations and, thus, expedite convergence of the iterative procedure. Low-pass filtering in real space is related to that in the conjugate space by means of the Faltung theorem in the theory of Fourier transforms. Alternatively, one may regard the filtering as a linear superposition of the impulse response of the filter with the past values of the function being filtered. In other words, this too may be regarded as a superposition, in the spirit of the Green's function, of the response of the filter to a unit stimulus weighted with past values of this stimulus, summed over these weighted products. Macroscopic quantities are then expressed merely as velocity moments over the distribution functions found.

There are very few assumptions made in this approach. The problem treated has planar symmetry, which makes finding the constants of the motion easy; yet, this matter is not regarded as intrinsic to the method. Further, the Boltzmann equation is regarded as a sufficient approximation and is used with all the assumptions embedded therein: Collisions are regarded as short-range and involving just two bodies; long-range effects are separated out into the electric field. Collisions are assumed to occur instantaneously. Quantum effects are neglected. So is gravity, although this is not necessary. The formulation is believed to be quite general otherwise, so long as the constants of the motion can be found. In multi-dimensional problems, the superposition of products of eigenfunctions, one having as an argument the source point, the other having as an argument the field point, might be used to express the Green's function, although we do not resort to this device here. It is disadvantageous when the Green's function can be found, as here, essentially as the product of the solutions of the differential equation that are, respectively, regular and irregular at the origin and contain the conditions of causality, all as needed.

1. The Poisson Equation

Poisson's equation relates the electric potential $\phi(z)$ to the net charge density at a point:[12]

$$\epsilon_o \frac{d^2\phi(z)}{dz^2} = e\,[n_i(z) - n_e(z)], \qquad (C.1)$$

where $n_i(z)$ is the total density of ions at z, $n_e(z)$ is the total density of electrons at the point z, e is the charge of a positron, and ϵ_o is the permittivity of a vacuum.

If it is presumed that the total net charge density is known, there are many ways of solving the above equation. For example, the potential is related to the net charge density by:[12]

$$\phi(\underline{r}) = \frac{1}{4\pi\epsilon_o} \int d\underline{r}' \, \frac{e[n_i(\underline{r}') - n_e(\underline{r}')]}{|\underline{r} - \underline{r}'|} \ . \qquad \text{(C.2)}$$

Since our present problem is one-dimensional, we may integrate once to determine the electric intensity and a second time to determine the potential. We find it more convenient to work in terms of the potential than in terms of the electric intensity. A double integral over the net charge density results. It is convenient to integrate this double integral by parts, so that only single integrals result. The potentials $\phi(z_\ell)$ and $\phi(z_r)$ at the end points, z_ℓ, z_r, are taken to be the boundary conditions, and the two constants of integration are selected to satisfy these boundary conditions, of course. Because all the operations are rudimentary, we merely cite the results. The electric intensity $\mathcal{E}(z)$ is given by either of two expressions, which can be easily shown to be equal to each other:

$$\mathcal{E}(z) = \frac{\phi(z_\ell) - \phi(z_r)}{(z_r - z_\ell)} + \frac{e}{(z_r - z_\ell)\,\epsilon_o} \int_{z_\ell}^{z_r} dz' \, [z' - z_r][n_i(z') - n_e(z')]$$

$$+ \frac{e}{\epsilon} \int_{z_\ell}^{z} dz' \, [n_i(z') - n_e(z')] , \qquad \text{(C. 3)}$$

$$\mathcal{E}(z) = \frac{\phi(z_\ell) - \phi(z_r)}{(z_r - z_\ell)} + \frac{e}{(z_r - z_\ell)\,\epsilon_o}\int_{z_\ell}^{z_r} dz' \, [z' - z_\ell][n_i(z') - n_e(z')]$$

$$+ \frac{e}{\epsilon}\int_{z_r}^{z} dz' \, [n_i(z') - n_e(z')]. \qquad \text{(C. 4)}$$

Likewise, the electric potential can be determined from either of two expressions, which can be easily shown to be equal to each other:

$$\phi(z) = \left(\frac{z - z_\ell}{z_r - z_\ell}\right)\phi(z_r) - \left(\frac{z - z_r}{z_r - z_\ell}\right)\phi(z_\ell) + \frac{e}{\epsilon}\int_{z_\ell}^{z} dz' \, [z' - z][n_i(z') - n_e(z')]$$

$$- \frac{e}{\epsilon}\left(\frac{z - z_\ell}{z_r - z_\ell}\right)\int_{z_\ell}^{z_r} dz' \, [z' - z_r][n_i(z') - n_e(z')], \qquad \text{(C. 5)}$$

$$\phi(z) = \left(\frac{z - z_\ell}{z_r - z_\ell}\right)\phi(z_r) - \left(\frac{z - z_r}{z_r - z_\ell}\right)\phi(z_\ell) + \frac{e}{\epsilon}\int_{z_r}^{z} dz' \, [z' - z][n_i(z') - n_e(z')]$$

$$- \frac{e}{\epsilon}\left(\frac{z - z_r}{z_r - z_\ell}\right)\int_{z_\ell}^{z_r} dz' \, [z' - z_\ell][n_i(z') - n_e(z')]. \qquad \text{(C. 6)}$$

In summary, both the electric intensity and the potential can be determined from integrals over the ion and electron density difference and in terms of the potentials at the boundaries.

2. Derivation of Integral Form of Boltzmann's Equation from Physical Principles

The integral form of Boltzmann's equation can be derived from the differential form of this equation, and we shall do this later. However, the integral form of Boltzmann's equation can also be derived from first principles ab initio. This method gives a much clearer physical picture and, for this reason, will be done first. The number of particles , N(z), moving with the direction of cosine μ with respect to the z-axis that gets from z' to z and experiences no collision between the two points is given by

$$\frac{dN(z)}{dz/\mu(z)} = - \Sigma(z)\, N(z) \; , \tag{C. 7}$$

the solution of which is

$$N(z) = N(0) \exp - \int_{z'}^{z} dz'' \, \frac{\Sigma(z'')}{|\mu(z'')|} \; . \tag{C. 8}$$

Here Σ is the probability a particle experiences a collision in going a unit distance.

The time taken for a particle travelling with the velocity component $v_{\parallel}(z', E, K_{\perp})$ parallel to the z-axis to cross the element $dz'/v_{\parallel}(z', E, K_{\perp})$. This time multiplied by the number of particles made per unit time from one particle is just the number of particles created at z' in the element dz'. This number times the probability $N(z)/N(z')$ of getting from z' to z with no collision between the two points is just the number of particles that arrive at z directly from dz' at z' The total number N(z) of particles at z arising from particles that originate from a source $S(z', E, K_{\perp})$ somewhere between z and a bounding surface, which, say, is at 0 is given by:

$$\int_{0}^{z} \left\{ \frac{dz' \, S(z', E, K_{\perp})}{v_{\parallel}(z', E, K_{\perp})} \right\} P(z, z') \; . \tag{C. 9}$$

We observe that the total energy and the contribution to the kinetic energy arising from the motion of the particle perpendicular to the z-axis will not change for these particles between their last collision at z' and the point of observation at z; these particles have already experienced their last collision. Thus, the variables E and $K_\perp$ are constants of the motion and will not change for these particles. The value of these quantities under the summation (integral) sign will be the same as outside; they serve as suitable labels for the particles. We must also remember that it is possible for a particle to arrive at z directly from the bounding surface at 0 with no collision in between. Thus, the number of particles at z originating at the boundary at 0 which arrive at z with no collisions between the two points is:

$$g(0, E, K_\perp, L)\ P(0, z), \tag{C. 10}$$

where L denotes the sense of the direction in which the particles move. Thus, the total number $g(z, E, K_\perp, L)$ of particles with coordinates z, E, $K_\perp$, and L is given by:

$$g(z, E, K_\perp, L) = g(0, E, K_\perp, L)\ P(0, z) + \int_0^z dz'\ \frac{S(z', E, K_\perp, L)}{v_\parallel (z', E, K_\perp)}\ P(z', z). \tag{C. 11}$$

We observe that this equation is really an integral equation for the particle density, for the source $S(z', E, K_\perp, L)$ is really a function of the particle density at z'. Second, we should be able to determine the density outside the integral to a much higher accuracy than the density inside the integral because of the summation and averaging over the density within the integral. Third, as with all integral equations, we observe that the boundary conditions are already incorporated in the equation, and no subsidiary conditions are needed to supplement the equation to impose the condition of particle conservation in phase space at the boundaries.

The matter is not yet finished, however It may be that the denominator $v_{\parallel}(z'', E, K_{\perp})$ vanishes at some point or that the denominator $\mu(z'', E, K_{\perp})$ vanishes at some point. Physically, these points correspond to points at which a particle runs out of kinetic energy; all its energy being potential, it turns around and moves in the opposite direction. This point can be seen more clearly by referring to Equation C. 40 or to Equation C.40 and C. 41, from which it is seen that $v_{\parallel} = v\mu$ and μ vanishes if and only if the total kinetic energy equals the total energy minus the potential energy As is physically obvious, certain regions are accessible and others are not.

This matter is important, for it enables us to avoid divergences in the numerical analysis, and it leads to an understanding of the various cases, illustrated in Figure II-1, that can occur. For particles that are reflected, we must integrate from the boundary to the point of reflection and back to the field point for certain directions of arrival of particles at the field point. Again, certain particles are trapped; they never escape from the potential energy wells in which they find themselves.

For particles that are trapped, it is impractical to integrate backwards infinitely far through infinitely many reflections. It is, however, still possible to consider these particles quite exactly as follows: Recall that we are interested only in those particles that have experienced their last collision. The perpendicular component of the velocity of these particles will not be altered by the reflection process. The potential is static, so the parallel component of the velocity merely reverses its temporal history; its path is traced backwards in time.

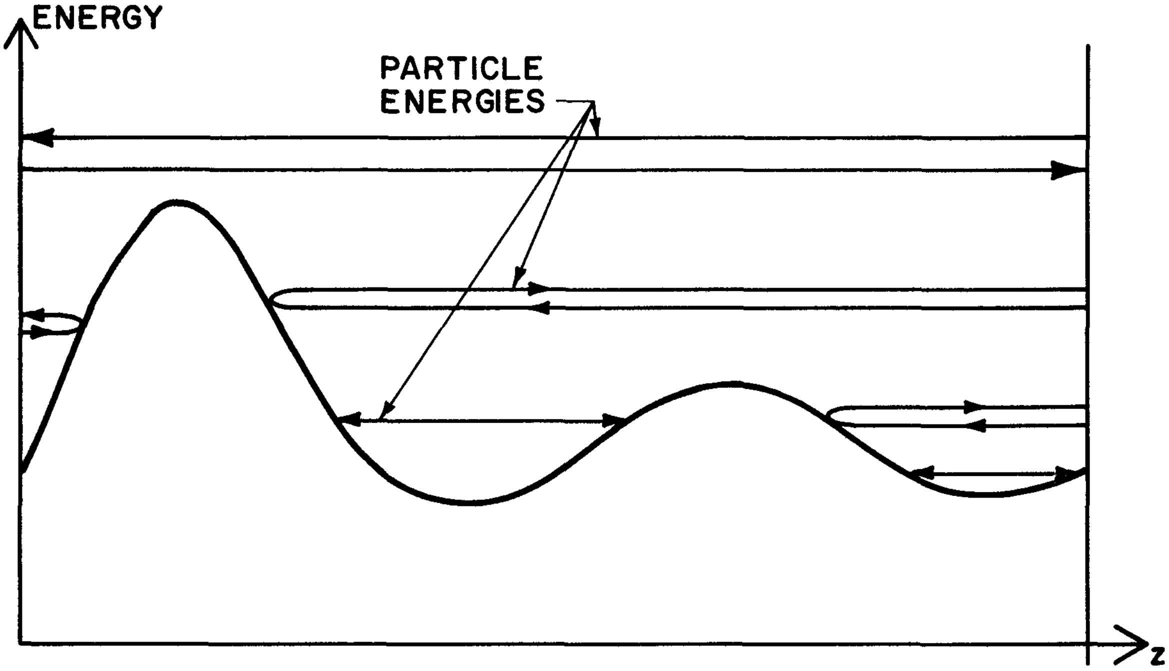


Figure II-1. Various Types of Trajectories
That Can Occur.

In other words, there is a kind of generalized Snell's law at work. We can handle the case of multiple reflections by integrating numerically over only one cycle. The remaining reflection cycles can be handled analytically: Consider the situation shown in Figure II-2. If we are integrating from z_1 to z, then the contribution to the density at z from the previous cycle will be equal to the above integral times

$$P = \exp - 2 \int_{z_\ell}^{z_r} dz'' \frac{\Sigma(z'')}{|\mu(z'')|} , \qquad (C.12)$$

because the trajectories are identical from one reflection to the next. Thus, the total contribution from all reflections is a geometric series:

$$1 + P + P^2 + P^3 + \ldots , \qquad (C.13)$$

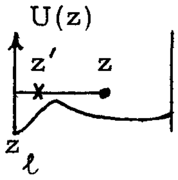
the sum of which is

$$\left\{ 1 - \exp -2 \int_{z_\ell}^{z_r} dz'' \frac{\Sigma(z'')}{|\mu(z'')|} \right\}^{-1} . \qquad (C.14)$$

We are now in a position to itemize the various cases that arise:

a. No reflection at all. Particles arrive at the field point from the left and move to the right.

$$g(z, E, K_\perp, +) = g(z_\ell, E, K_\perp, +)\, P(z_\ell, z) + \int_{z_\ell}^{z} dz' \frac{S(z')\, P(z', z).}{v_{||}(z)} \qquad (C.15)$$



b. No reflection at all Particles arrive at the field point from the right and move to the left.

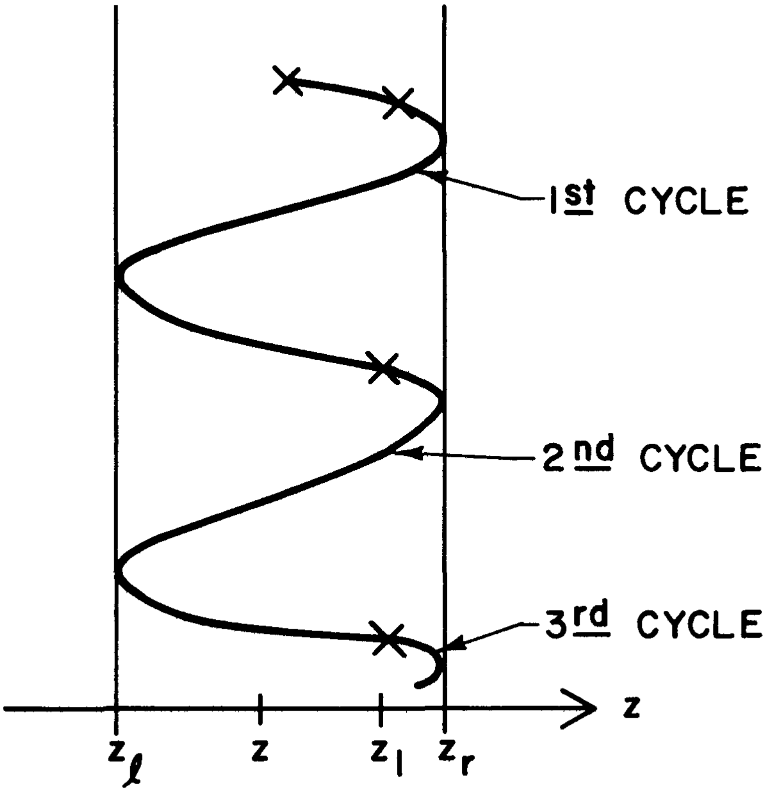
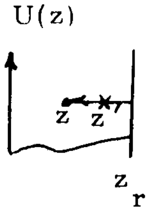


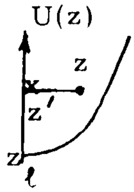
Figure II-2. Trajectories in Successive Reflections.

$$g(z, E, K_\perp, -) = g(z_r, E, K_\perp, -)\, P(z, z_r) + \int_z^{z_r} dz' \, \frac{S(z')\, P(z, z')}{v_\parallel(z')} \tag{C.16}$$



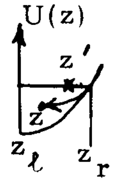
c. One reflection. Left-hand boundary. Particles arrive at the field point from the left and move to the right.

$$g(z, E, K_\perp, +) = g(z_\ell, E, K_\perp, +)\, P(z_\ell, z) + \int_{z_\ell}^{z} dz' \, \frac{S(z')\, P(z, z')}{v_\parallel(z')} \tag{C.17}$$



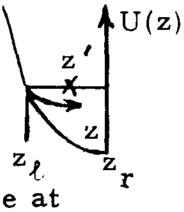
d. One reflection. Left-hand boundary. Particles arrive at the field point from the right and move to the left.

$$g(z, E, K_\perp, -) = g(z_\ell, E, K_\perp, +)\, P(z, z_r)\, P(z_r, z_\ell), + \int_z^{z_r} dz' \, \frac{S(z')\, P(z, z')}{v_\parallel(z')} + \int_{z_\ell}^{z_r} dz' \, S(z')\, P(z, z_r)\, P(z_r, z'). \tag{C.18}$$



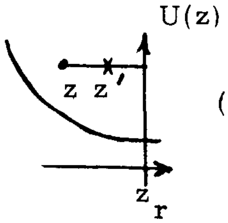
e. One reflection. Right-hand boundary. Particles arrive at the field point from the left and move to the right.

$$g(z, E, K_\perp, +) = g(z_r, E, K_\perp, -)\, P(z, z_\ell)\, P(z_\ell, z_r) + \int_{z_\ell}^{z} dz' \, \frac{S(z')\, P(z, z')}{v_\parallel(z')} + \int_{z_\ell}^{z_r} dz' \, \frac{S(z')\, P}{v_\parallel(z')}\, (z, z_\ell)\, P(z_\ell, z'). \tag{C.19}$$



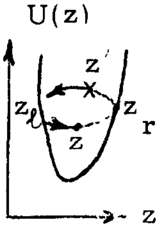
f. One reflection. Right-hand boundary. Particles arrive at the field point from the right and move to the left.

$$g(z, E, K_\perp, -) = g(z_r, E, K_\perp, -)\, P(z, z_r) + \int_z^{z_r} dz' \, \frac{S(z')\, P(z, z')}{v_\parallel(z')} \tag{C.20}$$



g. Multiple reflections at both left-hand and right-hand boundaries. Particles arrive at the field point from the left and move to the right.

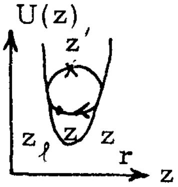
$$g(z,\, E,\, K_\perp,\, +) = \frac{\displaystyle\int_{z_\ell}^{z} dz' \frac{S(z')\, P}{v_\parallel(z')}(z',\, z) + \int_{z_\ell}^{z_r} dz' \frac{S(z')\, P}{v_\parallel(z')}(z, z_\ell) P(z_\ell,\, z')}{1 - P^2\,(z_\ell,\, z_r)} .$$



(C 21

h. Multiple reflections at both left-hand and right hand boundaries. Particles arrive at the field point from the right and move to the left.

$$g(z,\, E,\, K_\perp,\, -) = \frac{\displaystyle\int_{z}^{z_r} dz' \frac{S(z')\, P}{v_\parallel(z')}\ (z,\, z') + \int_{z_\ell}^{z_r} dz' \frac{S(z')\, P}{v_\parallel(z')}\ (z,\, z_r)\, P(z_r,\, z')}{1 - P^2\,(z_\ell,\, z_r)} .$$



(C. 22)

At this point it is interesting and important to observe that $g(z,\, E,\, K_\perp,\, L)$ is constant in the absence of scattering, in agreement with the result (C 45) (differential equation for g in the first place). Thus, we might expect better numerical accuracy as a result of using g than some other function, such as $n(z,\, E,\, K_\perp,\, L)$.* Indeed, we can formulate all of our integral equations in terms of this last quantity through the use of the Jacobian $J\left(\frac{v,\, \mu}{E, K_\perp}\right)$ It will then be observed that a number of singularities (a simple pole and a branch point of order 1/2, which is an essential singularity) appear. The singularities are more apparent than real, and, indeed, it can be shown that they do not lead to any real

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*See Q5, for a definition of $n(z,\, E,\, K_\perp,\, L)$, esp., (C. 43) and (C. 44). The issue is one of normalization divergences. Nevertheless, a computer does not know this; presumably, if our numerical differencing were to be carried out sufficiently finely and enough digits were carried in each word, a computer would have no trouble with all these apparent divergences. In practice, both the word length and the amount of machine time available are seriously bounded. It has been found that under practical conditions things get big near apparent singularities and results are much smoother and well-behaved if the whole subject is avoided and manifestly convergent procedures are used. For this reason, wherever possible Jacobians are avoided, $g(z, E, K_\perp, L)$ is used and $n(z, E, K_\perp, L)$ is avoided, even though from the theoretical point of view the practical procedure is somewhat less elegant.

Simpson's rule was used to integrate the argument of the exponential in the optical depth relation and the space integral in the density calculation, except possibly for the end interval. The end interval is computed by the trapezoidal rule if the number of intervals is even.

3. Boundary Conditions

The plasma forms one of the two boundaries of the sheath region. The electrons and ions in the plasma are distributed isotropically and have a Maxwell-Boltzmann speed distribution at any point. The temperatures and, therefore, the speed distributions of the electrons and ions will be different from each other, in general. Provision for this difference in temperature has been made in the program.

In a Maxwell-Boltzmann distribution, the number n(v) of particles moving between speed v and v + dv is[13]:

$$n(v) = 4\pi v^2 \left(\frac{m}{2\pi kT}\right)^{3/2} \exp - (mv^2/2kT), \tag{C.23}$$

where m is the mass of the particles, k is Boltzmann's constant, and T is the temperature. The number of particles moving between speed v and v + dv and with a direction cosine between μ and $\mu + d\mu$ is:

$$n(v, \mu) = 2\pi v^2 \left(\frac{m}{2\pi kT}\right)^{3/2} \exp - (mv^2/2kT). \qquad (C. 24)$$

The particle current J(z) at z is defined in terms of the directional density by:

$$\underline{J}(z) = \int_0^\infty dv \int_{-1}^{1} d\mu \, 4\pi v^2 \, \underline{v} \, n(z, v, \mu). \qquad (C. 25)$$

This current is given by Richardson's equation:

$$J(z) = \frac{4\pi m (kT)^2}{h^3} \exp - (\psi/kT), \qquad (C. 26)$$

where h is Planck's constant and ψ is the work function of the material from which the electrons are emitted. Thus, we may determine the distribution function for the electrons emitted from the hot electrode by multiplying the distribution function by a constant C and determining this constant C from the relation:

$$J_z = \frac{4\pi m(kT)^2}{h^3} \exp - (\psi/kT) = \frac{1}{2} \int_0^\infty dv \, v^3 \int_{-1}^{1} d\mu \, \mu C \left(\frac{m}{2\pi kT}\right)^{3/2} \exp - \left(\frac{mv^2}{2kT}\right). \qquad (C. 27$$

By solving the above expression for C and introducing the expression for C into the Boltzmann distribution, we find that

$$n_e(z, v, \mu) = 4\pi v^2 \left(\frac{m}{h}\right)^3 \exp - \left(\frac{\psi + \frac{mv^2}{2}}{kT}\right) = 2\pi \frac{Km^2}{h^3} \exp - \frac{\psi + K}{kT} . \qquad (C. 28$$

The current of ions emitted from a hot electrode is governed by the Saha-Langmuir equation:

$$\frac{p_g}{\sqrt{2\pi\, m_g\, kT_g}\;\{1 + 2\exp[e(V_i - \psi)/kT]\}}\,, \qquad (C.29)$$

where p_g is the pressure of the cesium atom gas, m_g is the mass of the gas molecules, T_g is the temperature of the gas, V_i is the ionization potential of cesium, and ψ is the work function of the material Again, the ion density corresponding to this current density may be found exactly as it was for the electrons The ion density is:

$$n_i(z, v, \mu) = \sqrt{\frac{m}{2\pi kT_g}}\;\frac{mp_g\, v^2 \exp -\left(\frac{mv^2}{2\,kT}\right)}{(kT)^2\,\{1 + 2\exp[e(V_i - \psi)/kT]\}}\,, \qquad (C\ 30)$$

$$= \sqrt{\frac{2m}{\pi\, kT_g}}\;\frac{p_g\, K}{(kT)^2}\;\frac{\exp -(K/kT)}{\{1 + 2\exp[e(V_i - \psi)/kT]\}} \qquad (C.31)$$

4 Derivation of Integral Form of Boltzmann's Equation from Differential Form

We turn now to a derivation of the integral equation for the particle density from the differential form of the Boltzmann equation. We believe there will be enough mathematics to convince one that the above result derived on the basis of common sense is in fact correct.[†]

The Boltzmann equation is merely a statement of particle conservation in phase space. The net number of particles crossing the boundaries of an element of volume in configuration and velocity space must equal the number scattered into or created in that volume element minus the number scattered out or absorbed in that volume element. Thus, the

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[†] Private communication from V Weisskopf

Boltzmann equation may be written as follows in the steady-state:

$$\underline{v} \cdot \nabla_{\underline{r}}\, n\,(\underline{r}, \underline{v}) + \underline{a} \cdot \nabla_{\underline{v}}\, n\,(\underline{r}, \underline{v}) = \left.\frac{\partial f}{\partial t}\right|_{\text{coll.}} . \tag{C. 32}$$

Here $n\,(\underline{r}, \underline{v})$ is the density of particles per unit volume in configuration space and per unit volume in velocity space, $\underline{r}$ is the position in configuration space of the field point at which the particle population is examined, $\underline{v}$ is the position in velocity space of the field point at which these particles are examined, $\underline{a}$ is the acceleration of the particle cloud, and $\left.\frac{\partial f}{\partial t}\right|_{\text{coll}}$ is the rate of change of the distribution due to collisions.

The electrons will be assumed to be isotropically scattered by the cesium atoms. Scattering by the ions and by other electrons is neglected because of the low degree of ionization, i.e., great preponderance of neutral particles The electrons will lose very, very little energy in their collisions with the neutrals. The ions are also assumed to be isotropically scattered. Because the masses of cesium atoms and ions are so nearly the same, the atoms and ions will come into equilibrium with each other very rapidly. Thus, we assume that the ions have the same temperature as the atoms. Any departure of the ions from an equilibrium distribution will strongly urge this distribution toward the equilibrium distribution.

We can write the Boltzmann equation as applied to our present problem:

$$v\mu \left.\frac{\partial n}{\partial z}\right|_{v,\,\mu} - \frac{e\mu}{m}\left(\frac{\partial \phi}{\partial z}\right)\left.\frac{\partial n}{\partial v}\right|_{\mu,\,z} - \frac{e}{m}\left(\frac{\partial \phi}{\partial z}\right)\frac{1-\mu^2}{v}\left.\frac{\partial n}{\partial \mu}\right|_{z,\,v} = \left.\frac{\partial f}{\partial t}\right|_{\text{coll.}} , \tag{C. 33}$$

where ϕ is the potential, z is the coordinate of the field point perpendicular to the plane of the electrodes, v is the speed of the particles, and μ is the direction cosine of the velocity with respect to the z-axis.

5. Transformation of Independent Variables

Consider now the following: The left-hand side of the conservation equation must be the same whether or not there is scattering in the problem, regardless of the transformation used to transform the independent variables. Let us consider the special case in which there is no collision in the problem. In this case, the total energy E of the particles and the contribution $K_\perp$ to the kinetic energy arising from the component of the motion of the particle parallel to the electrodes and perpendicular to the z-axis are constants of the motion. The contribution $K_\perp$ to the kinetic energy will be referred to as the perpendicular kinetic energy, for reasons of convenience, even though the term is somewhat inapt.

In the collisionless case, and, therefore, the case with collisions also, the left-hand side of the Boltzmann equation must reduce to one term when the independent variables z, v, and μ are re-expressed in terms of z, E, $K_\perp$ and L as the new independent variables, for the reason that a function of something that does not change, e.g., a constant of the motion, is not really a function at all of that something. It is a function of whatever independent variables still remain in the problem, the values of which change as the particles move about.

Be this as it may, one is usually much more convinced by a great amount of algebra, rather than mere abstract argument.[†] The old and new variables are related by the following expressions:

[†] Weisskopf, V., Private Communication.

$$z = z, \tag{C. 34}$$

$$E = K + V(z), \tag{C. 35}$$

$$K_\perp = K(1 - \mu^2), \tag{C. 36}$$

$$L = \text{sense of particle direction}, \tag{C. 37}$$

where

$$K = mv^2/2. \tag{C. 38}$$

It is necessary to introduce a variable, here called L, describing the sense in which the particle moves, i. e., whether it moves right or left, because this information is not carried by the new independent variables z, E, $K_\perp$, but is carried by the original independent variable μ. This information is lost because of the squaring process, as can be most easily seen from the inverse transformations, which are:

$$z = z \tag{C. 39}$$

$$v = \sqrt{2\,[E - V(z)]/m}, \tag{C. 40}$$

$$\mu = \pm\sqrt{1 - \frac{K_\perp}{E - V(z)}} \;. \tag{C. 41}$$

The Jacobian of the transformation will be of future use to us:

$$J\left|\frac{v, \mu}{E, K_\perp}\right| = -\left|\left\{2\sqrt{2m\,[E - V(z) - K_\perp]}\right\}\left\{E - V(z)\right\}\right|^{-1} . \tag{C. 42}$$

Before proceeding further, we need to consider another point of mathematics relating to the directional density. Originally, the directional density is some function n of z, v, and μ. These variables are replaced by z, E, $K_\perp$, and L:

$$g(z, E, K_\perp, L) = n(z, v, \mu). \tag{C.43}$$

The original directional density n is normalized per unit volume, per unit speed v, and per unit μ; i.e., this directional density is the number of particles per unit volume near z, per unit speed near v, per unit μ near μ. The normalization of the g function is exactly the same, even though it is a function of the variables z, E, $K_\perp$, and L. Since it is convenient to denote the normalization of a function with the arguments of that function, we introduce the new function $n(z, E, K_\perp, L)$ of the new variables, which will turn out to be more useful conceptually than practically.

$$n(z, E, K_\perp, L) = \left| J\left(\frac{v, \mu}{E, K_\perp}\right)\right| n(z, v, \mu). \tag{C.44}$$

6. Transformation of Boltzmann Equation

If, now, the old variables are replaced by the new ones and the partial derivatives carried out, a glorious amount of elementary mathematics results that ought to convince anyone that the Boltzmann equation reduces to:

$$\sqrt{\frac{2}{m}\,[E - V(z) - K_\perp]}\;\frac{dg\,(z, E, K_\perp, L)}{dz} = \left.\frac{\partial f}{\partial t}\right|_{coll}. \tag{C.45}$$

Note that

$$V_{\parallel} = \sqrt{\frac{2}{m}\,[E - V(z) - K_\perp]} \tag{C.46}$$

is merely the component of the velocity parallel to the z-axis. No cross section enters into the derivation of the above result; no mention was made of the presence or absence of collisions in this derivation Therefore, it must hold whether or not there are collisions in the problem

7. Collision Terms in Boltzmann Equation

We now consider the collision terms. These terms may be written in many ways.[14, 15] One way is as follows:

$$- \int d\underline{v}'' \, \Sigma \, (\underline{r}, \underline{v}, \underline{v}'') \, |\underline{v} - \underline{v}''| \, n \, (\underline{r}, \underline{v}) \, +$$

$$+ \int d\underline{v}' \int d\underline{v}'' \, \frac{F \, (\underline{v}' \rightarrow v, \underline{\Omega})}{v^2} \, c \, (v') \, \Sigma \, (\underline{r}, \underline{v}', \underline{v}'') \, |\underline{v}' - \underline{v}''| \, n \, (\underline{r}, \underline{v}'). \qquad \text{(C. 47)}$$

Here, $\Sigma (\underline{r}, \underline{v}, \underline{v}'')$ is the macroscopic cross section, i. e., the probability that a collision will take place at $\underline{r}$ with a particle of velocity $\underline{v}''$ when a particle of velocity $\underline{v}$ moves a unit distance, $f(\underline{v}' \rightarrow v, \underline{\Omega})$ is the probability that in a collision a particle of velocity $\underline{v}'$ disappears and is replaced by a particle of speed v and direction $\underline{\Omega}$, and $c(v')$ is the probable number of particles emerging from a collision induced by a particle of speed v'. The first term represents the number of particles leaving the phase volume of interest as a result of collisions; the second term represents the number of particles entering the phase volume of interest as a result of collisions. Unfortunately, these terms are very complicated; among other things, they are nonlinear; some approximations are required.

The approximations we make are as follows:

(1) Electrons experience only scattering collisions with neutral cesium atoms.

(2) In these scattering collisions, the electrons are scattered isotropically and lose no energy. The energy change is negligible because of the great disparity in masses of the electrons and cesium atoms.

(3) Ions experience only scattering collisions with neutral cesium atoms.

(4) The neutral cesium atoms are in thermodynamic equilibrium, i.e., in a Maxwell-Boltzmann distribution, which is characterized by some temperature.

(5) In a collision, the ions will on the average tend to the equilibrium distribution of the neutral atoms, because of the substantial equality of the masses of cesium ions and cesium atoms. The collision integrals for the ions will then be represented in the Krook approximation by the collision frequency times the difference between the equilibrium distribution function and the actual distribution function. The collision frequency is merely the macroscopic cross section times the speed of the particles.

Thus, the principal difference between electrons and ions is that the electrons do not and the ions do exchange energy with the neutrals, with the result that the ions do and the electrons do not tend to the distribution function of the neutrals. The interaction of electrons and ions with each other is neglected.

Ionization and recombination are not incorporated into the theory at this point, although they could very easily be, since we are primarily interested in sheath phenomena and since the probability of ionization or recombination is small over the short distances involved and compared with scattering collisions with neutrals.

The collision integrals are then represented in the Boltzmann equation for the electrons by:

$$-\Sigma(z)\, v\, n(z, v, \mu) + S_e(z, v), \tag{C.48}$$

where

$$S_e(z, v) = \frac{\Sigma v}{2} \int_{-1}^{1} d\mu'\, n(z, v, \mu'), \tag{C.49}$$

and in the Boltzmann equation for cesium ions by

$$-\Sigma(z)\, v\, n(z, v, \mu) + S_i(z, v), \tag{C.50}$$

where

$$S_i(z, v) = \Sigma(z)\, v\, \bar{n}(z, v, \mu) \tag{C.51}$$

and

$$\bar{n}(z, v, \mu) = 2\pi v^2 \left[m/2\pi kT(z)\right]^{3/2} \exp - \left[m v^2/2kT(z)\right] \tag{C.52}$$

is the equilibrium distribution at temperature T.

8. Reduction of Boltzmann Equation to Integral Equation

We are now ready to solve the Boltzmann equation. We have an equation for either electrons or ions of the form:

$$\sqrt{E - V(z) - K_\perp}\, \frac{dn}{dz} + \Sigma(z)\, vn = S \tag{C.53}$$

to solve, where S is a source function representing the collision integral in which particles are made in the phase element of interest. Solution proceeds by finding the Green's function $G(x, x')$ for the problem, i.e., the solution for the following equation:

$$\frac{dG(x, x')}{dx} + g(x)\, G(x, x') = \delta(x - x'). \tag{C.54}$$

The Green's function is:

$$G(x, x') = P(x, x')\, U(x - x'), \tag{C.55}$$

where

$$P(x, x') = \exp - \int_{x'}^{x} dx'' g(x''), \tag{C.56}$$

and U is zero if its argument is negative and 1 if it is positive.

We wish, then, to solve an equation of the form:

$$\frac{df(x)}{dx} + g(x) f(x) = h(x) . \tag{C.57}$$

The solution of this equation is:

$$f(x) = f_H(x) + \int dx' G(x, x') h(x') + f_H(x) , \tag{C.58}$$

where $f_H(x)$ is a solution of the homogeneous part of the original equation. Thus, the solution is:

$$f(x) = C_1 P(-\infty, x) + \int_{-\infty}^{x} dx' h(x') P(x', x), \tag{C.59}$$

where C_1 is chosen so that the solution satisfies the boundary conditions. Let us apply these techniques to the present problem. The Boltzmann equation then has the solution:

$$g(z, E, K_\perp, L) = g(0, E, K_\perp, L) P(0, z) + \int_0^z \frac{dz' S(z', E, K_\perp)}{v_\parallel(z', E, K_\perp)} P(z', z), \tag{C.60}$$

where

$$P(z', z) = \exp - \int_{z'}^{z} \frac{dz'' \Sigma(z'')}{|\mu(z'', E, K_\perp)|} . \tag{C.61}$$

9. Drift Velocity, Current, and Temperature

The drift velocity can be readily computed from the directional density. The drift velocity $\bar{v}(z)$ is defined to be:[13]

$$\underline{\bar{v}}(z) = \int_0^\infty dv \int_{-1}^{1} d\mu \, \underline{v} n(z, v, \mu)/n(z). \tag{C.62}$$

As applied to the present problem, the drift velocity is computed from:

$$\begin{aligned} \bar{v}_z(z) = \sqrt{\frac{2}{m}} \int_0^\infty dv \int_{-1}^{1} d\mu \sqrt{K_{\parallel}(z, E, K_{\perp})} \, \{ & g[z, E(z, v), K_{\perp}(z, v, \mu), +] + \\ & - g[z, E(z, v), K_{\perp}(z, v, \mu), -]\}/n(z), \end{aligned} \tag{C.63}$$

where

$$K_{\parallel}(z, E, K_{\perp}) = E - U(z) - K_{\perp}. \tag{C.64}$$

The integrals are carried out numerically, as follows:

$$\begin{aligned} \bar{v}_z(J) = \frac{2}{m} \Bigg[\sum_{N=2}^{NL} \frac{1}{2} \Bigg(\sum_{I=2}^{(IL+1)/2} \Bigg\{ & \frac{\sqrt{K_{\parallel}(J, N, I)}}{2} [g(J, N, I +) - g(J, N, I, -)] + \\ & + \frac{\sqrt{K_{\parallel}(J, N, I-1)}}{2} [g(J, N, I-1, +) - g(J, N, I-1, -)] \Bigg\} |\mu(J, N, I) - \mu(J, N, I-1)| + \\ & + \Bigg\{ \frac{\sqrt{K_{\parallel}(J, N-1, I)}}{2} [g(J, N-1, I, +) - g(J, N-1, I, -)] + \\ & + \frac{\sqrt{K_{\parallel}(J, N-1, I-1)}}{2} [g(J, N-1, I-1, +) - g(J, N-1, I-1, -)] \Bigg\} |\mu(J, N-1), I) \\ & - \mu(J, N-1, I-1)| + \sqrt{K_{\parallel}(J, N, (IL+1)/2)} [g(J, N, (IL+1)/2, +) + \\ & - g(J, N, (IL+1)/2, -)] |\mu(J, N, (IL/2)+1) - \mu(J, N, (IL+1)/2)| + \\ & + \sqrt{K_{\parallel}(J, N-1, (IL+1)/2)} [g(J, N-1, (IL+1)/2, +) - g(J, N-1, (IL+1)/2, -)] \\ & * |\mu(J, N-1, (IL/2)+1) - \mu(J, N-1, (IL+1)/2)| \Bigg) \\ & \left(\sqrt{K(J, N)} - \sqrt{K(J, N-1)} \right) / n(J) \Bigg]. \end{aligned} \tag{C.65}$$

Here J represents the quantized variable correlated to z, N to energy, I to perpendicular kinetic energy; NL is the limit of N, IL is the limit of I, + refers to directions in the positive sense, - refers to directions in the negative sense, and $K_{||}$ is the contribution to the kinetic energy resulting from the parallel component of the velocity (parallel kinetic energy for short) The quantized variables are integer constants and are processed according to the rules of integer arithmetic. For example, 1/2 = 0, 3.9999999/2 = 1, 4.000001/2 = 2, 2/2 = 1, 3/2 = 1, 4/2 = 2, and so on. The result is always the greatest integer less than or equal to the actual result.

The electric current then follows immediately and is:

$$\underline{j}(z) = q\, n(z)\, \bar{\underline{v}}(z) , \tag{C.66}$$

where q is the charge of the particles and n(z) is their total density.

The temperature can also be readily computed from the directional density. It is defined by:

$$\frac{3}{2} kT = \frac{\int_0^\infty dv \int_{-1}^{1} d\mu\, \frac{m}{2} (\underline{v} - \bar{\underline{v}})^2\, n(z, v, \mu)}{n\ (z)} , \tag{C.67}$$

and applied to the present problem as:

$$kT(z) = \frac{2}{3} \frac{\int_0^\infty dv \int_{-1}^{1} d\mu \left[\frac{mv^2}{2}\right] [g(z, E\ (z, v), K_\perp(z,v,\mu), +) + g(z, E(z, v), K_\perp(z, v, \mu), -)]}{n(z)} + - \frac{m}{3} \overline{v(z)}^2 . \tag{C.68}$$

The integrals are carried out numerically, as follows:

$$\begin{aligned}
kT(J) = {} & \sqrt{\frac{2}{9m}}\,\frac{1}{n(z)}\Bigg[\sum_{N=2}^{NL+1}\ \sum_{L=1}^{2}\Bigg(\sum_{I=2}^{(IL+1)/2}\frac{1}{2}\Bigg\{K\ (J, N)[g(J, N, I, L)+g(J, N, I-1, L)]* \\
& *\left|\mu(J, N, I, L) - \mu(J, N, I-1, L)\right| + K\ (J, N-1)[g(J, N-1, I, L)+g(J, N-1, I-1, L)]* \\
& *\left|\mu(J, N-1, I, L) - \mu(J, N-1, I-1, L)\right|\Bigg\} + K\ (J, N)\,g\left(J, N, \frac{(IL+1)}{2}, L\right)* \\
& *\left|\mu(J, N, (IL/2)+1, L) - \mu(J, N, (IL+1)/2, L)\right| + K\ (J, N-1)g\left(J, N-1\ , \frac{(IL+1)}{2}, L\right)* \\
& *\left|\mu(J, N-1, (IL/2)+1, L) - \mu(J, N-1, (IL+1)/2, L)\right|\Bigg)\left(\sqrt{K\ (J, N)} - \sqrt{K\ (J, N-1)}\right)* \\
& + \sum_{L=1}^{2}\ \sum_{I=2}^{(IL+1)/2}\Bigg\{K\ (J, 1)\,\frac{[g(J, 1, I, L)+g(J, 1, I-1, L)]}{2}\left|\mu(J, 1, I, L)-\mu(J, 1, I-1, L)\right|* \\
& *\frac{\sqrt{K\ (J, 1)}}{2} + K\ (J, NL+1)\,\frac{[g(J, NL+1, I, L)+g(J, NL+1, I-1, L)]}{2}\,\big|\mu(J, NL+1, I, L) + \\
& -\mu(J, NL+1, I-1, L)\,\frac{1}{2}\left(\sqrt{K\ (J, NL+2)} - \sqrt{K\ (J, NL+1)}\right)\Bigg\}\Bigg] - \frac{m}{3}\,\overline{v(z)}^{2}\ . \qquad \text{(C. 6}
\end{aligned}$$

It is necessary to compute the spectral distribution of electrons for the source term in the integral equation that determines the electron density. This can be easily done by noting from Equations C. 39 through C. 41 that the speed v is fixed if the indices N and J are fixed. Thus, if we sum over I and L, all values of μ will be spanned, and both the position and the speed will be constant, which is the meaning of integration over μ to determine the density for a particular position and speed:

$$n(z, v) = \int_{-1}^{1} d\mu\ g\,[z, E(z, v), K_{\perp}(z, v, \mu),\ L(\mu)]\ . \qquad \text{(C. 7}$$

$$= \sum_{L=1}^{2}\ \sum_{I=1}^{(IL/2)+1} \Delta\mu_{I}\ \{g[z, E(z, v), K_{\perp I}\,(z, v), L]\}. \qquad \text{(C. 7}$$

Likewise, the total density may also be found as:

$$\begin{aligned}
\imath(z) &= \int_0^\infty dv \int_{-1}^{1} d\mu\ g\,[z, E(z, v), K_\perp(z, v, \mu), L(\mu)] = \sum_{N=2}^{NL+1} \sum_{I=2}^{(IL+1)/2} \sum_{L=1}^{2} \\
&\Bigg\{\bigg[g_{N, I, L}\frac{1}{2}\left|\mu_{N, I, L}-\mu_{N, I-1, L}\right| + g_{N-1, I, L}\frac{1}{2}\left|\mu_{N-1, I, L}-\mu_{N-1, I-1, L}\right| + \\
&g_{N, I-1, L}\frac{1}{2}\left|\mu_{N, I, L}-\mu_{N, I-1, L}\right| + g_{N-1, I-1, L}\frac{1}{2}\left|\mu_{N-1, I, L}-\mu_{N-1, I-1, L}\right|\bigg] * \\
&* \frac{1}{2}\Big(v_N - v_{N-1}\Big) + g_{N, (IL+1)/2, L}\left|\mu_{N, (IL/2)+1, L}-\mu_{N, (IL+1)/2, L}\right| + g_{N-1, (IL+1)/2, L} * \\
&\left|\mu_{N-1, (IL/2)+1, L}-\mu_{N-1, (IL+1)/2, L}\right|\frac{1}{2}\,[v_N - v_{N-1}]\Bigg\}. \qquad \text{(C-72)}
\end{aligned}$$

However, the angular distribution at a fixed point cannot be determined in this manner, for one must sum over speed v, and if we vary N to accomplish this, μ will also vary. Therefore, the angular distribution must still be found through the use of the Jacobian and by integrating over the variables $K_\perp$ and L. See Appendix A for the details.

10. Convergence Procedures

To summarize the previous sections, we determine the potential in terms of the density difference between ions and electrons, and we determine the densities of ions and electrons in terms of the potential. Thus, an iterative procedure is required according to which we guess initially one of the quantities and compute the other, and then iterate. Although plasma problems, such as this one, are notorious for their instabilities, the integral formulation for all quantities to be determined does much to tame these problems.

Nevertheless, the mathematics, if correct, must reflect all of the physics inherent in the problem. Usually, the mathematics introduces additional special problems all of its own. We would expect then to see plasma oscillations, which involve the interplay of electrostatic fields and charged particles, if time dependence of the density distributions had been included in the problem, which it has not. Be this as it may, the iterative process introduces a kind of pseudo time dependence, not involving the masses of the particles. Thus, as a result of the iterative process we might expect to see oscillations in the iterations corresponding to plasma oscillations. Now, these oscillations occur at very high frequencies and with very short wavelengths. If we were to follow them with the computer, we would have to choose distance increments short compared with these wavelengths, and we would have to laboriously follow, again with short increments, these oscillations up and down in time. An enormous amount of computer time would be involved; further, these oscillations are of no particular interest. We are interested only in the static behavior of the system.

To side-step the problem of following all these oscillations, low-pass filtering is introduced. In fact, the results of both the Poisson and Boltzmann equations are so filtered. Now, filtering in the normal sense would consume a great amount of computer time, which we are hoping to economize. For this reason, we introduce the concept of filtering in the real domain instead of the conjugate domain.[16] Let us say we have a quantity f(s), where s is the iteration index that we wish to low-pass filter. This implies normally that the Fourier transform $F(\omega)$ of f(s) is computed:

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\ e^{-i\omega s}\ f(s), \qquad (C.\ 73)$$

and then the result $F(\omega)$ is multiplied by a function $G(\omega)$ corresponding to a low-pass filter, as shown in Figure II-3 . The output $f'(s)$ of the low-pass filter in the real domain will then be:

$$f'(s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega\ e^{i\omega s}\ F(\omega)\ G(\omega) \qquad (C.\ 74)$$

by the Fourier inversion theorem.

The same result can be achieved by operation in the real domain; there is no need to transform to the conjugate domain and transform back again to the real domain. This result follows from the Faltung theorem for Fourier transforms:

$$F(\omega)\ G(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds''\ e^{-i\omega s''} \int_{0}^{s''} ds'\ f(s')\ g(s - s'). \qquad (C.\ 75)$$

By the inversion theorem (C. 74) for Fourier transforms:

$$f'(s) = \int_{0}^{s} ds'\ f(s')\ g(s-s'). \qquad (C.76)$$

This result states that the low-pass filtered version $f'(s)$ of $f(s)$ is given by a kind of weighted average of past values $f(s')$ of $f(s)$ (acting as a source function), multiplied by the Green's function $g(s-s')$ (or impulse response, as it is called by some) of the low-pass filter. The Green's function can also be found from the Fourier inversion theorem (C. 74):

$$g(s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{i\omega s}\ G(\omega). \qquad (C.\ 77)$$

The trick then is to so choose $G(\omega)$ or $g(s)$ that the high frequency plasma oscillations are rejected by the filtering process, yet such that the low-frequency phenomena of interest are passed. Fortunately, we are only interested in truly static phenomena, so there is no real problem of choosing the filter.

A simple filtering scheme has proven very satisfactory for the present problem. For the potential $\phi(z)$, the following scheme was used:

$$\phi(z, N) = \sum_{s=1}^{N} \frac{\beta^{s-1}}{S_N} \phi(z, s) , \qquad (C.78)$$

where .

$$S_N = \sum_{s=1}^{N} \beta^{s-1} = \frac{(1-\beta^N)}{(1-\beta)} . \qquad (C.79)$$

(We are using the equality sign here in the sense in which it is always used with computers of "replaces," not "equals.")
Thus, the coefficients are a measure of the fraction to which a past iteration contributes to the present result. This scheme works very well indeed for N = 4 and $\beta = .75$.

For the filtering of the directional densities of the particles, a further development of the filtering process was used since it was impractical to store much past history of these densities in view of the huge amount of storage required to store these arrays for even the present values. With regard to the sums in Equation C. 78 we note the following:

$$\left[\left(\frac{1-\beta}{1-\beta^{N+1}}\right) \sum_{s=1}^{N+1} \beta^{s-1} n(z, E, K_\perp, L, s)\right] = \left(\frac{1-\beta}{1-\beta^{N+1}}\right) \beta^N n(z, E, K_\perp, L, N+1) +$$

$$+ \left(\frac{1-\beta^N}{1-\beta^{N+1}}\right) \left[\frac{1-\beta}{1-\beta^N} \sum_{s=1}^{N} \beta^{s-1} n(z, E, K_\perp, L, s)\right] . \qquad (C.80)$$

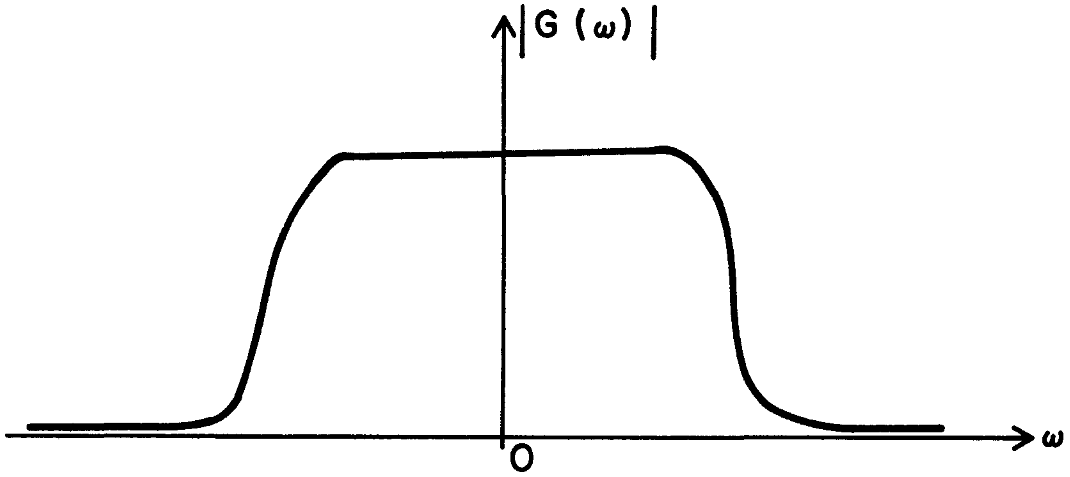


Figure II-3. Magnitude of Transfer Function of Low-Pass Filter.

In words, the new weighted average, which is in brackets on the left-hand side of the equation, can be computed from a suitable fractional multiple of the new density plus a suitable fractional multiple of the old weighted average, which the new weighted average upon calculation replaces, and, in turn, becomes the old weighted average for the next cycle. This method of weighting proved very effective. Here $\beta = .75$ and N, of course, kept going up with iterations, being, in fact, the iteration counter or index Thus, with this scheme one uses all past iterations in contrast to the previous one where one used only the past N iterations.

As a result of this filtering or averaging, convergence was never a problem Convergence is very rapid, usually occurring in just a few cycles, even with tight convergence criterion. Repeated iteration, after convergence has occurred, does not cause the solutions to change or move (In other words, the convergence is more than just apparent; it is real.)

The weighting coefficients for a few simple are listed in Table II-1

11 Results

The results may be briefly summarized before getting into the details. Plots of the potential and densities versus position will be presented momentarily. From these plots we find the following:

(1) The densities of electrons and ions are smaller near the collector than in the plasma.

(2) The densities of ions at the plasma-transition-region interface is approximately one-half that of the electrons, in keeping with the approximate result found by diffusion theory.

TABLE II-1

WEIGHTING COEFFICIENTS β^{s-1}/S_N

$\beta = .25$

n	β^0/S	β/S	β^2/S	β^3/S
1	1.000000 ...			
2	0.800000 ...	0.200000 ...		
3	0.76190476	0.19047619	.047619048	
4	0.75294118	0.1882353	.04705882	.01176471

$\beta = .50$

n	β^0/S	β/S	β^2/S	β^3/S
1	1.000000 ...			
2	.666666 ...	.333333 ...		
3	.57142857	.28571428	.14285714	
4	.533333 ...	.266666 ...	.133333 ...	.066666 ...

β / .75

n	β^0/S	β/S	β^2/S	β^3/S
1	1.000000 ...			
2	0.57142857	.42857143		
3	0.432432 ...	.324324 ...	.243243 ...	
4	0.36571428	.2742857	.20571428	.1542857

(3) Reflection of particles (electrons in the present case) at a potential barrier leads to discontinuities in the particle densities.

(4) These discontinuities are the smaller, the larger the number of speed groups used.

(5) Convergence was rapid with filtering. In a number of cases the convergence was ideal in that convergence could have not occurred with fewer iterations irrespective of the perfection of the method.

(6) The current for each species was not constant; i. e., particles were not conserved to the accuracy desired. This matter was not corrected by the time the project was terminated.

(7) In the case where the regions of integration were several scattering mean free paths thick, the presence of the plasma should have made itself manifest by the potential having zero slope. This phenomenon was not observed and the problem was not ferreted out by the time the project was terminated. It is believed that correction of the current inconstancy may very likely eliminate the problem with the potential.

(8) Convergence was more rapid with potential filtering than without.

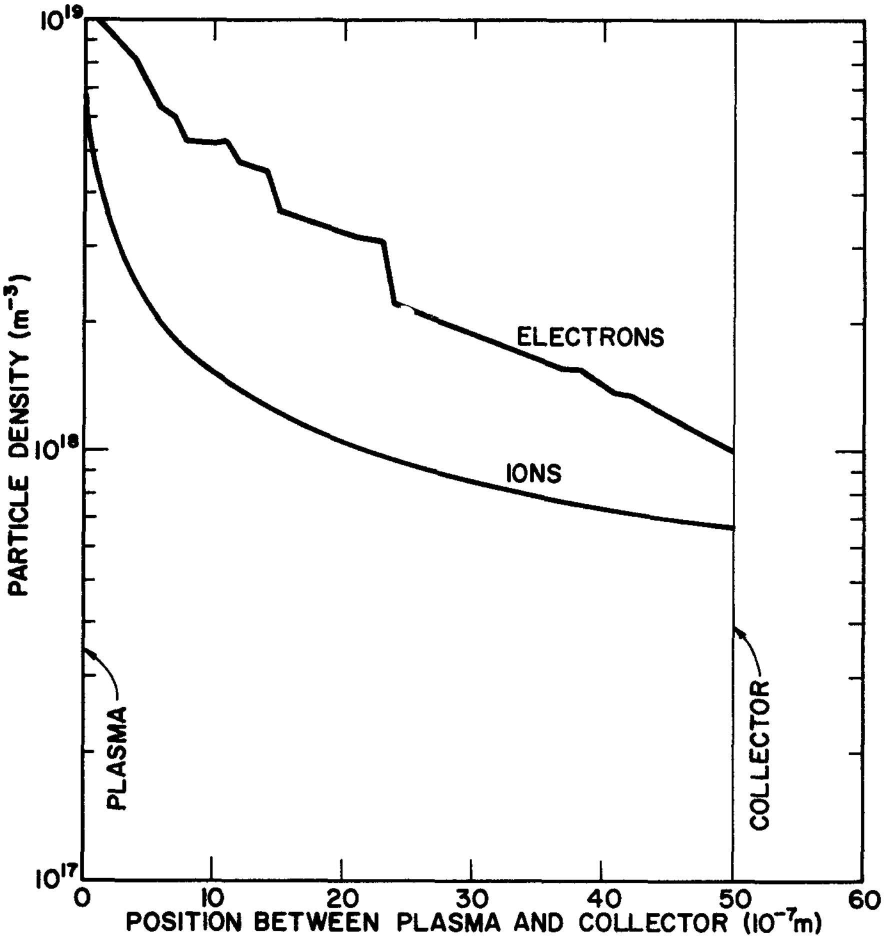
(9) The inner loop would converge without any filtering. The outer loop would just oscillate, even with potential filtering, in the absence of particle filtering. (Only a few outer loop iterations were ever followed, of course, since with filtering the convergence was so rapid.)

(10) Convergence of the inner loop is faster, the closer the outer loop is to convergence.

(11) More iterations are required with problems having scattering than without scattering.

(12) The heavier the scattering, the more iterations required.

In connection with checking out the program and correcting the errors, a great many runs were made of a program under more or less standard conditions. The standard conditions are illustrated by the example of the input data presented in connection with the program. With four speed groups, the electron and ion densities with filtering turned on are displayed on Figure II-4. The discontinuities in the electron densities correspond to points at which electrons belonging to a particular speed group were reflected by the potential barrier and returned to the plasma. These discontinuities can be seen even more clearly by observation of Figure II-5, which is a plot of the electron and ion densities with filtering turned off. There is a one-to-one correspondence between these discontinuities and the reflection points of electrons in respective speed groups, as can be proved by examining the directional density arrays for the electrons, not presented here. Ions are not reflected, and their density experiences no discontinuities as a result. The result of using eight speed groups, instead of four, is shown in Figures II-6 and II-7 for the filtered and unfiltered electron and ion densities. In each case, the problem was iterated to convergence, as shown in Figures II-8 and II-9, for four and eight speed groups, and then iterated once more with the filtering turned off. This had the effect of removing past history from the directional density arrays, thereby making it much easier to observe



Number of Speed Groups	4
Number of Angular Groups	4
Convergence Tolerance	± .02 volt
Plasma Density	$1.1 \times 10^{19}/m^3$
No Scattering	
Spacing	5 μm
Collector Temperature	910°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
Filter Factors	.75 (Potential) .75 (Particle)
Collector Work Function	1.711 volts

Figure II-4. Particle Density Versus Position.

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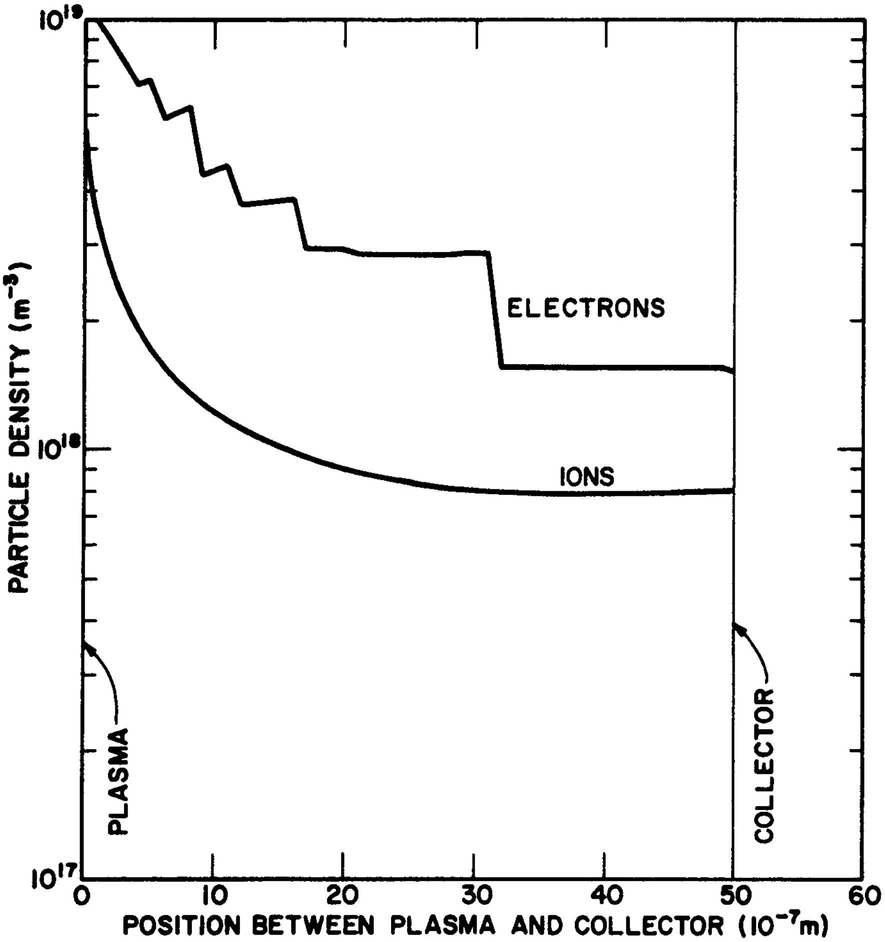
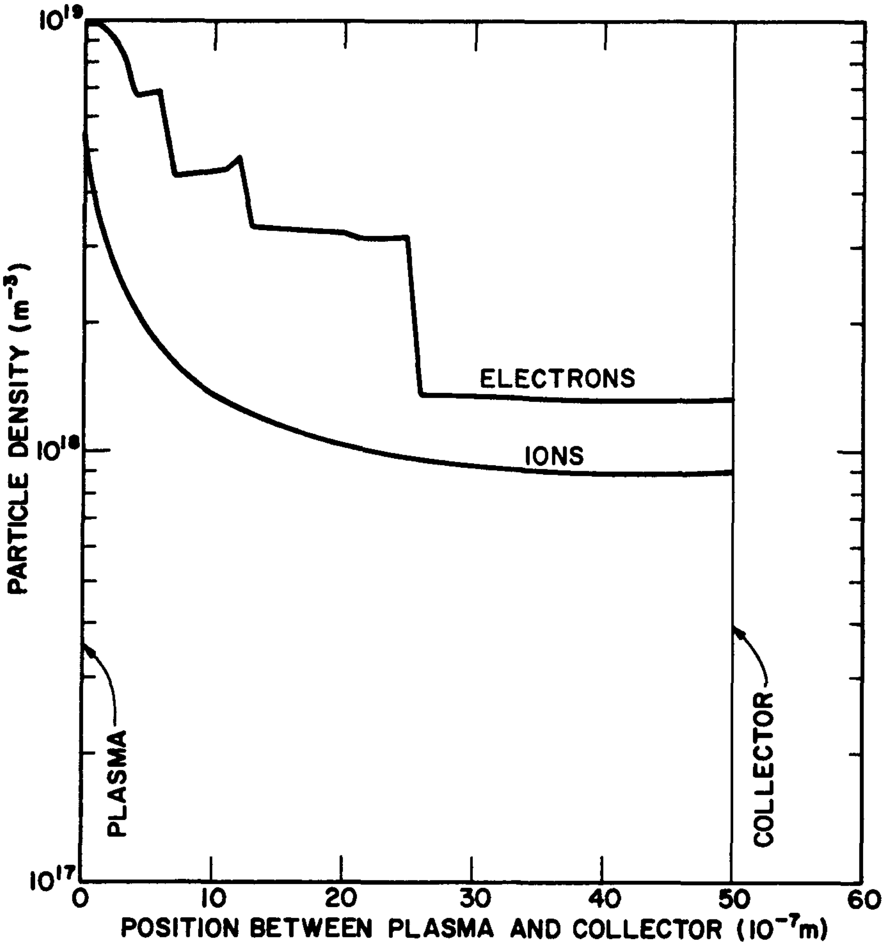


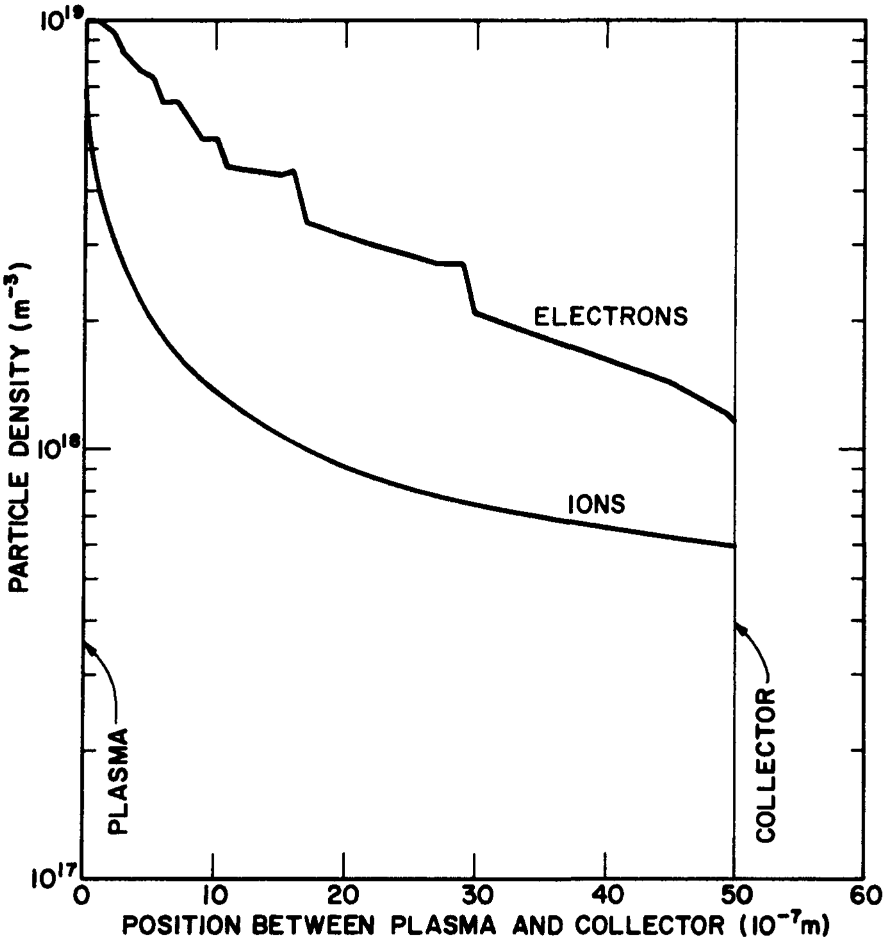
Number of Speed Groups	8
Number of Angular Groups	4
Convergence Tolerance	± .02 volt
Plasma Density	$1.1 \times 10^{+19}/m^3$
No Scattering	
Spacing	5 μm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
No filtering this iterate only	
Collector Work Function	1.711 volts

Figure II-5. Particle Density Versus Position.



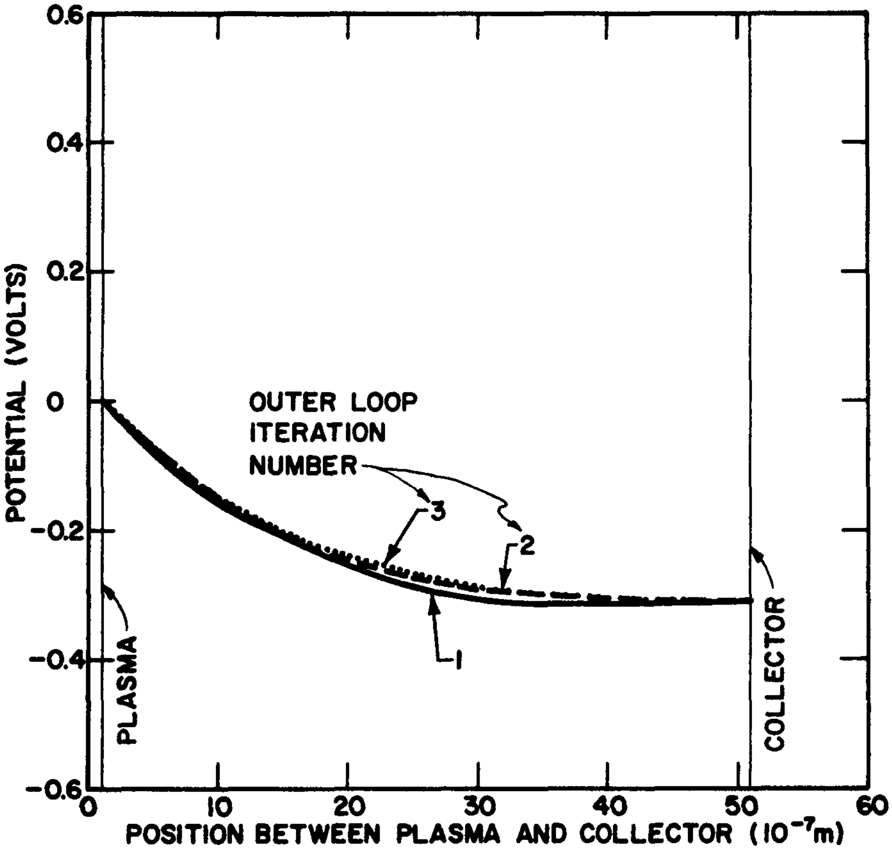
Number of Speed Groups	4
Number of Angular Groups	4
Convergence Tolerance	±.02 volt
Plasma Density	$1.1 \times 10^{19}/m^3$
No Scattering	
Spacing	5 μm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
No filtering this iterate only	
Collector Work Function	1.711 volts

Figure II-6. Particle Density Versus Position.



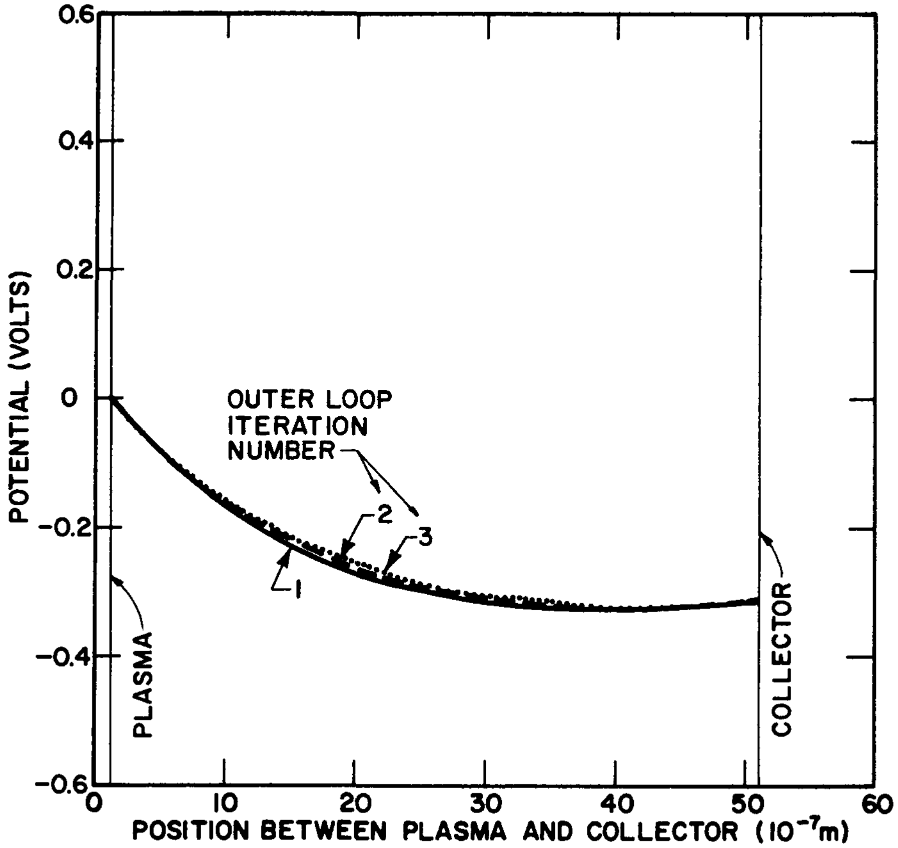
Number of Speed Groups	8
Number of Angular Groups	4
Convergence Tolerance	±.02 volt
Plasma Density	$1.1 \times 10^{19}/m^3$
No Scattering	
Spacing	5 μm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
Filter Factors	.75 (Potential) .75 (Particle)
Collector Work Function	1.711 volts

Figure II-7. Particle Density Versus Position.



Number of Speed Groups	4
Number of Angular Groups	4
Convergence Tolerance	±.02 volt
Plasma Density	$1.1 \times 10^{19}/m^3$
No Scattering	
Spacing	5 µm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415 K
Electron Temperature in Plasma	2300°K
Filter Factors	.75 (Potential) .75 (Particle)
Collector Work Function	1.711 volts

Figure II-8. Potential Versus Position.



Number of Speed Groups	8
Number of Angular Groups	4
Convergence Tolerance	± .02 volts
Plasma Density	1.1 x $10^{19}/m^3$
No Scattering	
Spacing	5 µm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
Filter Factors	.75 (Potential) .75 (Particle)
Collector Work Function	1.711 volts

Figure II-9. Potential Versus Position.

the constancy of the directional density in these collisionless cases.

Figures II-8 and II-9 are plots of the potential as a function of position. Since all printing was suppressed until the time for the run was nearly up, we can present only the results printed out. Rates of convergence for the inner and outer loops are displayed in Table II-2. (The upper limit had been set at 20 iterations of the inner loop.) Convergence of the inner loop was achieved in each case. These results are quite representative. Convergence in either loop is fast, and is faster in the inner loop, the closer the outer loop is to convergence. The convergence criterion was that the potential differ from its previous value by less than 0.02 volt at all points. Figure II-8 is a plot of the potential as a function of position for the first, second, and third iterates of the outer loop for four speed groups. Figure II-9 is a plot of the potential as a function of position for the first, second and third iterates of the outer loop for eight speed groups. The third iterate is an extra one with the filtering turned off. One can hardly expect any problem or method to converge faster than in the two iterations displayed in each case in Table II-2. The 0th iteration is the user's guess, which consisted of a linear function for the electron and ion directional densities between their respective values at the plasma-sheath interface and the corresponding values at the collector and which implies that the potential changes linearly between its value at the plasma-sheath interface and its value at the collector; the first iterate is the computer's calculation from the user's guess; the second iterate is needed to confirm the accuracy and validity of the first iterate.

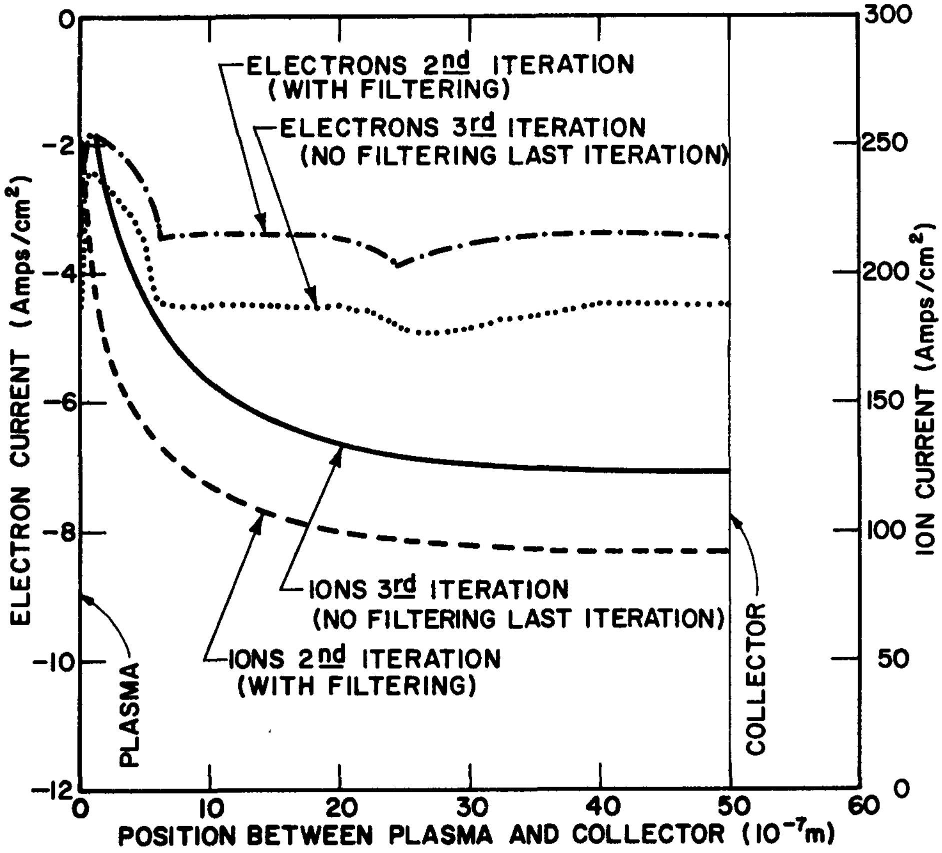
TABLE II-2

RATES OF CONVERGENCE UNDER VARIOUS CONDITIONS

Number of Speed Groups	Outer Loop Iterate	Number of Iterations of Inner Loop	Number of Iterations of Outer Loop	Comment
4	0	4	2	
	1	2		
	2	1		
	3	1		Extra iteration after convergence with filtering turned off
8	0	4	2	
	1	2		
	2	1		
	3	1		Extra iteration after convergence with filtering turned off

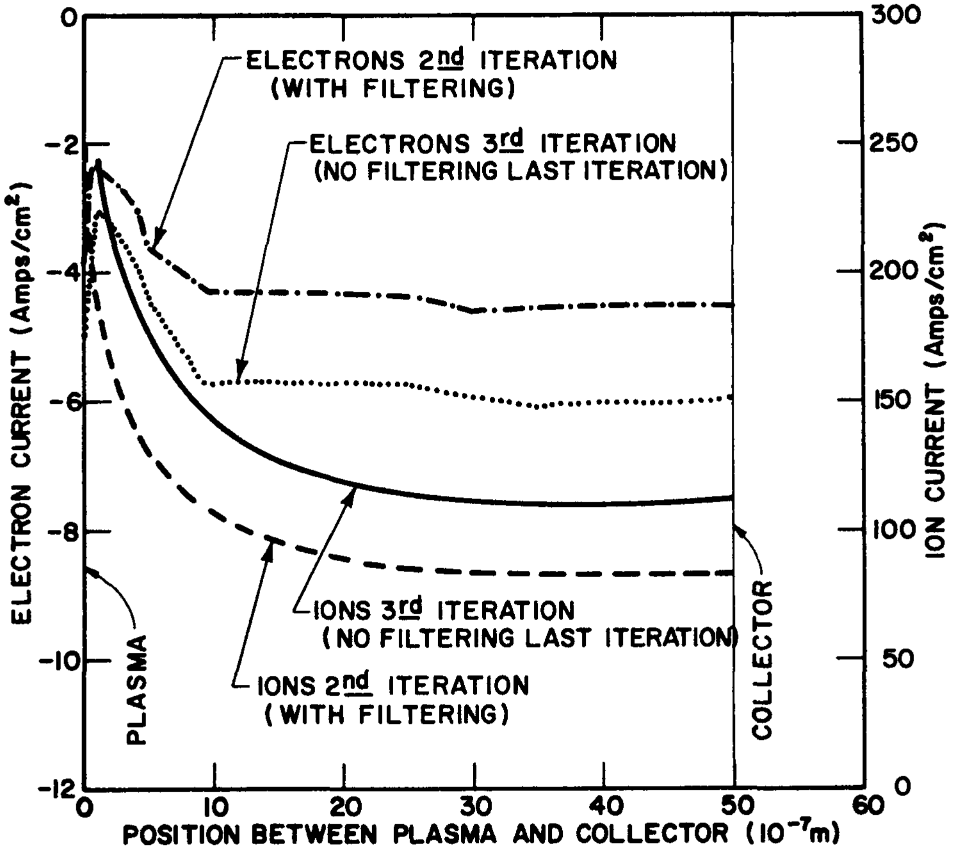
Figures II-10 and II-11 are plots of the electron and ion currents as a function of position for the 4 and 8 speed group case, respectively. These results are disturbing: each current should be constant in the absence of any net production or absorption of particles, as must be the case in the absence of collisions.[17] If the current is not constant in the collisionless case, then particles are not being conserved. Since our current is changing by a factor of about 2, either there must be some mistake in the current calculation or particles are not being conserved. Because the directional density is rigorously constant in the collisionless case (with the filtering turned off, of course, since the filtering averages over past history), we believe that particles are conserved, but that the calculation of the current is somehow in error. We did not have time to check into this question at the time the project was terminated. It is seen that the current jumps upon turning off the filtering, whereas the potential, which is an extremely sensitive function of the net difference between positive and negative charges, changes hardly at all, again providing further evidence that there is something peculiar in the calculation of the current. Of course, the current will be somewhat sensitive to changes in the directional density in that it involves the difference in the directional density in different directions.

We have run a large number of other cases before the program got to its present status, and we now briefly summarize our experience with these other cases: More iterations were required with problems involving scattering, especially heavy scattering. Turning off potential filtering slowed convergence. Turning off particle filtering caused the potential to oscillate; at the end of six iterations of the outer loop, no convergence was in sight, even with potential filtering present.



Number of Speed Groups	4
Number of Angular Groups	4
Convergence Tolerance	±.02 volt
Plasma Density	1.1 x $10^{19}/m^3$
No Scattering	
Spacing	5 µm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
Filter Factor	.75 (Potential) .75 (Particles)
Collector Work Function	1.711 volts

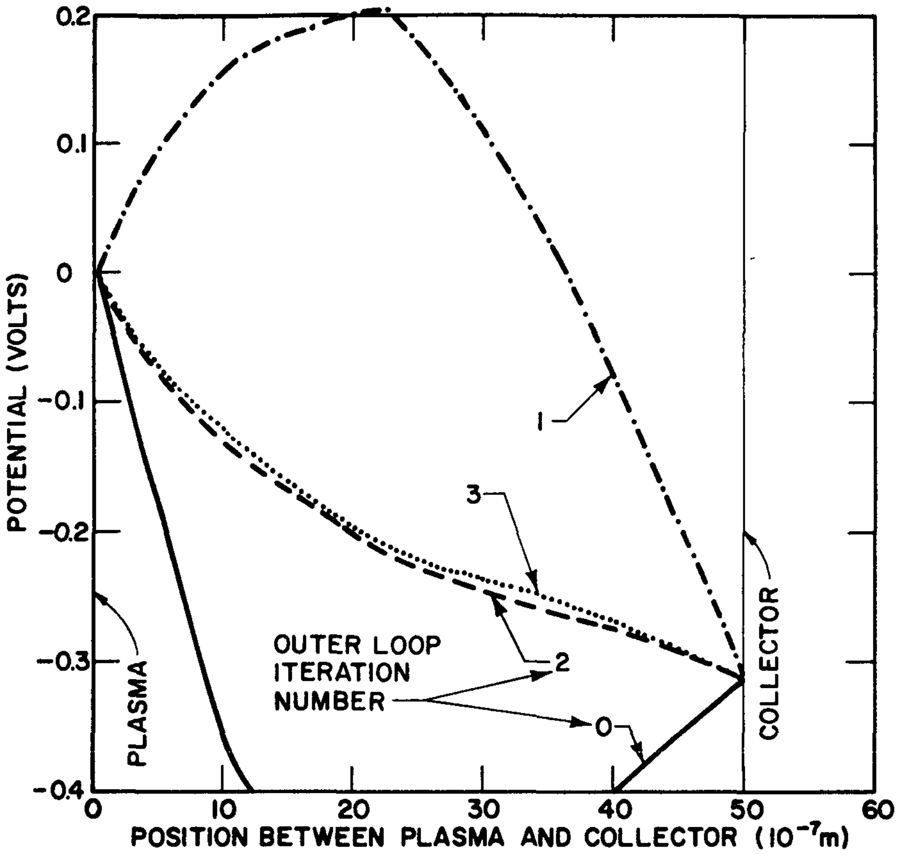
Figure II-10. Electron and Ion Currents Versus Position.



Number of Speed Groups	8
Number of Angular Groups	4
Convergence Tolerance	±.02 volt
Plasma Density	1.1 x $10^{19}/m^3$
No Scattering	
Spacing	5 µm
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
Filter Factor	.75 (Potential) .75 (Particles)
Collector Work Function	1.711 volts

Figure II-11. Electron and Ion Currents Versus Position.

With a mixture of integration methods, i. e., with some integrals done using the variables z, v, and μ, and no Jacobian, the inner loop would converge by itself, but the outer loop would just oscillate using no filtering of any sort. Even with all integrals done using the variables, z, E, $K_\perp$, and L, and the Jacobian, convergence for the outer loop of the sort shown in Figure II-12 was obtained. Because of the nonmanifest convergence of the integrals involved (the Jacobian has both a simple pole and a branch point of order 1/2 for singularities), the particle densities behaved poorly: At each point of reflection, the density would have a sharp maximum because of the singularities in the Jacobian, which define the points of reflection. However, in this case the inner loops converged poorly, requiring many more iterations for convergence than was found above with the method that did all integrals in terms of the variables z, v and μ. Nevertheless, convergence was obtained With all the integrals done in terms of the variables, z, E, $K_\perp$, and L, convergence could not be obtained without filtering. The singularities of the Jacobian seemed to be just too much; filtering provided a means for smoothing out these singularities so that the problem had a chance to converge. The problem with no filtering is that a particle of given energy is either reflected or it is not. If it is reflected, then the density of particles of this energy suddenly goes to zero in the inaccessible region. While this circumstance is true in reality, it is also true in reality that there are many more energy groups of particles than just the four usually in most of our runs for reasons of machine time and memory requirements. Actually, the particle densities change continuously with energy, instead of being bunched into energy groups, so that there is a continuous distribution of rejected particles and consequently a



Number of Speed Groups	4
Number of Angular Groups	4
Convergence Tolerance	10% of most recent value
Plasma Density	1.1 x $10^{19}/m^3$
Maximum Total Energy	2.7 volts
Minimum Total Energy	.1 volt
No Scattering	
Spacing	5μ
Collector Temperature	910°K
Reservoir Temperature	614°K
Gas Temperature	1415°K
Electron Temperature in Plasma	2300°K
Filter Factor	.75 (Potential) .75 (Particles)
Collector Work Function	1.711 volts

Figure II-12. Potential Versus Position.

continuous density change with distance, instead of the discontinuous changes modeled here. Filtering helped to smooth out these distribution functions by introducing enough history into the particle density that the potential and particle density no longer oscillate from iteration to iteration in a futile attempt to adjust to each other.

The problems involving heavy scattering did not show evidence of a plasma being established, i. e., of the potential having zero slope at the plasma end of the region of integration. We believe this difficulty may very well be connected with the problem involving nonconservation of particles mentioned above.

12. Future Work

Future work could extend the realm of applicability of the present method substantially:

(1) Ionization and recombination might be introduced into the program so that the entire interelectrode space could be treated by the method, instead of merely the transition region near the collector.

(2) Actual scattering laws could be introduced, thereby removing the assumption of isotropy. It is known, for example, that Rutherford scattering varies as $\csc(\theta/2)$,[4] where θ is the scattering angle. This phenomenon would be of primary importance in the transition region.

Several variants of the mathematical method might also be examined more closely:

(1) The use of higher order (Adams) integration formulas than trapezoidal or Simpson's rules should be studied to determine if any advantages result from their use. One may gain more accuracy for a given number of mesh points in E or $K_{\perp}$. If so, one could reduce the size of the directional density arrays $n(z, E, K_{\perp}, L)$, which now consume large amounts of fast memory, even with only a few speed groups and directional groups.

(2) The densities and/or potential could be approximated by functions having arbitrary parameters in them. These functions could then be inserted into the integral relations for the densities and/or potentials. The parameters could then be adjusted numerically until the error of the solution was minimized. The error of a solution might be taken as the magnitude of the difference between the right- and left-hand sides of an equation. The functions could be taken of such a form, for example, that they satisfied all the physical requirements that one knows ahead of time have to be satisfied by the solution. The function representing the potential might be of such a form that at the plasma-sheath interface it always has zero slope in problems where scattering is present, for example. Again, the densities might be represented with a reasonably simple functional form in the sheath region, rather than merely with a graph or set of numbers. The method has the disadvantage that the accuracy of the results is limited, but great accuracy in problems of this sort is of little value anyway. Further, by choosing functions with more and more

parameters in them, it would be possible to fit the solution as accurately as desired. Of course, the goal is to achieve the desired accuracy with as few parameters as possible.

D. OTHER METHODS

1. General

The analyses described below consider the sheath region with increasing levels of complexity. Starting with the usual collisionless sheath approximation, integration of this assumption through the sheath shows there is no solution which satisfies all the boundary conditions. The next step of working from the physical phenomena likely in the sheath preserves a good understanding of the relative importance of the processes involved in the different portions of the sheath. The resulting analysis resembles diffusion theory. However, when numerical integration is attempted, the analysis becomes unreasonable due to the instabilities encountered. The more direct approach of the S_n method, which treats the sheath as a whole, likewise has instabilities. A study of these instabilities showed that they are intrinsic to the differencing scheme used in the S_n method when applied to charged particles moving in an electric field. Investigation of other differencing arrangements developed a method likely to converge under the sheath conditions. This method was not pursued numerically because of the progress made with the integral method described earlier in this report.

2. Collisionless Sheath

Wang, Lieb, and Pigford have treated the problem of the collisionless sheath in which the electrons and ions are constrained to move along the z-axis.[1] Space charge effects were taken into account by use of Poisson's equation; electrons and ions are introduced at the emitter and the plasma boundaries of the sheath as half maxwellian distributions. Vlasov's equation for one dimension with particles constrained to move along the z-axis was used to describe the conservation of particles in phase space.

The distribution function is as follows for the various cases listed:

a. Retarding field: See Figure II-13.

(1) Forward-going particles

$$n(z, v) = n_0 \exp - [|e(\phi-\phi_0)|/kT] \exp - (mv^2/2kT). \tag{D. 1}$$

(2) Backward-going particles

$$n(z, v) = \begin{cases} 0, \text{ if } \frac{mv^2}{2} + e(\phi-\phi_0) > e\,\phi_{max}, & \text{(D. 2)} \\ n_0 \exp - [|e(\phi-\phi_0)|/kT] \exp - (mv^2/2kT), \text{ if } \frac{mv^2}{2} + e(\phi-\phi_0) < e\,\phi_{max}. & \text{(D. 3)} \end{cases}$$

b. Accelerating field: See Figure II-14

(1) Forward-going particles

$$n(z, v) = \begin{cases} 0, \text{ if } \frac{mv^2}{2} < e(\phi - \phi_0), & \text{(D. 4)} \\ n_0 \exp [|e(\phi-\phi_0)|/kT] \exp - (mv^2/2kT), \text{ if } \frac{mv^2}{2} > e(\phi-\phi_o). & \text{(D. 5)} \end{cases}$$

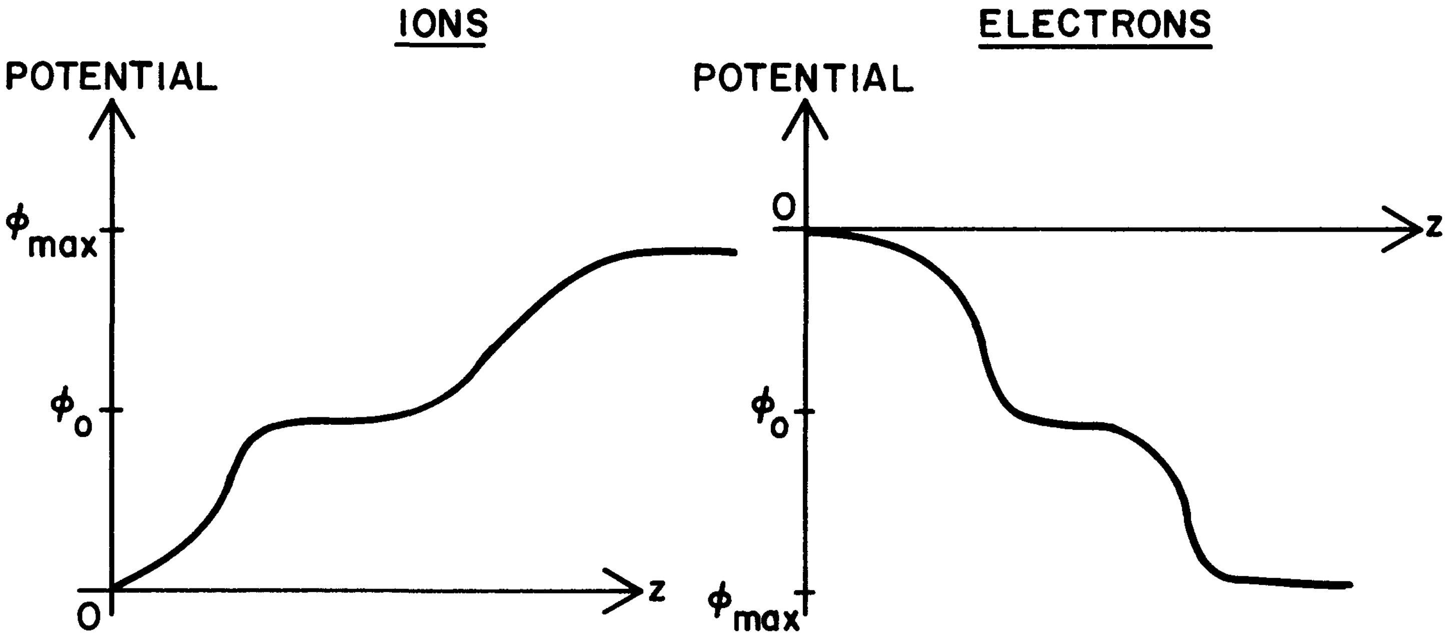


Figure II-13. Potential as a Function of Position for Retarding Fields.

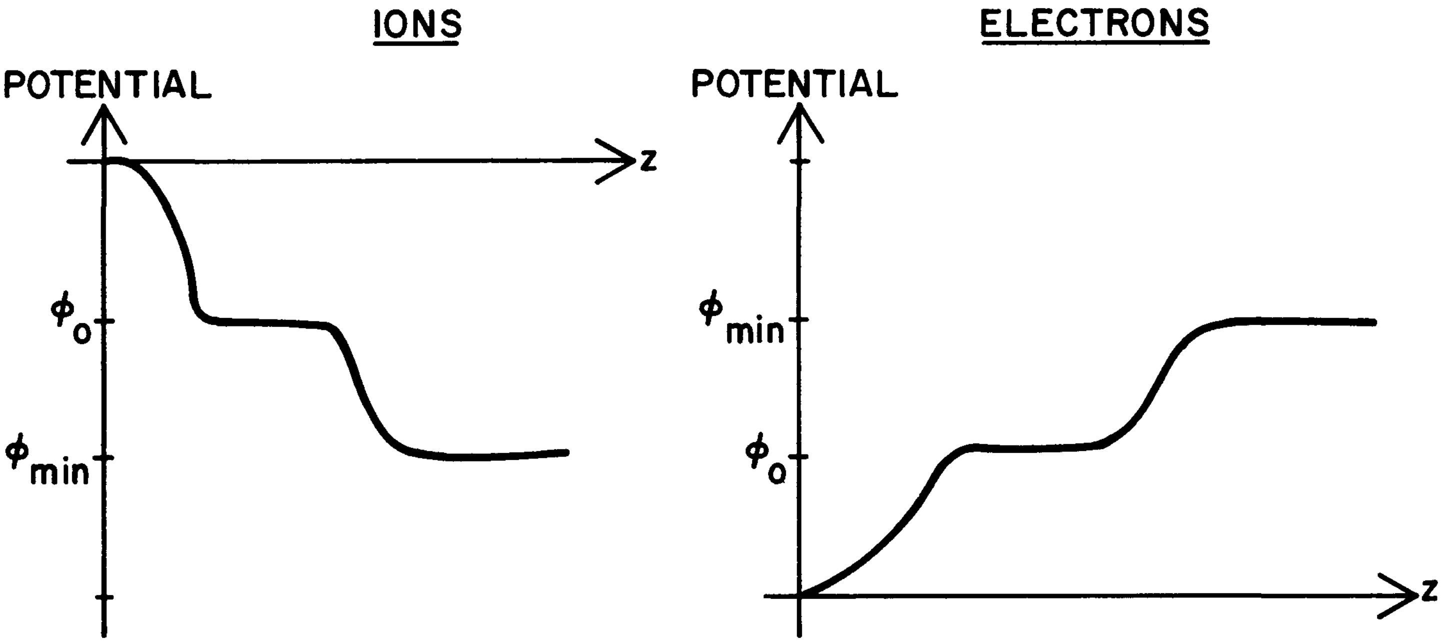


Figure II-14. Potential as a Function of Position for Accelerating Fields.

The results of Wang, Lieb, and Pigford may then be found from the definitions

$$\xi = z/\lambda_D, \tag{D. 6}$$

$$\psi = e\phi/kT_E \tag{D. 7}$$

$$n_\alpha^\pm = \int_{-\infty}^{\infty} dv\; f_\alpha^\pm(\psi, v)/N_e(0), \tag{D. 8}$$

where λ_D is the Debye length calculated at the electron density at the electrode of temperature T_E, and from the revised form of the reduced Poisson equation:

$$\frac{d^2\psi}{d\xi^2} = 1/2 \left[n_e^{(+)}(\psi) - n_i^{(+)}(\psi) + n_e^{(-)}(\psi) - n_i^{(-)}(\psi) \right] . \tag{D. 9}$$

Here, $n_\alpha^+(\psi)$ is the density of particles of type α moving in the positive direction at point $\psi(z)$, and $n_\alpha^-(\psi)$ is the density of particles of type α moving in the negative direction at point $\psi(z)$. The definitions

$$L(\psi) = \exp(\psi)\ \text{erf}\sqrt{\psi} - 2\sqrt{\psi/\pi}, \tag{D. 10}$$

$$M(\psi) = \exp(\psi)\ (1 - \text{erf}\sqrt{\psi}) + 2\sqrt{\psi/\pi}, \tag{D. 11}$$

$$N(\psi) = \exp(\psi)\ (1 + \text{erf}\sqrt{\psi}) - 2\sqrt{\psi/2}), \tag{D. 12}$$

were used by these authors, and their last equation (Eq. D. 4) is correctly given by

$$\begin{aligned}\left(\frac{d\psi}{d\xi}\right)^2 = {} & \exp\left(\psi_{\min}\right)\left[M(\psi-\psi_{\min}) - 1\right] + \frac{N_i(o)}{N_e(o)}\left[\exp -(\psi_p)\left\{N(\psi_p-\psi)\right.\right. \\ & \left.\left. - N(\psi_p-\psi_{\min})\right\} + 2\,L(-\psi_{\min})\right] + \frac{N_e(p)}{N_e(o)}\,\frac{1}{C_1}\exp\left[C_1\,(\psi_{\min}-\psi_p)\right] \\ & \left[N\left\{C_1\,(\psi-\psi_{\min})\right\} - 1\right] + \frac{N_i(p)}{N_e(p)}\,\frac{1}{C_2}\left[M\left\{C_2\,(\psi_p-\psi)\right\} + \right. \\ & \left. - M\left\{C_2\,(\psi_p-\psi_{\min})\right\}\right], \quad \psi \geqq 0 . \qquad \text{(D. 13)}\end{aligned}$$

The subscript p or argument p denotes that the associated quantity is evaluated in the plasma.

$$C_1 = T_E/T_{pe} , \qquad \text{(D. 14)}$$

$$C_2 = T_E/T_{pi} . \qquad \text{(D. 15)}$$

In the method of Wang, Lieb, and Pigford,[1] the charged particles from the emitter are assumed to isotropically distributed over a hemisphere and to have a Maxwell speed distribution. An exact form of the solutions of the Boltzmann equations is easily found, and a first integral can be found analytically for Poisson's equation. The second integral must be found by numerical integration. The integration constant that results can be determined only by a boundary condition.

The plasma region has been treated by numerous authors[2-5] by the diffusion equations for electrons and ions. The nearly isotropic distribution of the plasma region must then somehow be joined to the anisotropic distribution of the sheath region. The problem here is that if one requires continuity of the charge density, the potential, and the electric intensity, no solution at all can be found. If only one or two of these quantities are continuous, then a multitude of solutions exist, and the solution is nonunique.

Now, a plasma is generally positive with respect to the electrodes. Consequently, electrons in the plasma are reflected for the most part by the positive sheath potential back into the plasma, whereas ions are expedited out of the plasma by the positive sheath potential. If n is the density of electrons or ions in the plasma, n/2 of the ions are headed out of the plasma and never come back. This is the number of ions injected into the program at the interface. The emission of ions from the emitter is neglected. In contrast, of the n/2 electrons headed into the sheath (and injected into the program), nearly all come back Thus, near the interface between the sheath and the plasma, the density of electrons is nearly n, half going one way and half going the other way; the density of ions is only n/2 because none of those leaving return. There is, therefore, a net charge of n/2 at this interface and a concomitant source of electrical fields.

Next, let us consider the boundary condition on the potential. We know the collisionless solution must be valid up to the order of at least λ_{in} away from the emitter. Indeed, we can think of the solutions for the collisionless region extrapolating to a distance beyond λ_{in} before the collisionless solution meets the plasma potential. The positive and negative charge densities and the potential energy of electrons as a function of distance for a typical case are shown in Figure II-15, where it has been assumed that there is zero electric

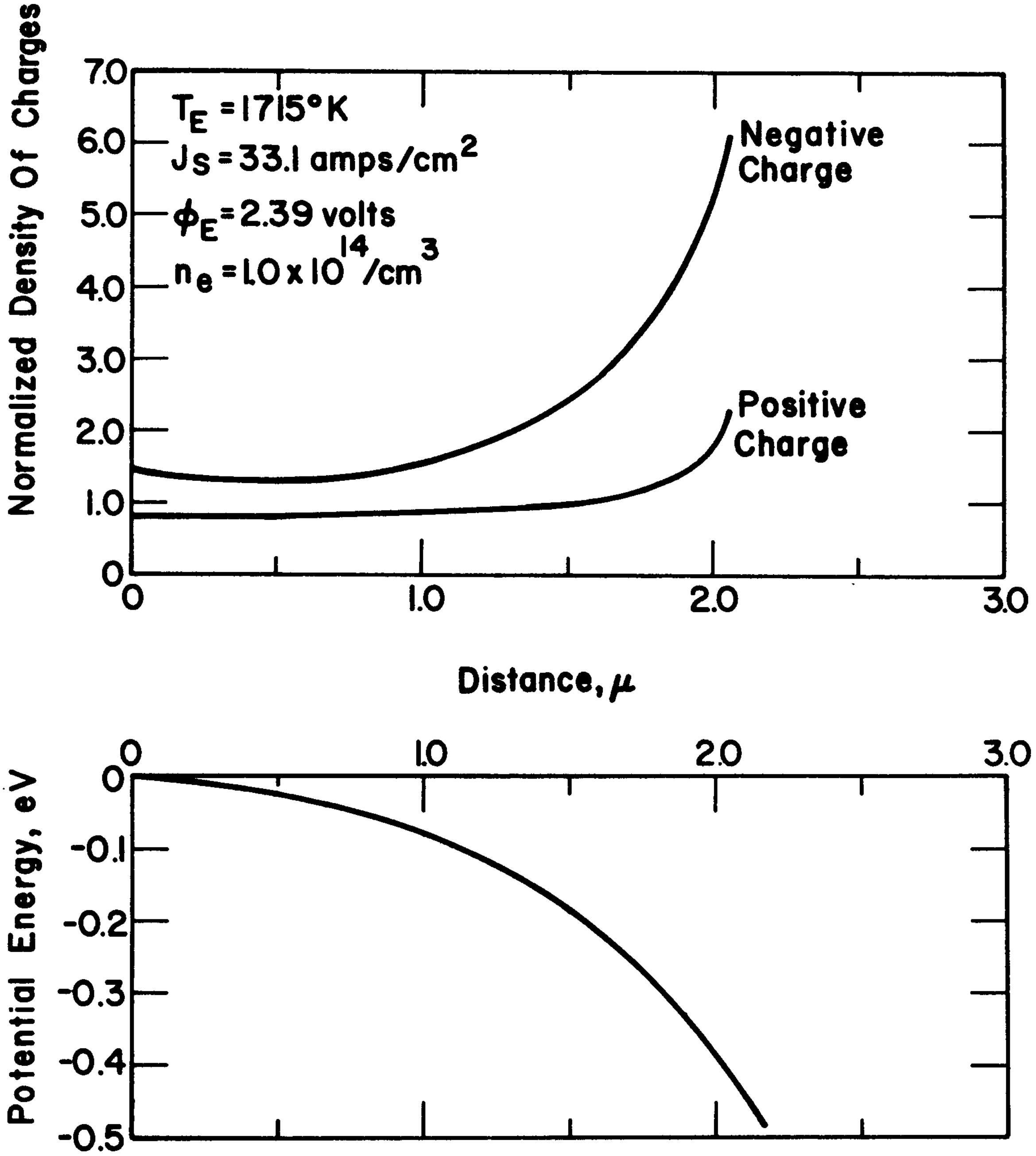


Figure II-15. Positive Charge Density, Negative Charge Density, and Motive of Electrons in Collisionless Region as a Function of Distance Away from the Emitter Assuming Zero Electric Intensity at the Emitter.

field at the emitter. The plasma conditions were adapted from results of Wilkins and McCandless[2] for one of their cases. Under our present criterion, a solution is valid if and only if the computed potential equals the plasma potential at a distance λ_{in} away from the emitter. In the present case, the solution is not valid because the potential energy of an electron in the collisionless region becomes equal to that of an electron in the plasma at a distance closer to the emitter than λ_{in}. At such short distances, charges, on the average, will not have experienced a collision, and diffusion processes, which are characteristic of a plasma, cannot be said to have begun. A more negative slope near the emitter of the potential energy would have put the equality point even closer to the emitter. A more positive slope would imply a maximum of the potential energy of the electrons in the collisionless region, as shown in Figure II-16. This figure displays the positive and negative charge densities, and the potential energy of electrons as a function of distance. The solution obtained is valid under the present criteria, for the potential energy of an electron becomes equal to that of an electron in the plasma at the distance λ_{in} away from the emitter. It is observed that the slope of the potential energy is positive at the emitter and that a maximum of the potential energy function occurs.

Despite the assumption by Wilkins and McCandless of monotonic sheaths for all the cases they treated, it is possible to apply their results to situations where sheaths possess a potential minimum by imagining a virtual emitter with the properties of their emitter for the corresponding case. The potential of the plasma was found by requiring that our electron current density, the random electron

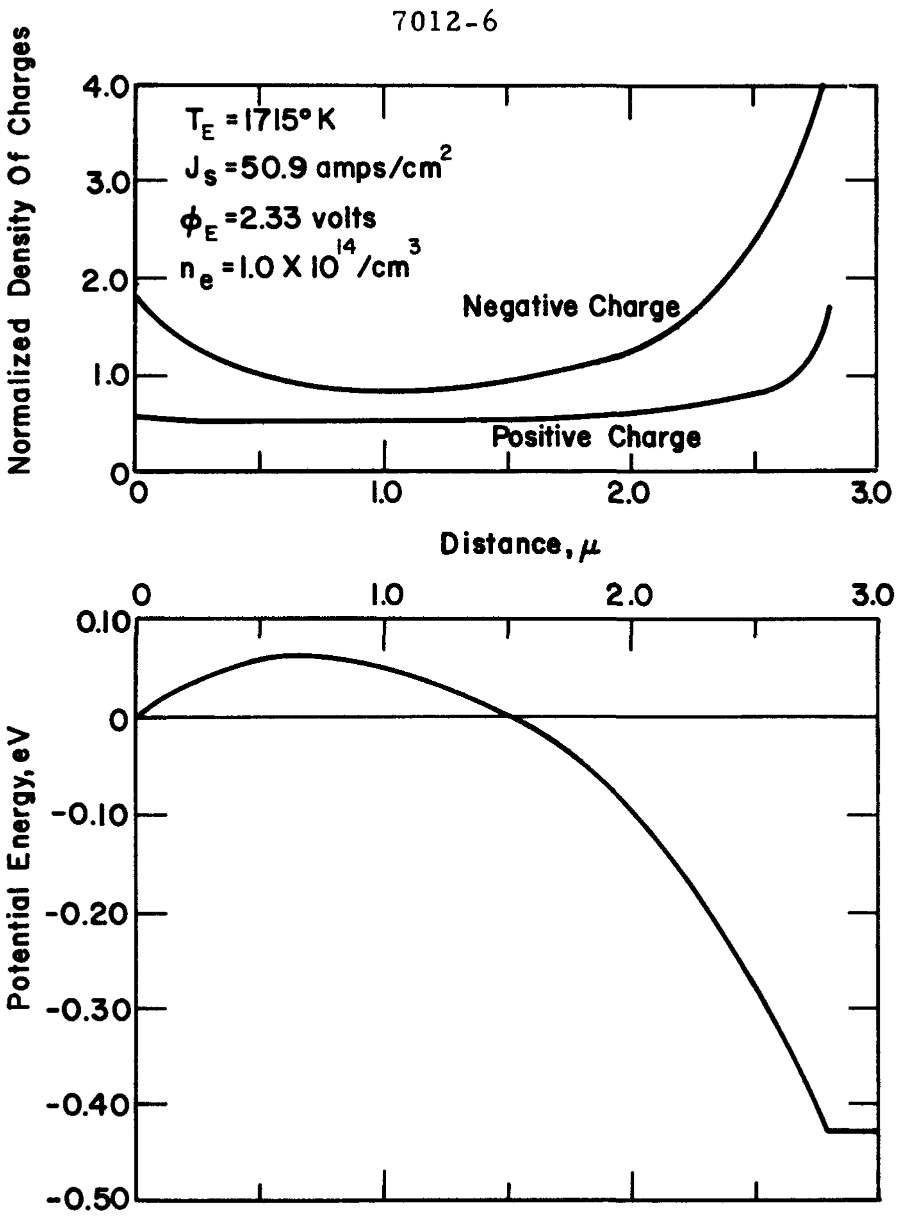


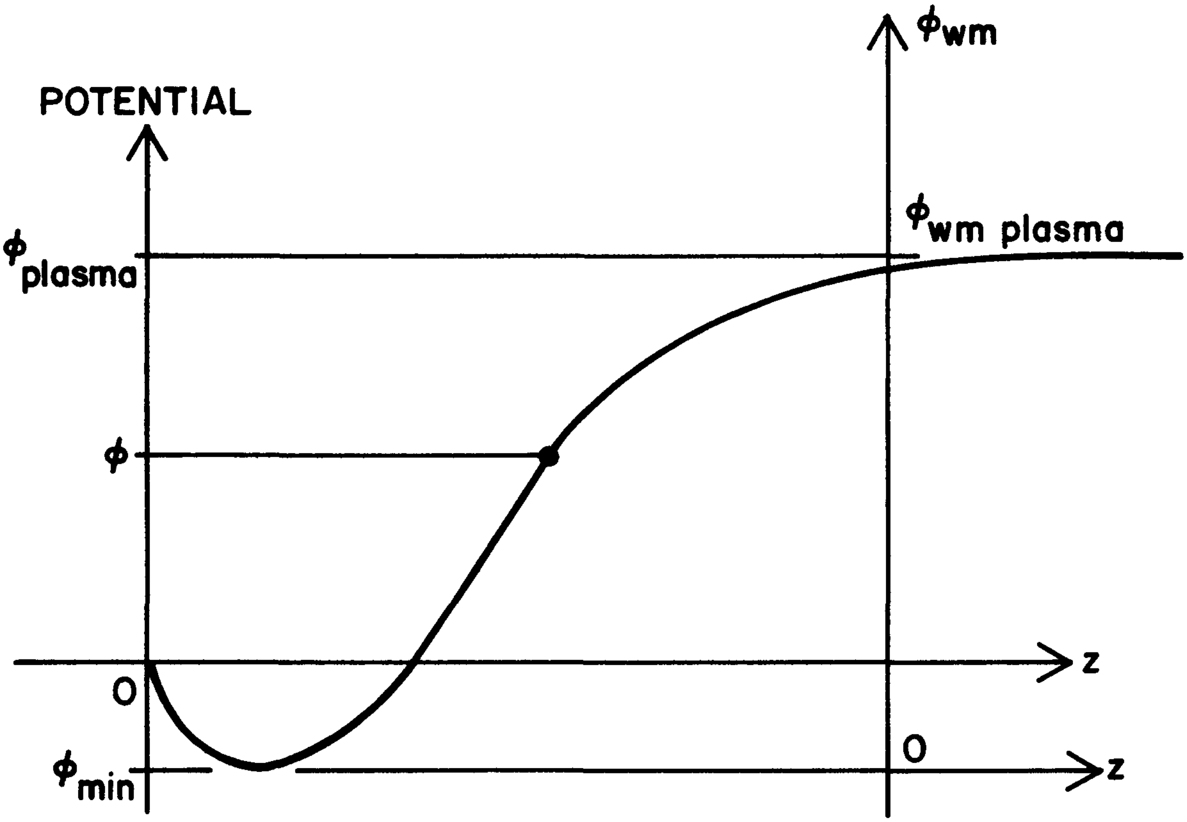
Figure II-16. Positive Charge Density, Negative Charge Density, and Motive of Electrons in Collisionless Region as a Function of Distance Away from the Emitter when the Motives of the Electrons in the Collisionless and Plasma Regions are Equal at One Ion-Neutral Mean Free Path Away from the Emitter.

current density, and the saturation current density be the same as those of a corresponding case of theirs at the plasma-sheath interface. Thus, the saturation currents are related by

$$J_{e\,E\,sat} = J_{e\,sat,\ monotonic}\, \exp + \left| \phi_{min}/k\,T_E \right| \ .$$

Their values for the Schottky correction and the work function were used also The work function and the potential of the plasma used in our calculation was then related to the corresponding quantities used by them, as shown in Figure II-17.

It is impossible to avoid a minimum of the potential for this case. If a longer collision distance is assumed, then the minimum potential required for a solution will be even deeper. Therefore, if a minimum of the potential is to be avoided, the distance at which collisions occur must be made shorter. But we have already picked the shortest collision distance that occurs in the problem as the point at which the potential of an electron is to equal the potential of an electron in the plasma. For the electrons we probably should have picked λ_{en} as the distance at which the potential of the electrons in the collisionless region equals the potential in the plasma. Again, the true solution will smoothly joint the potential function of the plasma, a matter that will somewhat round the corner in the present very approximate theory. To the first order, the effect of such smoothing is represented by the extrapolated boundary. It is readily seen that the extrapolated boundary is further from the emitter than the boundary chosen; therefore, rounding will not diminish the distance at which the collisionless theory stops and diffusion theory begins. In the just limiting case for the present problem, where a potential minimum just fails to occur, the crossing occurs at 2.2 μ, whereas $\lambda_{in} = 2.8\ \mu$.



$$\phi_{wm} = \phi - \phi_{min}$$

$$\phi_{wm\ plasma} = \phi_{plasma} - \phi_{min}$$

Figure II-17. Relationship of Potential in the Plasma and the Work Function Used in Our Calculations to the Potential in the Plasma and the Work Function Used for Monotonic Sheath Calculations.

It is obvious that a negative charge density is a necessary but insufficient condition for the existence of a minimum of the potential. A sufficient condition for the existence of a minimum of the potential requires that the necessary condition be supplemented by some other conditions, such as the distance from the emitter at which the solutions for the collisionless and plasma regions join.

The existence of a minimum in the potential implies that not all electrons originating from the emitter will get to the plasma. Since it is necessary to know the fraction of electrons getting to the plasma in order to perform plasma calculations, it appears necessary to compute the potential function in the collisionless and transition regions.

Again, the electric intensity computed from the potential across the collisionless region and the Debye length in the plasma is 11,400 volts/cm, and from the Debye length at the emitter is 7, 400 volts/cm. The electric field computed from the collisionless theory is 1, 540 volts/cm. Thus, because the collisionless region appears to be substantially wider than a Debye length, the electric intensity at the emitter is lower than that computed from either Debye length.

Figure II-18 displays the density of positive and negative charges, and the potential for a higher temperature case. A solution can be obtained in which the potential of an electron in the collisionless region is equal to that in the plasma without using a minimum in the potential. The reversal of the sign of the net charge density is interesting. The electric intensity computed from the potential across the collisionless region and the Debye length in the plasma is 47, 000 volts/cm, and from the Debye length at the emitter is 12, 000 volts/cm.

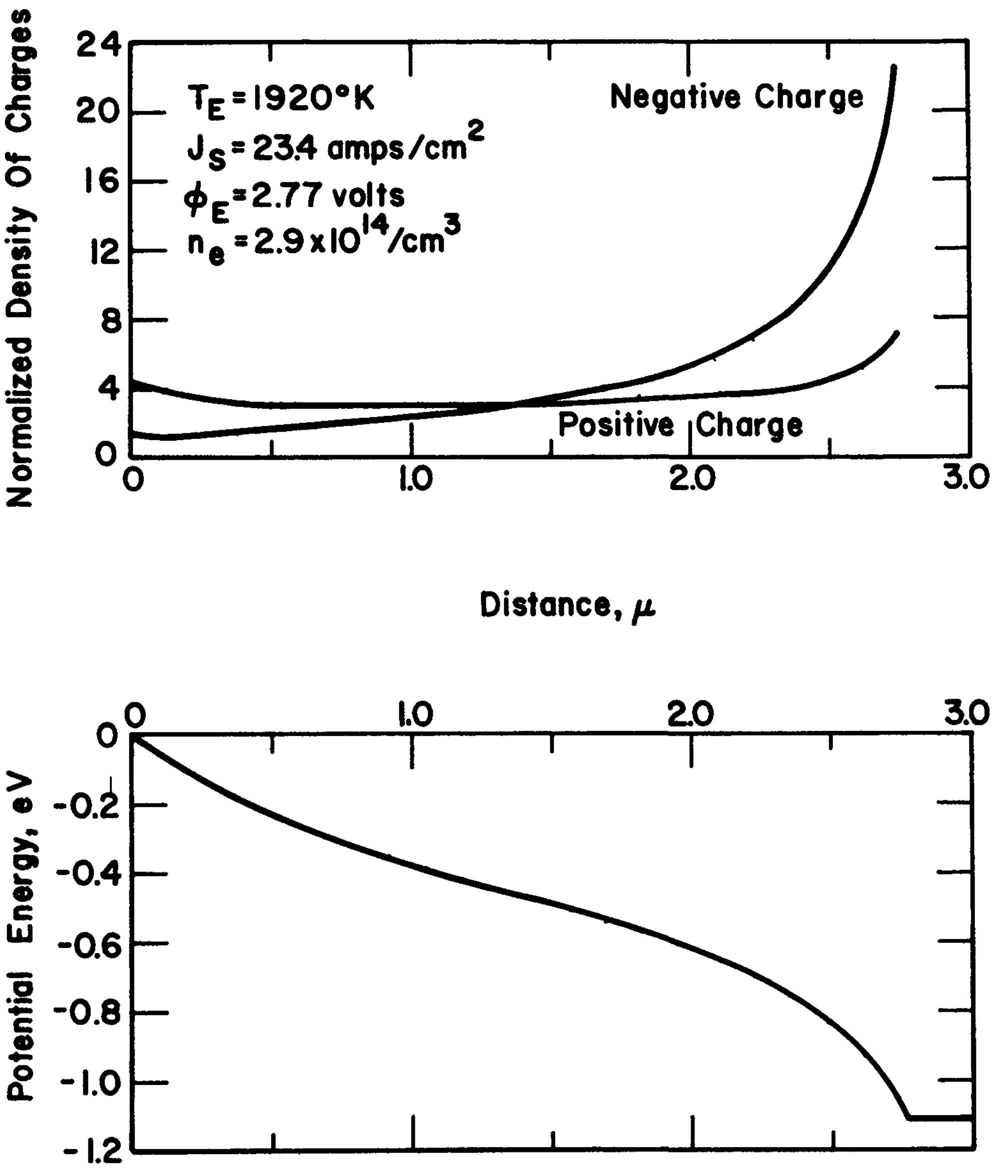


Figure II-18. Positive Charge Density, Negative Charge Density, and Motive of Electrons in Collisionless Region as a Function of Distance Away from the Emitter when the Motives of the Electrons in the Collisionless and Plasma Regions are Equal at One Ion-Neutral Mean Free Path Away from the Emitter.

The electric intensity computed from the collisionless theory is 4,100 volts/cm. Again, because the collisionless region appears to be substantially wider than the Debye length, the electric intensity at the emitter is rather lower than that computed from the Debye length. Thus, even in the case of the monotonic accelerating sheath, the present result reduces the magnitude of the correction to the work function resulting from the Schottky effect and will, thus, reduce the saturation current somewhat.

It is very interesting to note the decidedly constant behavior of the ion density as a function of distance away from the electrode in all the cases presented here, as well as many others computed, but not presented.

3. Diffusion Theory Approach to a Thermionic Energy Converter

In a thermionic diode, the interelectrode gas is only slightly ionized. The temperature and density of the neutral cesium atoms are determined quite independently of the temperatures and densities of the ions and electrons.

The masses of the ions and neutral atoms are very nearly equal. For this reason, several consequences follow: First, the temperature of the ions will be nearly equal to that of the neutral atoms. Second, the ion distributions can become maxwellian isotropic by collisions with neutrals or with themselves.

Several conclusions follow from the fact that the electrons are very much less massive than the neutrals or ions. First, the temperature distribution of the electrons will be entirely independent of that of the ions or neutral atoms. Second, the electrons may exchange momentum with the ions or neutrals, but not energy. The electron distributions can become isotropic by collisions with neutrals or ions, or with themselves. Third, the electron distributions may become maxwellian by collisions with themselves.

The electric fields created by a very slight inequality of electron and ion densities are very intense. For this reason, the densities of electrons and ions will be equal to a very good approximation everywhere outside a Debye sphere around these ions.

The electrons or ions emitted from an electrode are isotropically distributed over a hemisphere in a maxwellian distribution over the hemisphere. The electron distributions can become maxwellian by momentum-only-changing collisions with ions or neutrals. The temperature of the maxwellian distribution will be the same as the temperature parameter characterizing the half maxwellian.

There are a number of characteristic lengths associated with this problem. The Debye length is always much shorter than any mean free path for parameters of interest in thermionic diodes. The Debye length λ_o is given by

$$\lambda_o = (\epsilon_o kT_e/n_e e^2)^{\frac{1}{2}} . \qquad \text{(D-16)}$$

If the electron and ion temperatures are equal, then the mean free path for electron-electron collisions equals the mean free path for ion-ion collisions, and the mean free path for electron-electron collisions equals to a good approximation the mean free path for electron-ion collisions. The ion-neutral mean free path is shorter than the electron-neutral mean free path. The mean free paths for the electron-electron, ion-ion, and the electron-ion collisions are as follows:

$$\lambda_{ee} = \frac{103 \cdot \epsilon_o^2 (kT_e)^2}{e^4 n_e \ln \Lambda} \tag{D. 17}$$

$$\lambda_{ii} = \frac{103 \cdot \epsilon_o^2 (kT_i)^2}{e^4 n_i \ln \Lambda}, \tag{D. 18}$$

$$\lambda_{ei} = \frac{103 \cdot \epsilon_o^2 (kT_e)^2}{e^4 n_i \ln \Lambda}. \tag{D. 19}$$

Here λ is the mean free path for the interaction denoted by the subscripts, e being for an electron and i for an ion, ϵ_o is the permittivity of the vacuum, e is the charge of an electron, n is the density of particles denoted by the subscript, k is Boltzmann's constant, T is the temperature of the particles, and

$$\Lambda = \frac{12\pi (\epsilon_o kT/e^2)^{3/2}}{n_e^{\frac{1}{2}}} \tag{D. 20}$$

Except within a Debye distance (where applicable),

$$n_e = n_i \tag{D. 21}$$

to a very good approximation. If $T_e = T_i$, then we observe that

$$\lambda_{ei} = \lambda_{ii} = .805 \ \lambda_{ei}. \tag{D. 22}$$

For our discussion of the diffusion approximation, we take the electron-electron, electron-ion, and ion-ion mean free paths all equal. Three cases of interest occur as shown in Figure II-19, and the properties of the particles are summarized in Tables II-3, II-4 and II-5.

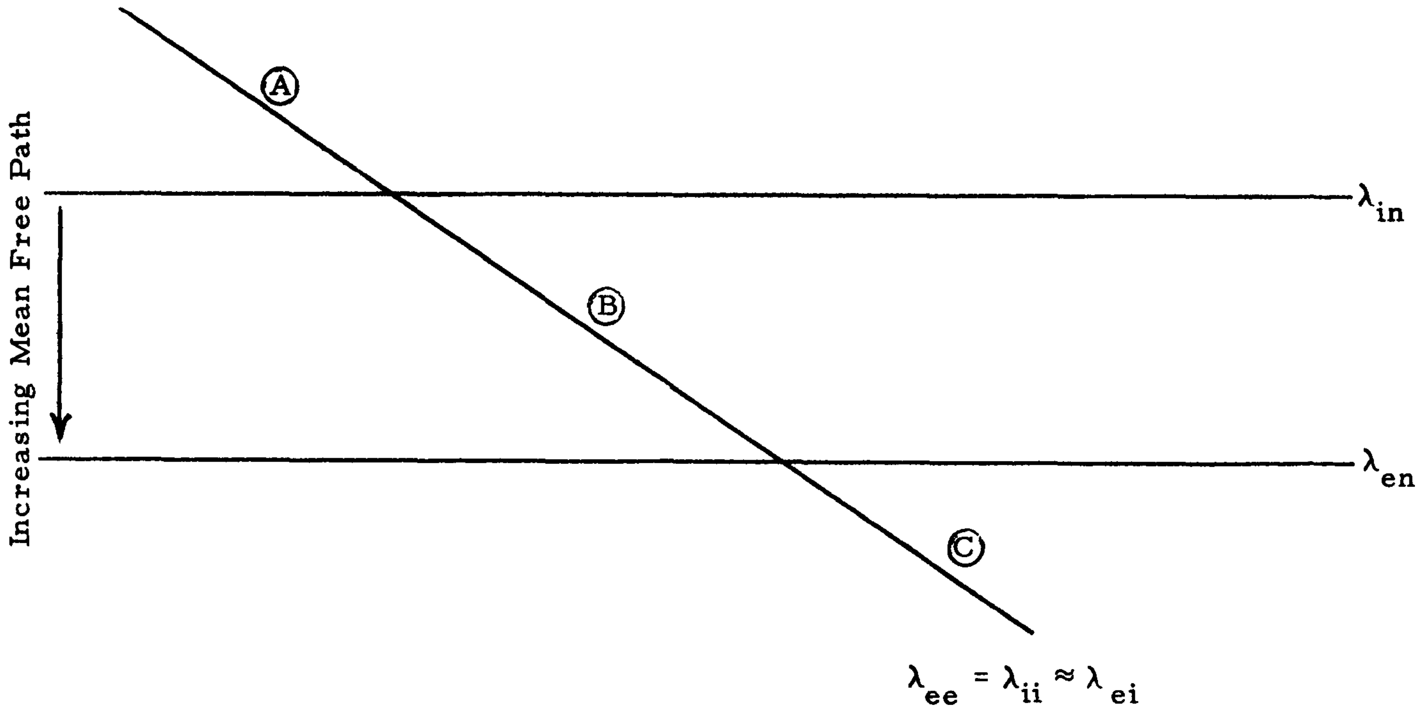


Figure II-19. Three Cases of Interest in a Thermionic Energy Converter.

TABLE II-3

Case A $\lambda_{ee} = \lambda_{ii} \approx \lambda_{ei} < \lambda_{in} < \lambda_{en}$

		$\lambda_{ee} = \lambda_{ii} \approx \lambda_{ei}$	λ_{in}	λ_{en}
Electrons	Maxwellian ½ isotropic No collisions	Maxwellian Isotropic ee ei collisions	Maxwellian Isotropic ee, ei, in collisions	Maxwellian Isotropic All collisions
Class	1 Free molecular flow	3 Diffusion	3 Diffusion	3 Diffusion
Ions	Maxwellian ½ isotropic No collisions	Maxwellian Isotropic ii, ie collisions	Maxwellian Isotropic ii, ie, in collisions	Maxwellian Isotropic All collisions
Class	1 Free molecular flow	2 Inertial flow	3 Diffusion	3 Diffusion

TABLE II-4

Case B. $\lambda_{in} < \lambda_{ee} = \lambda_{ii} \approx \lambda_{ei} < \lambda_{en}$

λ_{in} $\lambda_{ee} = \lambda_{ii} \approx \lambda_{ei}$ λ_{en}

Electrons	Maxwellian ½ isotropic No collisions	Maxwellian ½ isotropic No collisions	Maxwellian Isotropic ee, ei collisions	Maxwellian Isotropic All collisions
Class	1 Free molecular flow	1 Free molecular flow	3 Diffusion	3 Diffusion
Ions	Maxwellian ½ isotropic No collisions	Maxwellian Isotropic in collisions	Maxwellian Isotropic ii. ie, in collisions	Maxwellian Isotropic All collisions
Class	1 Free molecular flow	3 Diffusion	3 Diffusion	3 Diffusion

TABLE II-5

Case C $\lambda_{in} < \lambda_{en} < \lambda_{ee} = \lambda_{ii} \approx \lambda_{ei}$

λ_{in} λ_{en} $\lambda_{ee} = \lambda_{ii} \approx \lambda_{ei}$

Electrons	Maxwellian ½ isotropic No collisions	Maxwellian ½ isotropic No collisions	Maxwellian Isotropic en collisions	Maxwellian Isotropic All collisions
Class	1 Free molecular flow	1 Free molecular flow	3 Diffusion	3 Diffusion
Ions	Maxwellian ½ isotropic No collisions	Maxwellian Isotropic in collisions	Maxwellian Isotropic in collisions	Maxwellian Isotropic All collisions
Class	1 Free molecular flow	3 Diffusion	3 Diffusion	3 Diffusion

Three classes of particle transport may be identified:

a. Free Molecular Flow

There are no collisions of charged particles. Particles are accelerated by the electric field present. The charged particle distribution is half isotropic.

b. Inertial Flow

The rate of change of kinetic energy (or inertia) dominates greatly any collisional drag. There is no energy exchange among the particles.

c. Diffusion

Collisional drag dominates the rate of change of kinetic energy (or inertia)

In formulating the problem we would like to find the electron density $n_e(z, v)$, the ion density $n_i(z, v)$, the average drift speed $\bar{v}_e(z)$ of the electrons, the average drift speed $\bar{v}_i(z)$ of the ions, the electric current $j_e(z)$ created by the electrons, the electric current $j_i(z)$ created by the ions, the temperature $T_e(z)$ of the electrons, the temperature $T_i(z)$ of the ions, and the potential energy $U(z)$ all as a function of position. The equations involved will be listed by class and the equations must be selected from the class appropriate to the type of charged particle being described. In general, the class of equations for electrons is different from that for ions. Poisson's equation is always used in the diffusion approximation:

$$\frac{d^2 U(z)}{dz^2} = \frac{e^2}{\epsilon_o} \int dv \left[n_i(z, v) - n_e(z, v) \right] \quad . \tag{D. 23}$$

Case A occurs quite infrequently because a high degree of ionization is required. Cases B and C occur more frequently. In case C, which is probably the most frequently occurring case, an ion starting from the emitter will, on the average, make its first collision at the distance λ'_{in}. Collisions of the charged and neutral particles among themselves will make the distribution functions isotropic; collisions of the electrons with the ions or neutrals will have essentially no influence on the respective speed distributions. Thus, in this case, ions become isotropic nearer the emitter than the electrons, and we can think of treating the ions by diffusion theory in the transition region and the electrons by the collisionless Boltzmann equation for part of the transition region.

The equations for particle conservation in each of the three cases are as follows:

a. Free Molecular Flow

Case 1 Conservation of particles in phase in which the particles are restricted to move only along the z-axis:

$$v \frac{\partial n(z,v)}{\partial z} - \frac{1}{m} \left(\frac{dU}{dx} \right) \frac{\partial n(z,v)}{\partial v} = 0 . \qquad (D.24)$$

b. Inertial Flow

Case 2.

(a). Conservation of particles: Current defined: For each species of particles

$$\Gamma = n(z)\, \bar{v}(z) = \text{const.} \qquad (D.25)$$

(b) Conservation of momentum: For each species of particles

$$n(z)\,\frac{d}{dz}\left[\frac{m}{2}\,\bar{v}^{2}(z)\right] + U(z) \quad + \frac{d}{dz}\,\Big[n(z)\,kT(z)\Big] = 0. \tag{D.26}$$

(c) Conservation of energy: For each species of particles

$$\frac{d}{dz}\left\{\Gamma\left[\frac{5}{2}\,kT(z) + \frac{m}{2}\,\bar{v}^{2}(z)\right] - \varkappa(z)\,\frac{dT(z)}{dz}\right\} = -\Gamma q\mathcal{E} - Q. \tag{D.27}$$

c. <u>Diffusion</u>

Case 3.

(a) Conservation of particles:

$$\frac{d\Gamma_e}{dz} = eS_e = e\beta_r\,n_e\left[n_{es}\,n_{is} - n_e^2\right] \approx 0\ , \tag{D.28}$$

$$\frac{d\Gamma_i}{dz} = eS_i = e\beta_r\,n_e\left[n_{es}\,n_{is} - n_e^2\right] \approx 0\ . \tag{D.29}$$

$$\left(\frac{1}{\mu_{ei}} + \frac{1}{\mu_{en}}\right)\Gamma_e = -\left[\frac{dp_e}{dz} + e\,n_e\,\mathcal{E} + R_{ie} + n_e\,\frac{d}{dz}\left(\frac{m_e\,\bar{v}_e^{2}}{2}\right)\right], \tag{D.30}$$

$$\left(\frac{1}{\mu_{ie}} + \frac{1}{\mu_{in}}\right)\Gamma_i = -\left[\frac{dp_i}{dz} - en_i\,\mathcal{E} - R_{ie} + n_i\,\frac{d}{dz}\left[\left(\frac{m_i\,\bar{v}_i^{2}}{2}\right)\right]\right]. \tag{D.31}$$

(b) Conservation of energy:

$$\frac{dq_e}{dz} = -\,j_e\,\mathcal{E} - Q_e\ , \tag{D.32}$$

where

$$q_e = j_e\left(\frac{5}{2}\ \frac{kT_e}{e}\right) - \varkappa_e\,\frac{dT}{dz} + \frac{1}{2}\,m_e\,\bar{v}_e^{2}\ . \tag{D.33}$$

Here, Γ is the particle current of the subscripted particle (not electric current created by the particles), n(z, v) is the number of particles per unit volume and per unit speed, of mass m and charge q, T(z) is their temperature, h(z) is the thermal conductivity of the subscripted particle, Q is the rate of energy transfer from one species of particles to the other, R_{ie} is the rate of transfer of momentum, i. e., force, to ions from electrons as a result of collisions between these two species. $\mathcal{E}$ is the electric intensity and ϕ is the electric potential, S is the number of particles created per unit volume, n_{es} and n_{is} are the electron and ion equilibrium particle densities, β_r is the recombination coefficient, μ is the mobility of the first subscripted particle as a result of collisions with the second subscripted particle, p is the pressure of the subscripted particle, q is the kinetic energy flux of the subscripted particle, e as a subscript refers to electrons, and i as a subscript refers to ions.

The various equations in the above theory are readily derived in several different ways. One method consists in noting that they are physically obvious, which is one of the pleasant things about this theory. Perhaps it should be mentioned that the effects of the drift velocity of either species are taken into account by the $m\bar{v}^2/2$ term, which represents the kinetic energy of macroscopic motion of the relevant species. The terms involving the mobility describe the effects of drag on the movement of the related species. The enthalpy of a perfect gas is (5/2) kT and is the energy transported across a surface by a unit mass.[22] The equations for inertial flow describe the anisotropic distribution in the transition region only to the lowest order. It is to be hoped that this accuracy is sufficient. The hope of the theory is that it will successfully join the answer from the Vlasov equation for the collisionless region to the answer from diffusion theory for the plasma region.

The various equations in the above theory can also be readily derived by taking corresponding velocity moments of the Boltzmann equation.[5] The resulting equations are really those of magnetohydrodynamics. The collisionless equation D. 24 for the sheath region is just the collisionless Boltzmann equation where the charges are constrained to move along the z-axis in an electric field of intensity $-\nabla\phi$. The particle conservation equation is really just the zeroth velocity moment of the time-independent Boltzmann equation:[5]

$$\nabla_r \cdot [n(\underline{r})\,\overline{\underline{v}\,(r)}\,] = \int dv\, \frac{\partial\, f(\underline{r}, \underline{v})}{\partial t}\bigg|_{coll}, \tag{D. 34}$$

the right-hand side of which is the case of no net production or absorption reduces immediately to Eq. D. 25. The momentum conservation equation (D. 26) is almost as immediate and follows by taking the first velocity moment of the time-independent Boltzmann equation in an electrostatic force field:[5]

$$\begin{aligned} mn(\underline{r})\,\overline{\underline{v}(\underline{r})\cdot\nabla\underline{v}(\underline{r})} &= -n(\underline{r})\,\nabla\,\left[e\phi(\underline{r})+\nabla\cdot\underline{\underline{P}}\,(\underline{r})\right] + \\ &- m\overline{\underline{v}(\underline{r})}\int d\underline{v}\,\frac{\partial f(\underline{v}, \underline{v}}{\partial t}\bigg|_{coll} + \int d\underline{v}\; mv\,\frac{\partial f(\underline{r}, \underline{v})}{\partial t}\bigg|_{coll}, \end{aligned} \tag{D. 35}$$

where

$$\underline{\underline{P}}\,(\underline{r}) = m\int d\underline{v}\,\underline{v}\,\underline{v}\,f\,(\underline{r}, \underline{v}). \tag{D. 36}$$

The above equation is simplified by approximating the kinetic stress tensor with an isotropic velocity Maxwell-Boltzmann distribution functions and by neglecting any collisions. The energy conservation equation (D. 27) is found by computing the second velocity moments of the time-independent Boltzmann equation. After some algebraic reduction one finds that[5]

$$1/2 \; m\overline{v}^2 \, \nabla \cdot (n\overline{\underline{v}}) + 1/2 \; n m \overline{\underline{v}} \cdot \nabla \overline{v}^2 + 5/2 \; \overline{\underline{v}} \cdot \nabla p + 5/2 \; p \nabla \cdot \overline{\underline{v}}$$

$$= -\underline{j} \cdot \nabla \phi + \int d\underline{v} \left(\frac{mv^2}{2} \right) \frac{\partial f}{dt} \bigg|_{coll} . \qquad (D.37)$$

To apply this result to the present problem, we use the result from Eq. D. 25, and approximate the integral involving the collisions solely by a heat conduction term:

$$\int d\underline{v} \left(\frac{mv^2}{2} \right) \frac{\partial f}{\partial t} \bigg|_{coll} = \varkappa (z) \frac{d}{dz} T(z) . \qquad (D.38)$$

The result (Eq. D. 27) immediately follows.

The derivation of the source and sink terms describing ionization and recombination follows from the law of detailed balance: The rate of increase of a population of electrons is given by

$$\frac{dn_e}{dt} = \alpha \, n_n \, n_e - \beta \, n_i n_e^2 , \qquad (D.39)$$

where α is the proportionality factor for the ionization process

$$Cs^o + e^- \rightarrow Cs^+ + e^- + e^- , \qquad (D.40)$$

and β is the proportionality factor for the recombination process

$$Cs^+ + e^- + e^- \rightarrow Cs^o + e^- . \qquad (D.41)$$

At equilibrium $dn_e/dt = 0$, so that

$$\frac{\alpha}{\beta} = \left(\frac{n_i n_e}{n_n}\right)_s ,$$

the subscript s denoting the equilibrium condition. Thus,

$$\frac{dn_i}{dt} = \frac{dn_e}{dt} = \beta n_e \left[n_{es} n_{is} - n_e^2\right] , \tag{D. 42}$$

$$= \beta n_e \left[n_{es}^2 - n_e^2\right] . \tag{D. 43}$$

The equations valid for the diffusion regime can be derived in a variety of ways. We refrain from repeating these derivations which are readily available elsewhere.[23, 24] Again, one starts from the Boltzmann equation, defines the current as a first velocity moment of the distribution function, approximates the actual distribution function by the Maxwell-Boltzmann distribution that is isotropic plus a small perturbation that is not, in general, isotropic, defines the mobility as the proportionality factor between the particle current per unit particle density and the electric intensity, and defines the diffusion coefficient as the second velocity moment over the distribution function divided by 3 times the collision frequency.

The mobilities, collision frequency, and thermal conductivity are taken from the literature.[23, 25, 26] The mobility μ_e of electrons is

$$\mu_e = \frac{.98\ e}{m_e \nu_{en}} = \frac{.521\ e}{\sqrt{m_e kT_e}\ N_o \sigma_{en}} , \tag{D. 44}$$

and μ_i of ions is

$$\mu_i = \frac{0.90\, e^2}{m_i\, \nu_{in}} = \frac{.677\ e}{\sqrt{m_i\, kT_i}\ N_o\, \sigma_{in}} \quad . \qquad \text{(D. 45)}$$

The collision frequency ν_{en} of electrons against neutrals is

$$\nu_{en} = \frac{3}{2}\sqrt{\frac{\pi k T_e}{2\, m_e}}\ N_o\, \sigma_{en} \ , \qquad \text{(D. 46)}$$

and ν_{in} of ions against neutrals is

$$\nu_{in} = \frac{3}{4}\sqrt{\frac{\pi k T_i}{m_i}}\ N_o\, \sigma_{in} \ . \qquad \text{(D. 47)}$$

The thermal conductivity of the plasma ia

$$\varkappa_e = 1.92\ \frac{n_o\, \mu_e\ k^2\, T_e}{e} \quad . \qquad \text{(D. 48)}$$

The vapor pressure P_{cs} of Cs is given by

$$P_{cs} = 3.27 \times 10^{10}\ \frac{\exp - 8910/T_R}{\sqrt{T_R}}\ \text{newtons}/\text{m}^2 \ . \qquad \text{(D. 49)}$$

The electron cesium recombination coefficient β is given by:

$$\beta = 5.6 \times 10^{-27}\, (kT_e)^{-4.5} . \qquad \text{(D. 50)}$$

The electron-ion mobility μ_{ei} is given by

$$\mu_{ei} = \frac{93.0 \cdot \epsilon^{2} (kT_{e})^{3/2}}{e^{3} m_{e}^{\frac{1}{2}} \ln\left[\frac{12\pi}{\sqrt{n_{e}}} \left(\frac{kT}{\epsilon}\right)^{3/2}\right]} . \qquad (D.51)$$

The following procedure was used to solve these equations numerically: In the absence of any ionization and recombination, the current of electrons and the current of ions are constant. These facts may be used to eliminate the average drift speeds of ions and electrons from their respective equations in terms of the electron and ion densities and the constant electron and ion currents. The perfect gas law is used to eliminate the electron and ion partial pressures from their respective equations. The ion temperature is taken to be constant, equal to the arithmetic average of the emitter and collector temperatures. The ion temperature is, therefore, constant. Poisson's equation D.23, the diffusion equation (D.31) for the ion density, and the diffusion equation for the electron density (D.30) are differenced. The electric intensity is determined from

$$\mathcal{E}_{j+1} = \mathcal{E}_{j-1} + \frac{2\Delta ze}{\epsilon_{o}} (n_{ij} - n_{ej}); \qquad (D.52)$$

the ion density is determined from

$$n_{ij+1} = n_{ij-1} + 2\Delta z \left\{\frac{\Gamma_{i} e}{\mu_{inj}} - |e|\, \mathcal{E}_{j}\, n_{ij}\right\} \Big/ \left\{\frac{m_{i} \Gamma_{i}^{2}}{n_{ij}^{2}} - k T_{i}\right\}; \qquad (D.53)$$

and the electron density and temperature are determined by the simultaneous solution of

$$\begin{cases} a_{11}\, T_{ej+1} + a_{12}\, n_{ej+1} = c_1 \,, & \text{(D. 54)} \\ a_{21}\, T_{ej+1} + a_{22}\, n_{ej+1} = c_2 \,, & \text{(D. 55)} \end{cases}$$

where

$$a_{11} = \frac{1}{2\Delta z}\left[\frac{5}{2} k\, \Gamma_e + \frac{2\,(\varkappa_{j-1} - 3\varkappa_j)}{2\Delta z}\right], \tag{D. 56}$$

$$a_{12} = \frac{-m_e\, \Gamma_e^3}{2\,\Delta z\, n_{ej}^3}\,, \tag{D. 57}$$

$$a_{21} = \frac{-k\, n_{ej}}{2\,\Delta j}\,, \tag{D. 58}$$

$$a_{22} = \frac{1}{2\Delta z}\left[\frac{m_e\, \Gamma_e^2}{n_{ej}^2} - k\, T_{ej}\right]. \tag{D. 59}$$

$$c_1 = -\,|e|\, \Gamma_e\, \mathcal{E}_j - Q_{ej} \quad \frac{1}{2\Delta z}\left[\frac{5}{2} k\, \Gamma_e + \frac{\varkappa_{j-1} + \varkappa_j}{\Delta z}\right] T_{e\,j-1}$$

$$- \frac{2\varkappa_{ej}}{(\Delta z)^2}\, T_{ej} - \frac{m_e\, \Gamma_e^3\, n_{ej-1}}{2\,\Delta z\, n_{ej}^3}\,, \tag{D. 60}$$

$$c_2 = \frac{1}{2\Delta z}\left[\frac{m_e\, \Gamma_e^2}{n_{ej}^2} - k\, T_{ej}\right] n_{e\,j-1} + \left[\,|e|\, \mathcal{E}_j - \frac{k\, T_{ej}}{2\,\Delta z}\right] n_{ej}$$

$$+ \left[\frac{1}{\mu_{enj}} + \frac{1}{\mu_{eij}}\right] e\, \Gamma_e \,. \tag{D. 61}$$

In the practical case tried by this method, the integration proceeded outward from the plasma, starting at a point in the plasma where the electric field was zero, and the electron and ion densities were equal to each other and to the plasma particle density. The region of interest was taken near the collector so the source could be taken to be zero, at least for our initial attempts.

A flow diagram of the program is presented in Fig. II-20. In view of the very elementary character of the logic, it is believed that the flow diagram is self explanatory.

The method was abandoned, despite its simplicity and intuitive physical nature, because it appeared to be afflicted with instabilities, i. e., we found negative electron or ion densities on occasion. If this diffusion type of equation were linear, then there is a simple method of getting around the instabilities using recurrence relations. Unfortunately, the present problem is nonlinear, and the method is not applicable to nonlinear problems. No method is known by the writer for suppressing the undesired, divergent, second solution for the nonlinear problem. Problems of this sort inherently involve the application of a boundary condition at both ends of the region of interest The problem is either undetermined or unstable by the application of boundary conditions at only one end of the region of interest.[27] For this reason, the method was abandoned in favor of the S_n method, which appeared to and had the reputation for avoiding all these difficulties. Further, the S_n method is intrinsically more accurate

4. S_n Method

The S_n method has been widely applied to the treatment of problems involving neutron transport in reactive assemblies. Although no proof of the stability of the S_n difference method seems to have been found, many experiments seem to indicate that it is stable.[18] The

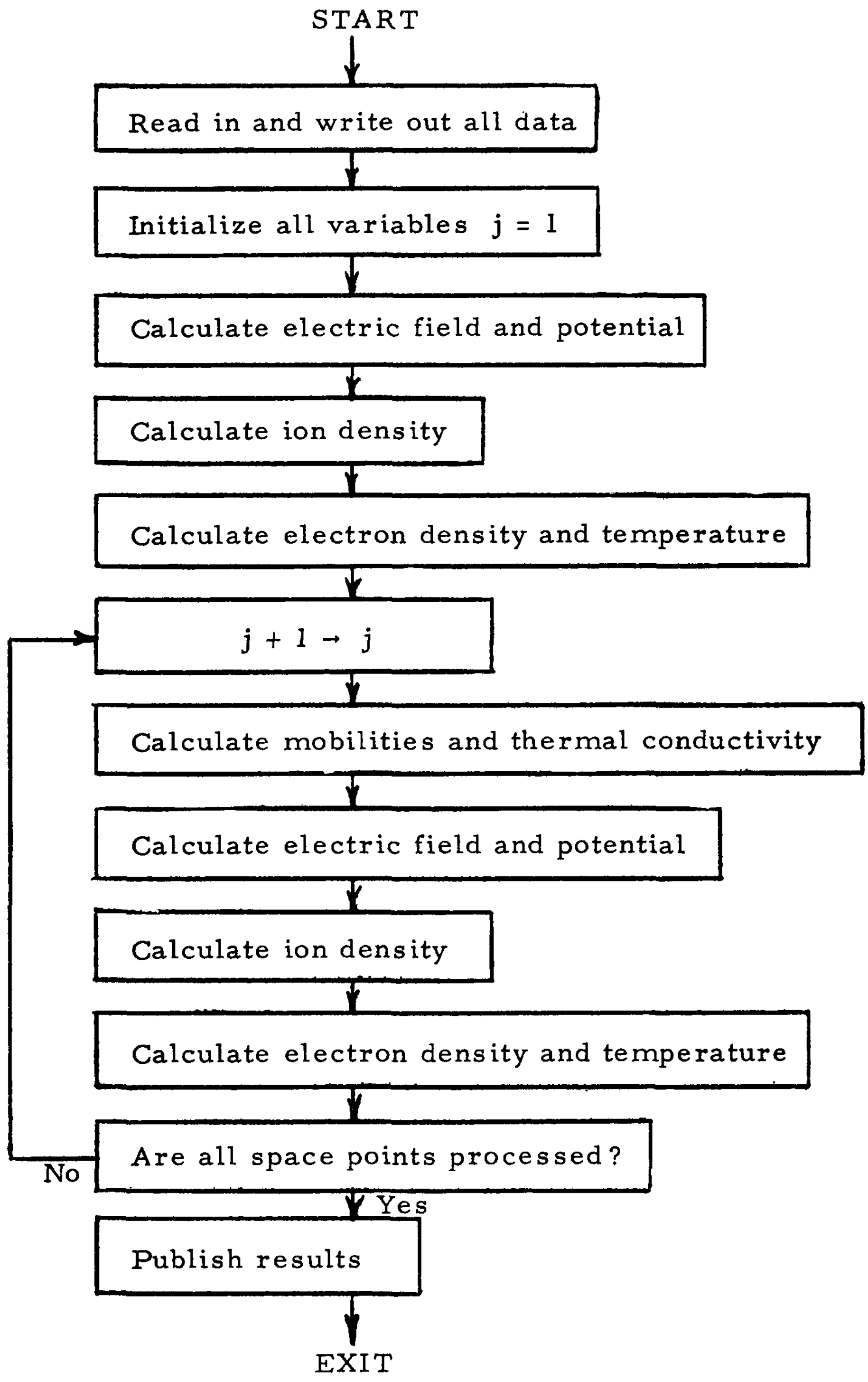


Figure II-20. Flow Diagram of Program to Compute Particle Densities and Electron Temperature by Modified Diffusion Theory method in essence consists in subdividing μ-space usually in equal subdivisions, and then approximating the directional density at intermediate points in μ space by straight lines drawn between the discrete points.[18] We extended the method here to approximate the speed dependence in a similar manner in order to get more accuracy in the speed dependence than is provided by the usual multigroup step. Likewise, the spatial dependence is similarly approximated. We must also extend the S_n method to incorporate the acceleration terms in the Boltzmann equation in order to describe the crossing of bounding surfaces in velocity space; in particular, the effects of the electric field must be incorporated into the S_n method. All this is quite easy to do and very straightforward. The details are given in Appendix C.

The essential trouble with the S_n method was that we obtained negative electron densities frequently and occasionally even negative ion densities. Since this was thought to be caused by instabilities, we investigated this problem. It was decided that the phenomena which had been observed were not instabilities, but were rather the consequence of choosing speed or increments too large, compared with the increments in z, so that the densities oscillated. Be this as it may, we seemed to find from the instability investigation that the S_n method was unconditionally unstable. This investigation was, however, more characterized by its vigor than rigor. For this reason, further work on the S_n method was abandoned in favor of the much more promising integral technique discussed elsewhere.

It is to be hoped that a mathematician will rigorously investigate the stability of the S_n method with an electric field present. Our vigorous, nonrigorous treatment of this point follows: As is the custom in the study of complicated equations involving a number of independent variables, we start with an equation involving just two independent variables that has the form of several terms of the original equation. Further, we regard the equation to have constant coefficients. Third, we observe that the time independent Boltzmann equation may be likened to a time dependent Boltzmann equation in that the derivative with respect to z may be thought of as corresponding, insofar as any mathematics is concerned, to t, the time, in a time dependent equation. Our problem is then really reduced to an initial value problem. Thus, we shall be studying the following equation, when treated by the S_n approach, with respect to stability along the z axis, which is the axis that has been causing the trouble:

$$v\mu \frac{\partial n(z,\mu)}{\partial z} - \frac{e\mathcal{E}}{m} \frac{(1-\mu^2)}{v} \frac{\partial n(z,\mu)}{\partial \mu} + v\Sigma n(z,\mu) = \frac{v\Sigma}{2} \int_{-1}^{1} d\mu' \, n(z,\mu') \quad . \tag{D.62}$$

Stability is usually examined by the von Neumann method.[19, 21] The S_n equation relating the densities at various points in the position-speed (say) mesh is

$$c_{00}\, n_{ji} + c_{10}\, n_{j-1i} + c_{01}\, n_{ji-1} + c_{11}\, n_{j-1i-1} = s \sum_{i=1}^{IL} n_{ji} \, , \tag{D.63}$$

the c_{00}, c_{10}, $c_{01, t}$ and c_{11} being rather complicated coefficients. The densities at the various points are Fourier transformed to yield:

$$\left\{ c_{00}\, e^{\ell k i \Delta\mu} + c_{01} e^{\ell k(i-1)\Delta\mu} - s \sum_{i'=1}^{IL} e^{\ell k i' \Delta\mu} \right\} \underline{n}_{ji}$$

$$= \left\{ -c_{10} e^{\ell k i \Delta\mu} - c_{11} e^{\ell k(i-1)\Delta\mu} + s \sum_{i'=1}^{IL} e^{\ell k i' \Delta\mu} \right\} \underline{n}_{j-1i} \, . \tag{D.64}$$

From this result, we can deduce the amplification matrix $G(\Delta\mu, k)$ immediately:

$$G(\Delta\mu, k) = \frac{c_{10}(e^{-\iota k\Delta\mu}-1) + c_{11}(e^{-2\iota k\Delta\mu}-e^{-\iota k\Delta\mu}) + s(e^{\iota k(IL-i)\Delta\mu}-e^{-\iota ki\Delta\mu})}{c_{00}(1-e^{-\iota k\Delta\mu}) + c_{01}(e^{-\iota k\Delta\mu}-e^{-2\iota k\Delta\mu}) + s(e^{-\iota ki\Delta\mu}-e^{\iota k(IL-i)\Delta\mu})} . \qquad \text{(D. 6}$$

From this, we see the condition for stability is that

$$\sin^2\left(\frac{k\Delta\mu}{2}\right)\left[c_{00}^2 + c_{01}^2 - c_{10}^2 - c_{11}^2 + 2\left(c_{10}c_{11} - c_{01}c_{00}\right)\cos k\Delta\mu\right]$$
$$+ s\sin\left(\frac{k\Delta\mu}{2}\right)\sin\left(\frac{Nk\Delta\mu}{2}\right)\left\{\left[c_{11}-c_{01}\right]\cos k\Delta\mu\left(i-\frac{IL+3}{2}\right) + \right.$$
$$\left. + \left[c_{10}-c_{00}\right]\cos k\Delta\mu\left(i-\frac{IL+1}{2}\right)\right\} \geq 0 . \qquad \text{(D. 6}$$

To simplify our considerations, we take the case in which there is no source, i. e., $s = 0$. In this case, the stability condition becomes:

$$\left(a_i d_i' + \bar{a}_i e_i'\right) + \left(a_i e_i' + \bar{a}_i d_i'\right)\cos(k\Delta\mu) \geq 0 . \qquad \text{(D. 6}$$

(See Appendix 2 and below for the definition of various quantities.)

The left-hand side of this expression has no maximum or minimum. For $\cos(k\Delta\mu) = -1$, we find that

$$\left[\mu_i - \mu_{i-1}\right]\left[d_i' - e_i'\right] \geq 0. \qquad \text{(D. 6}$$

Since $\mu_i > \mu_{i-1}$, this condition requires that

$$d_i' \geq e_i' . \qquad \text{(D. 6}$$

For cos $(k\Delta\mu) = 1$, we find that

$$\left|\mu_i + \mu_{i-1}\right| \left|d_i' + e_i'\right| \geq 0. \tag{D. 70}$$

We conclude that if $\mu_i + \mu_i \geq 0$,

$$e_i' \leq \pm d_i' \tag{D. 71}$$

and that if $\mu_i + \mu_{i-1} \geq 0$, (D. 72)

$$-d_i' \leq e_i' \leq d_i' . \tag{D. 73}$$

Here,

$$d_i' = \frac{\Sigma}{2} - \frac{e\mathscr{E}\, b_i}{2\, mv^2} , \tag{D. 74}$$

$$e_i' = \frac{\Sigma}{2} + \frac{e\mathscr{E}\, b_i}{2\, mv^2} . \tag{D. 75}$$

If $\mu_i + \mu_{i-1} \leq 0$, stability requires that

$$\Sigma \leq -\Sigma, \tag{D. 76}$$

which is obviously impossible unless the cross section is zero. Stability also requires that

$$\frac{e\mathscr{E}\, b_i}{mv} \leq -\frac{e\mathscr{E}\, b_i}{mv} , \tag{D. 77}$$

which is true only if $\mathscr{E} \leq 0$. If $\mu_i + \mu_{i-1} \geq 0$.

stability requires that

$$-v\Sigma + \frac{e\mathscr{E}\, b_i}{mv} \leq v\Sigma + \frac{e\mathscr{E}\, b_i}{mv} \tag{D. 78}$$

and that

$$\frac{e\mathcal{E}b_i}{mv} \le -\frac{e\mathcal{E}b_i}{mv}. \qquad (D.79)$$

The first condition is automatically true; the second is true if $\mathcal{E} \le 0$. Thus, we conclude that the method is unconditionally unstable, since there is no increment which if chosen properly would enable us to satisfy the various stability conditions. Of course, we have only shown that instability occurs with no source, and we have only shown that local instability occurs, since we have assumed various coefficients to be independent of our independent variables. However, stability in the large can hardly occur if there is instability locally; further, it is not likely that appending source terms will help matters.

In the above tests it was assumed that integration was always carried out in a particular direction. Let us now choose our direction of integration in accord with the dictates of the usual S_n procedure: In this case, $\underline{n}_j$ is determined from $\underline{n}_{j-1}$, and $\mu_i > 0$. $d'_i \ge e'_i$ and $-d'_i < e'_i$ are required:

$$v\Sigma - \frac{e\mathcal{E}b_i}{mv} \le v\Sigma + \frac{e\mathcal{E}b_i}{mv} , \qquad (D.80)$$

$$-v\Sigma + \frac{e\mathcal{E}b_i}{mv} \le v\Sigma + \frac{e\mathcal{E}b_i}{mv} . \qquad (D.81)$$

The first condition is true only if $\mathcal{E} < 0$; the second condition is automatically satisfied. If $\mu_i < 0$, $\underline{n}_{j-1}$, is determined from n_j, then the amplification matrix is just the inverse of that written above. In this case, the stability requirements become

$$d_i \le e'_i , \qquad -d_i \le e' \qquad (D.82)$$

$$v\Sigma - \frac{e\mathcal{E}b_i}{mv} \le v\Sigma + \frac{e\mathcal{E}b_i}{mv} , \qquad (D.83)$$

$$-v\Sigma + \frac{e\mathcal{E} b_i}{mv} \leq v\Sigma + \frac{e\mathcal{E} b_i}{mv} \quad . \tag{D. 84}$$

The first condition is satisfied only if $\mathcal{E} > 0$; the second condition is automatically satisfied.

Unlike the usual situation, there is no increment or ratio of increments we can adjust to achieve stability. For each directional sense, we can find a direction of integration in which to integrate that will give us unconditional stability insofar as the increment sizes are concerned, but which is conditioned upon the sign of the electric intensity, and the requirement is just the opposite for each sense of the direction. Thus, there is no choice of the sense of the electric intensity that will make stability possible. The method seems to be unconditionally unstable. (Even if there were a sense of the electric field making stability possible, the fact would not help much, because reversals of the direction are almost bound to occur during the course of the numerical calculation.)

While we have been neither careful nor rigorous, the picture for the S_n method was sufficiently discouraging and the picture for the integral method was by this time so bright that no more time was spent trying to get the S_n method to work, even though the original difficulties that lead to the investigation of the stability were probably not due to instabilities in retrospect and could have been cured. To cure these difficulties with instabilities looming over the horizon made the method unattractive for further work.

It is interesting to note that the method used presently for studying the stability of a numerical process gives the correct results when applied to the S_n method for neutral particles, viz., when one integrates in the direction in which particles flow, the method is unconditionally stable for neutral particles.

Nevertheless, a number of cases did run without any particle density becoming negative. These are listed in Table II-6. In a large number of other cases, the density of the electrons became negative at some point during the integration in phase space, at which point the integration was stopped. Although it is believed that the particular source of these oscillations could be corrected, the spectre of instabilities and the virtues of the integral method appear so great that we believe our efforts will be much better invested by improvements in the integral method.

The details of the program for the S_n method will be found in Appendix 4 .

5. A Stable Differencing of the Boltzmann Equation

Some effort was made to find methods of differencing the Boltzmann equation that are stable, especially those that had already been used elsewhere. Such a method has been developed by Killeen[21] and Killeen and Rompel,[28] based, in part, on the work of Leith,[29] which, in turn, is based on the work of Marchuk,[30] Pagrinovsky[22] and Godunov,[31] and D'yakonov.[32] Killeen treated the time-dependent buildup of a cylindrical layer of relativistic electrons for the Astron in a static magnetic induction where the azimuthal current created by the electrons creates a magnetic induction larger than that applied. This problem requires the use of Vlasov's and Maxwell's equations. (Space charge effects, i. e., Poisson's equation, were neglected.) It is Killeen's treatment of the Vlasov equation that interests us.

TABLE II-6

CASES TREATED BY THE S_n METHOD IN WHICH THE DENSITY DID NOT BECOME NEGATIVE

Electric Field	Scattering	Number of Speed Groups	Direction of Integration
OFF	Present	4	Collector to plasma and back
ON	Absent	1	Collector to plasma and back
OFF	Absent		Plasma to collector and back
OFF	Present		Plasma to collector and back

The essence of the method is that to solve

$$\frac{\partial \rho}{\partial \tau} + \gamma \frac{\partial \rho}{\partial \eta} = 0 \tag{D. 85}$$

one uses the differencing scheme

$$\rho^{\nu+1,\beta} = \rho^{\nu,\beta} - \frac{\alpha}{2}\left(\rho^{\nu,\beta+1} - \rho^{\nu,\beta-1}\right) + \frac{\alpha^2}{2}\left(\rho^{\nu,\beta+1} - 2\rho^{\nu,\beta} + \rho^{\nu,\beta-1}\right). \tag{D. 86}$$

This scheme is stable if $|\alpha| \leq 1$, where $\alpha = \gamma\Delta\tau/\Delta\eta$, is accurate to second order in $\gamma\Delta\tau$ and $\Delta\eta$, and is a two level formula, so that the step size is easy to change, as may be required by stability conditions, as compared with a three or more level formula. Instabilities result if the method is directly extended to another dimension. However, the method of Leith, Marchuk, Pagrinovsky, Godunov, and D'yakonov can be used to extend the method to more dimensions. The essence of the idea is that, if a differencing scheme is stable with respect to either of two sets of two independent variables, to increment forward first with respect to one set, then with respect to the second set to complete a full cycle In other words, a complete iteration cycle is subdivided into two subcycles, each of which is stable. Extensions to more sets of independent variables are obvious and valid. Thus, if we write the differencing algorithm in matrix form,

$$\rho^{\nu + 1/2} = (I + A)\,\rho^{\nu} \tag{D. 87}$$

and

$$\rho^{\nu + 1} = (I + B)\,\rho^{\nu + 1/2}, \tag{D. 88}$$

then

$$\rho^{\nu} = (I + B)(I + A)\,\rho^{\nu} \tag{D. 89}$$

for two sets of two independent variables.

To apply the above method to the present problem let

$$\zeta = \frac{-q\,\mathcal{E}\,\Delta z}{m\,v\,\Delta v} \qquad (D.90)$$

and

$$\xi = \frac{-q\,\mathcal{E}\,(1-\mu^2)\,\Delta z}{m\,v^2\,\mu\,\Delta\mu}\,. \qquad (D.91)$$

The particle density of either charge is then determined from the three equations

$$n_{j+1/2,\,n,\,i} = n_{j,\,n,\,i} + 1/2\,\zeta_{j,\,n,\,i}\left[n_{j,\,n+1,\,i} - n_{m,\,n-1,\,i}\right] +$$
$$+ 1/2\,\zeta^2_{j,\,n,\,i}\left[n_{j,\,n+1,\,i} - 2n_{j,\,n,\,i} + n_{j,\,n-1,\,i}\right], \qquad (D.92)$$

$$n_{j+1,\,n,\,i} = n_{j+1/2,\,n,\,i} + 1/2\,\xi_{j,\,n,\,i}\left[n_{j+1/2,\,n,\,i+1} - n_{j+1/2,\,n,\,i-1}\right]$$
$$+ 1/2\,\xi^2_{j,\,n,\,i}\left[n_{j+1/2,\,n,\,i+1} - 2\,n_{j+1/2,\,n,\,i} + n_{j+1/2,\,n,\,i-1}\right], \qquad (D.93)$$

$$n_{j+1,\,n,\,i} = n_{j+1,\,n,\,i} + \frac{\sigma_n N_n \Delta_z}{2\,\mu_i}\sum_{i'} n_{j+1,\,n,\,i'} - \frac{\sigma_n N_n \Delta_z}{\mu_i}\,n_{j+1,\,n,\,i}. \qquad (D.94)$$

All three equations for each charge species (here electrons and Cs^+) must be processed for each cycle of iteration. Further, to insure stability one must satisfy both

$$\Delta z \le \left|\frac{mv}{q\mathcal{E}}\right|\Delta v \qquad (D.95)$$

and

$$\Delta z \le \left|\frac{mv}{q\mathcal{E}}\right|\left|\frac{v\mu}{1-\mu^2}\right|\Delta\mu \qquad (D.96)$$

for both electrons and ions. However, if the speeds for electrons and ions are chosen to equate their kinetic energies, then

$$\frac{m_e v_e^2}{2} = \frac{m_i v_i^2}{2} \tag{D. 97}$$

so that

$$|\zeta_e| = |\zeta_i| \tag{D. 98}$$

and

$$|\xi_e| = |\xi_i| \; . \tag{D. 99}$$

Thus, the same upper limit exists for both electrons and ions. Further, in a system there is a tendency for the electrons and ions to have very approximately the same energies, so that both species will be well described by choosing the respective energies according to Eq. D. 97.

The inequalities above and the practicalities of running a program imply that the space increment Δz changes from time to time. This fact means that variables computed for a particular choice of space increment must be related to those referring to a subsequent space increment. Coding for this method was about half completed when it was decided to concentrate all our energy on the integral method, because of its greater promise. At least, even in principle the integral method could never give a negative density of any sort (a problem that haunted the S_n method), whereas it appeared that the above method could give negative densities.

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APPENDIX 1

CALCULATION OF THE COLLISION INTEGRAL

The integral

$$I = \frac{v\Sigma}{2} \int_{-1}^{1} d\,\mu\, n(z, v, \mu) \tag{1.1}$$

is needed in the calculation of the source term for electrons. If one desires to write this integral in terms of the variables z, E, $K_\perp$, and L (as we do not) then the following method may be used:

$$I = \frac{v\Sigma}{2} \int_{0}^{\infty} dv' \int_{-1}^{1} d\mu\ \delta\,(v - v')\ n\ (z, v', \ \mu), \tag{1.2}$$

$$= \Sigma\sqrt{\frac{2}{m}\,[E - U(z)\,]}\ \sum_{L=1}^{2} \int_{0}^{\infty} dE' \int_{0}^{\infty} dK_\perp\ n(z, E, K_\perp, L)$$

$$\left(\delta\left\{\sqrt{\frac{2}{m}\,[E' - U(z)] + } - \sqrt{\frac{2}{m}\,[E - U(z)]}\right\}\right). \tag{1.3}$$

This result can now be trivially integrated to yield:

$$I = \Sigma \left|E - U(z)\right| \sum_{L=1}^{2} \int_{o}^{\infty} d\,K_\perp\ n(z, E, K_\perp,\ L)\ . \tag{1.4}$$

Of course, normally in these variables one will want to normalize the result per unit volume, per unit total energy, and per unit perpendicular kinetic energy. The present result is the number of particles created per unit time, per unit volume, per unit speed, and per unit μ. The Jacobian provides us with the necessary transformation to change the normalization:

$$\frac{\Sigma}{2\sqrt{2\,m\ \ [E - U(z) - K_\perp]}}\ \sum_{L=1}^{2} \int dK_\perp n(z, E, K_\perp,\ L). \tag{1.5}$$

The angular distribution, spectral distribution, and total density can be easily expressed in terms of the variables z, E, $K_\perp$, and L:

$$n(z, K_\perp) = \sum_{L=1}^{2} \int_0^\infty dE \, \frac{g(z, E, K_\perp, L)}{2\sqrt{2m}\,[E - U(z)\,\sqrt{E - U(z) - K_\perp}} \tag{1.6}$$

$$n(z, E) = \sum_{L=1}^{2} \int_0^\infty dK_\perp \, \frac{g(z, E, K_\perp, L)}{2\sqrt{2m}\,[E - U(z)]\sqrt{E - U(z) - K_\perp}} \, , \tag{1.7}$$

$$n(z) = \sum_{L=1}^{2} \int_0^\infty dE \int_0^\infty dK_\perp \, \frac{g(z, E, K_\perp, L)}{2[E - U(z)]\sqrt{2m[E - U(z) - K_\perp]}} \, . \tag{1.8}$$

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APPENDIX 2

THE COMPUTER PROGRAM FOR THE INTEGRAL METHOD

In this appendix several of the details of the computer program for the integral method are discussed. For the most part, the program is entirely straightforward.

a. Genealogy Chart

Figure 2. 1 is a genealogy chart for the program. It shows the relation of one program to another; in other words, it shows which programs call which other programs and, in turn, are called by which programs. Control flows generally from top to bottom and from left to right.

We now list the various functions of the program:

Program Name	Function
MAIN	Controls everything.
BLOCK DATA	Initializes various variables and asserts the values of various constants.
BOUCON	Calculates the boundary conditions at the electrodes.
DEBUG	A service program generally used to debug all other programs, usually by printing out various arrays, such as the density and potential arrays.
DENSIT	Computes the particle densities.
DEPTH	Computes the optical depth.
DETEJL	Determines the grid point of the left boundary or left reflection point.
DETEJR	Determines the grid point of the right boundary or right reflection point.
ELIODE	Controls the calculation of particle densities.
INITIA	Initializes all variables not initialized by Block Data, esp. arrays.

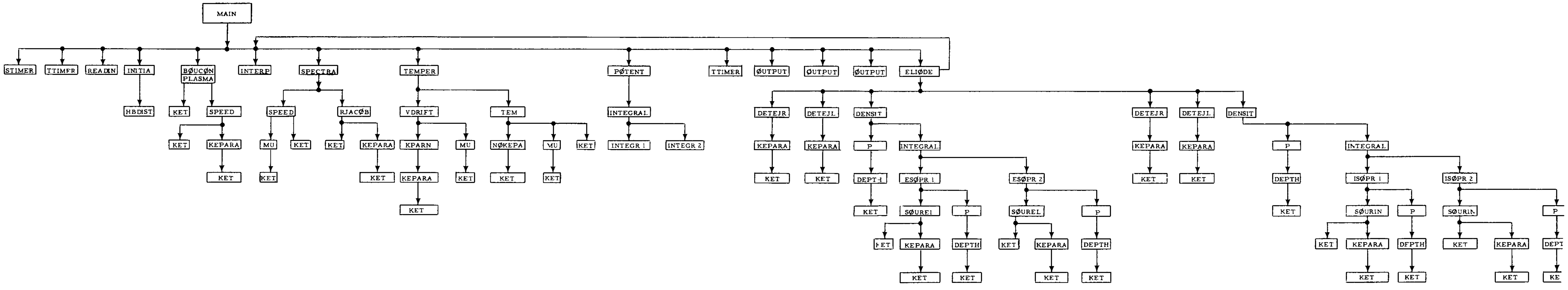

Figure 2. 1 Genealogy Chart of Programs Used in Integral Method.

Program Name	Function
INTEGRAL	Integrates over z by Simpson's rule.
INTERP	Interpolates initial charge distribution.
KEPARA	Calculates the component of the kinetic energy resulting from the parallel component of the velocity.
KET	Calculates the total kinetic energy.
KPARN	Calculates particle flux along axis.
MU	Calculates the direction cosine with respect to the z-axis.
NOKEPA	Calculates the integrand for the temperature calculation.
OUTPOT	Writes potential out.
OUTPUT	Writes out all results.
P	Computes the probability of not scattering between two points.
PLASMA	Computes the boundary condition in the plasma, if required.
POTENT	Computes the potential.
READIN	Reads in all data.
RJACOB	Computes the reciprocal of the Jacobian of the transformation from $z, v, \mu,$ to $z, E, K_{\perp}, L$.
SOUREL	Calculates the source of electrons.
SOURIN	Computes the source of ions.
SPECTRA	Computes the spectral distribution of electron density and ion density.
SPEED	Calculates the speed spectrum.
STIMER	Initializes the clock.
TEM	Calculates the temperature.
TEMPER	Controls the calculation of the drift velocity and the temperature.
TTIMER	Reads out the time elapsed since initialization.
VDRIFT	Calculates the drift velocity.

b. Flow Diagrams

Figures 2. 2, 2. 3 and 2. 4 are flow diagrams of the MAIN program, a program that controls the calculation of particle densities (ELIODE), and a program that determines the grid point of the right boundary or right reflection point (DETEJR). The logic of other programs, except that for DETEJL, is trivial.

The MAIN program consists of an inner iterative loop and an outer iterative loop. In the collisionless case, the directional densities are independent of position, although dependent on both the total energy and perpendicular kinetic energy. Nevertheless, the total densities are dependent on position because the elements of integration are. Additionally, the limits of integration will be dependent on the potential, because the potential defines the accessible and inaccessible regions. It is the purpose of the inner loop to make the potential and total electron and ion density difference self-consistent. The outer loop makes the calculation of the electron and ion directional densities consistent with the potential computed from the inner loop. The total densities are, of course, computed from the directional densities, and these must be used, in turn, to compute the potential.

At present the program may stop because the maximum number of iterations of the outer loop have been carried out, the maximum allotted time has elapsed, or the problem has converged and the specified number of extra ("superconvergence") iterations, if any, have been carried out. Unless the maximum allotted time has elapsed, the program looks for the next case in the data stack. If none is present, the problem is finished, and the computer goes on to the next job. Printing out of results, both formal and informal, of each individual

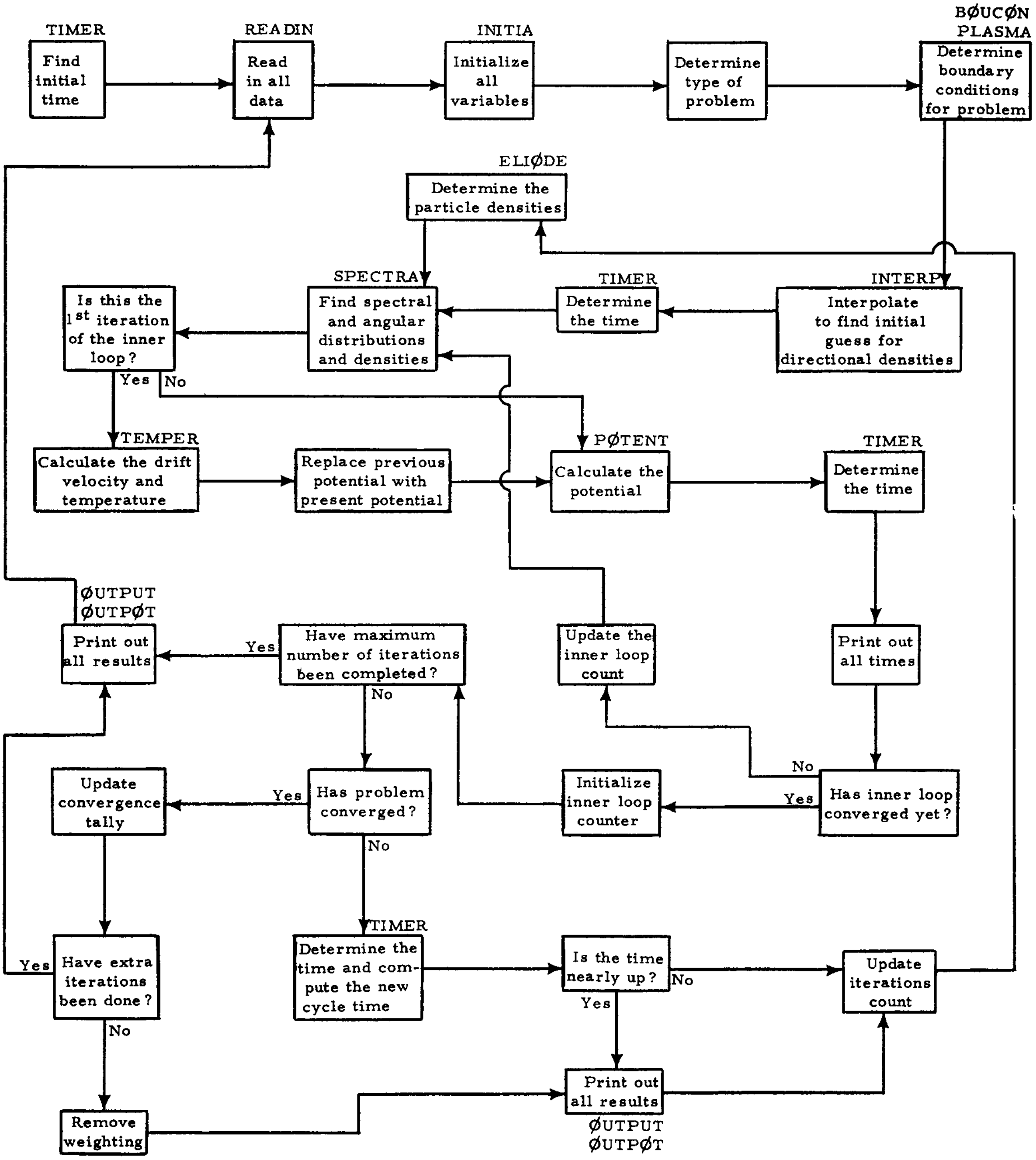

Figure 2. 2 Flow Diagram of Main Program.

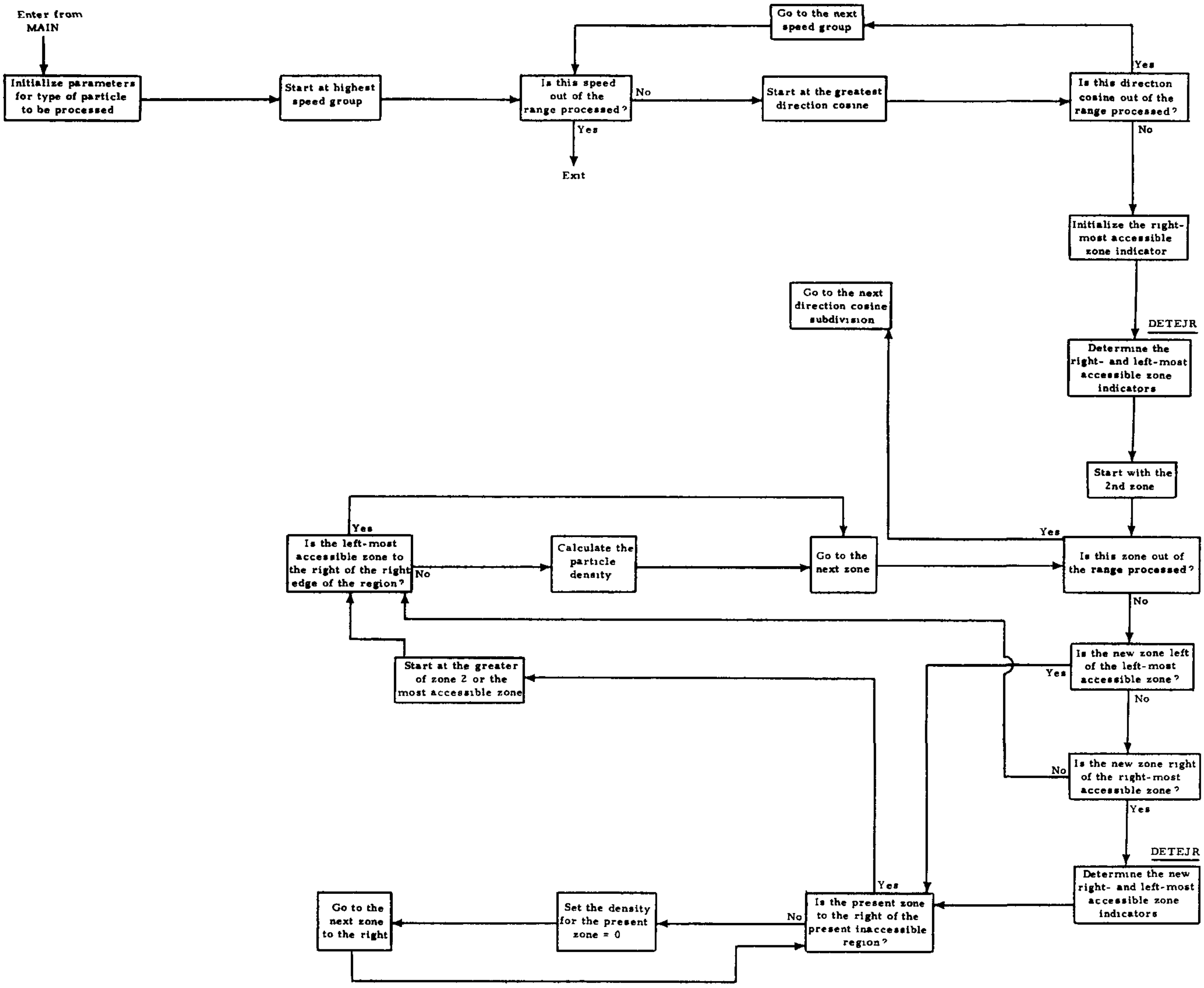

Figure 2. 3 Flow Diagram of the Part of ELIØDE for Particles of One Species Moving from Left to Right. This program controls the calculation of particle densities.

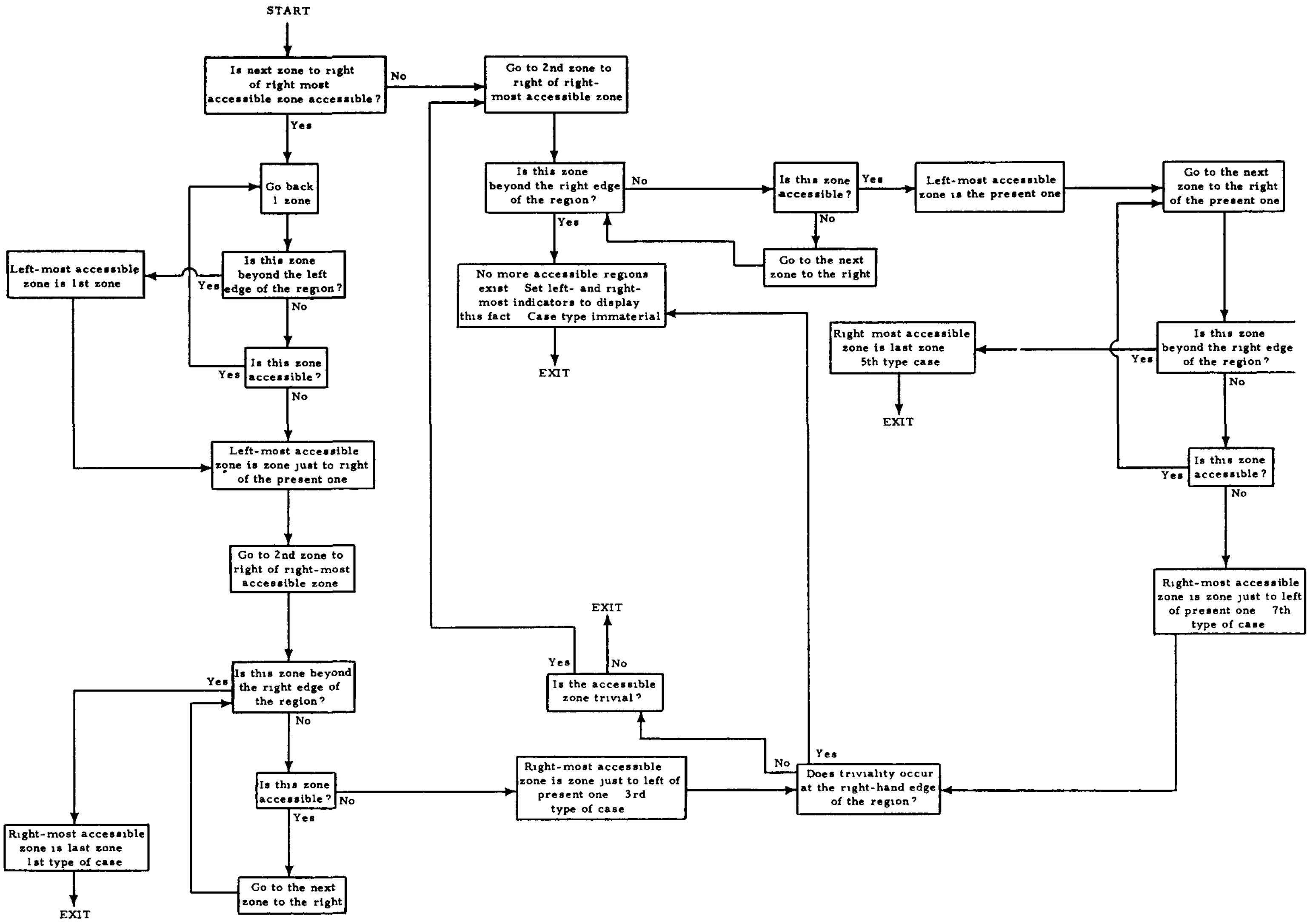

Figure 2.4 Flow Diagram of DETEJR. This program determines the grid point of the right boundary accessible to the particles or the right reflection point at which particles moving to the right are reflected and commence moving to the left.

iteration is suppressed now until the maximum amount of time for the particular case (which may be different from the job time) has nearly elapsed. Thus, one can get more iterations done in the allotted time since printing out does cost machine time. There is also a maximum number of inner loop iterations permitted to prevent the machine from looping endlessly in case convergence does not occur. It has been found repeatedly that the closer the outer loop is to convergence, the more rapidly the inner loop converges.

The convergence criterion is adjustable at object time. Convergence is reckoned by the agreement of the new potential with the old potential. The potential is presumably a very sensitive function of the density difference between the electrons and ions[34] and should form a sensitive test of convergence.

Only a quarter of ELIODE is flow diagrammed because the other parts are substantially identical to the part drawn. Two of the parts relate to electrons and two of the parts relate to ions. One part processes electrons moving to the right (this is the part diagrammed); a second part processes electrons moving to the left. Third and fourth parts process ions moving to the right and left, respectively. These parts are logically identical to the corresponding parts for the electrons. The corresponding parts differ only in the sign of the charge of the particle, the source term, and the scattering cross section. The first and second parts differ from each other only in the interchange of the words (and corresponding symbols) "right" and "left", and the values of the position index denoted the limits of integration are interchanged. Consequently, there is no need to flow diagram these other three parts of ELIODE.

The program DETEJL is logically complex, but it is substantially identical to DETEJR, which is diagrammed. As with ELIODE, only "right" and "left" and the associated end points along the z-axis are interchanged. The logic is otherwise identical to that for DETEJR.

The other logic is relatively trivial, so no flow diagrams of the other subroutines are presented. Such logic as this is usually concerned with calculating the value of some quantity for all spatial zones, all speed groups, or all direction cosines. Tests appear with some frequency for not allowed values of some quantity being evaluated; if the value is not allowed, some value is assigned or some course of action is taken to bypass a calculation as irrelevant for such a case.

c. The Program

Much of the program is believed to be self-explanatory in view of the numerous comments made throughout it and in view of the material already presented concerning the basis for the program. There are also numerous checks throughout the program; these are identified by an X in column 1. These checks may be suppressed by deleting an X on the FORTRAN run card. The checks generally seek to determine if a quantity is unreasonably small, unreasonably large, or absurd for some other reason, or if there has been any overflow in the calculation. There were originally many more checking features in the program, but these have been removed gradually as we gained confidence with the program.

Generally symbols are mnemonic and stored in labelled COMMON (really GLOBAL) for transmission to other programs. Occasionally variables are put into argument lists for transmission to subroutines, where it seemed convenient or advantageous. The program has been constructed solely with the thought of quick debugging in mind. It is obvious that it could be enormously speeded up by a different scheme. Basically, to do this one observes that the densities and potentials are computed at all space points, and that the value of the respective quantity at a subsequent space point can be easily related to that at the previously calculated space point, thereby obviating the need to recompute all the relevant integrals for the new space point, as is now done. It was felt that this better method was fancier and, therefore, would be harder to debug, so no effort was expended on it, other than working out the analytical relations needed.

The program prints out all input data immediately after it is read in so that one may check to determine that all data have been entered correctly and to permanently label the case run. Input is further facilitated greatly by use of NAMELIST. The variables may be written in any order, without regard to the field in which they appear, and without justification of any sort. The formal output consists of four tables. The first table lists the position, potential, electric intensity, electron density, ion density, electron current, ion current, electron kinetic energy, and ion kinetic energy. The second table lists the electron speed spectrum as a function of position. The third table lists the ion speed spectrum as a function of position. The fourth table lists the angular distribution of electrons and the angular distribution of ions as functions of position. Output for checking purposes consists of various tables. One table lists the potential of the previous major loop iteration, and the last four potentials of the minor loop iteration (if that many exist), the electron density, the ion density, and the net charge as a function of position. Another form of output lists the complete electron and ion directional density arrays as functions of perpendicular kinetic energy, energy group, and position. The times at which the various points in the program are passed are printed out too. Another table lists the electric potential, the electron density in double precision, the ion density in double precision, the electron temperatures, and the ion temperatures, all as a function of position. All of these nonformal outputs are very useful for debugging, especially the directional density arrays, which give one a feeling that one really knows what is going on.

The program automatically chooses the energy groups consistent with the total number of groups such that approximately equal numbers of particles occur in each group, be they electrons or ions, in the plasma where a Maxwell-Boltzmann distribution obtains.

The program was compiled and run on XDS Sigma 5 computer having 65, 586 words of memory, using XDS extended Fortran IV. Words are either 32 bits or 64 bits long. In floating point numbers the characteristic consumes 8 bits, leaving 24 bits for single precision and 56 bits for double precision words, corresponding to 7 and 15 digits of precision, respectively. The program was coded in double precision throughout because of the need to know the ion-electron density difference very accurately in order to compute the scalar potential with some significance. There seemed to be no trouble whatever from loss of significance in calculating this density difference in double precision. Single precision was never tried, although the program would occupy substantially less fast memory and would run significantly faster. Numbers as small as 5. x 10^{-79} (other than 0 itself) and as large as 7. x 10^{75} can be represented as a result. Integer constants may be as large as 2, 147, 483, 647 or as small as -2, 147, 483, 648. The principal extended Fortran features found to be of use were GLOBAL, REPEAT, and compound statements. GLOBAL can be replaced by labelled common statements in which the label is the same as the variable name stored in the concommitant control section. REPEAT triple statements cannot be replaced by DO statements, but can only be replaced by the appropriate control-variable initialization and IF statements at the beginning, and arithmetic statement for updating the control variable, GO TO, and CONTINUATION statements at the end of the nest of statements enclosed within the loop. It is frequently important that the nest of statements be NOT executed even once if the condition for execution of the nest is NOT satisfied initially. Approximately 49, 000 words were available to the user for his program and library routines. However, by limiting the number of spatial points, angular subdivisions, and speed groups rather severely, it was possible to keep the arrays for the electron and ion directional densities sufficiently small to be able to fit into fast memory for testing purposes. For the actual execution of programs, it would be highly desirable to have at least 8192 more words of fast memory. Removal of the checking features, which may be accomplished by not specifying "X" on the FORTRAN control card, is also quite effective in reducing the demands for fast memory and in speeding up the program. However, the checks were invaluable in quickly isolating errors (which is by far the chief problem in debugging), so the writer was very reluctant to suppress them. The character representation is hexadecimal within the machine.

The input data that must be specified in order to run the program are as follows, together with typical data:

CASE = 2	• A label for the case being run.
EPS = .02	• The maximum potential in volts by which the potential of the previous major iteration may differ from that of the present major iteration after convergence.
IL = 4	• The number of angular subdivisions, counting the perpendicular as one if IL is even, and not counting this line if IL is odd.
JL = 50	• The number of spatial zones.
ML = 4	• The number of historical values used in filtering the potential, including the present value as 1.
NEP = 1.1×10^{19}	• The density of electrons in the plasma, m^{-3}.
NIP = 1.1×10^{19}	• The density of ions in the plasma, m^{-3}.
NL = 4	• The number of speed groups.
PHIR = 1.711	• The work function of the right electrode, volts.
PHIL = 2.798	• The work function of the left electrode, volts.
SIGMAE = .0	• The electron-neutral cross section, m^{-2}.
SIGMAI = 0.	• The ion-neutral cross section, m^{-2}.

SPACIN = 5. x 10^{-6}	• The distance over which the integration occurs, such as the distance from the plasma to the collector, m.
TL = 1920.	• The temperature of the left electrode, °K.
TR = 910.	• The temperature of the right electrode, °K.
TEMRES = 614.	• The temperature of the Cs reservoir, °K.
TPLE = 2300.	• The temperature of electrons in the plasma, °K.
TG = 1415.	• The temperature of the neutral gas in the plasma, °K.
TYPE = 2	• The type of problem being run. If TYPE =1, integration is from one electrode to the other. If TYPE = 2, integration is from the plasma to the right electrode. If TYPE = 3, integration is from the plasma to the left electrode. If TYPE = 4, integration is only along the z axis from the right electrode to the left one. If TYPE = 5, integration is only along the z axis from the right electrode to the plasma. If TYPE = 6, integration is only along the z axis from the plasma to the left electrode.
VL = -1.922	• The potential of the left electrode, volts.
VR = -2.237	• The potential of the right electrode, volts.

VI = 3.893	• The ionization potential of Cs, volts.
ITL = 30	• The maximum number of major loop iterations permitted.
TLEL = 2500	• Temperature of electrons at left electrode, °K.
TREL = 2000	• Temperature of electrons at right electrode, °K.
BETA = .75	• Filter function weighting parameter for low-pass filtering of potential.
BIGNO = $1. \times 10^{56}$	• A big number of intermediate size used to check variables for unreasonably big size.
JMIN = 1	• A parameter that defines the width of a potential minimum as being trivial, z-axis mesh points.
BBIGNO = $1. \times 10^{74}$	• A big number of the biggest size used to check variables for unreasonably big size.
GAMMA = .75	• Filter function weighting parameter for low-pass filtering of the particle density.
IMMAX = 20	• The maximum number of inner loop iterations permitted before an outer loop iteration is performed.
ITIMPR = 120	• The time associated with the printing of output, seconds.

ITIMAX = 1000	• The maximum time the program is to run with suppression of the printing of the output results (to save time), seconds.
IEXTRA = 1	• The number of iterations to be performed over and above those needed for convergence of the outer loop.

All units in the program are MKS. The data may be entered in any order, in any column on a card, providing the last datum is followed with *.

d. Program Improvements

There are several ways in which the present program could be improved with future work also:

1. The checking should be completed.
2. The calculation of the potential itself and the particle density should be recorded so that results already computed are used for the next integration, instead of starting all over again ab initio as done in the present program. Some work has already been done on this subject; it is easy to accomplish; it should greatly speed up the program, which is already running amazingly fast. It is thought that with such reprogramming, each iteration would run as fast as an iteration of the corresponding differential equation. (It is iteresting to observe that integral equations have been used very, very little for the numerical solution of problems, and that books on numerical analysis seldom discuss integral

equations. The writer has never understood this, because integral equations offer many advantages, as mentioned elsewhere in this report. Sometimes the objection is mentioned that the integral equation will take a lot longer for each iterate. It is usually not mentioned that it will converge in far fewer iterates. Certainly, as far as the present integral equation goes, the objection is not well taken.) The integral formulation has proved that it will converge in just a few iterations for many problems, and will probably be much faster indeed, for this reason, than the solution of the corresponding problem by differencing of the related differential equations. Possibly this reprogramming should be done before item 1 is accomplished because some of the checking runs get to be longer than desired, since some of them involve running many speed groups or many angular groups to determine the effects of numerical accuracy, or iterations many times after convergence to determine if the problem has really converged.

3. The total density should be perturbed away from neutrality in such a way that the resulting potential can be computed analytically. This result should then be compared with that computed numerically to ascertain that the numerical calculation of the potential is correct. Preferably, the perturbation should be made in the directional densities so that one also checks the validity of the numerical calculation of the spectrum and total density.

4. It will be observed in some parts of the program, such as PLASMA, RJACOB, SPEED, TEM, VDRIFT, decisions are made as to whether or not a particular zone is accessible, depending upon the sign of the kinetic energy or the perpendicular kinetic energy, rather than going through the complicated logic of DETEJL or DETEJR. As it were, a decision can be made on the spot at the instant needed as to whether a particular zone is or is not accessible. This technique could be employed in ELIODE to simplify this program considerably and to get rid of DETEJL and DETEJR. The parallel kinetic energy (KEPARA) would be used to make this particular decision. The program would run somewhat faster and take somewhat less space too.

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APPENDIX 3

DETAILS OF THE S_n METHOD

In this appendix the details of the S_n method used in the present work are presented.

Since expositions of the S_n method are readily available,[18] we limit ourselves to an outline of the method followed:

The operation

$$\frac{8}{\Delta_n \; \Delta_j \; \Delta_i} \int_{v_{n-1}}^{v_n} dv \int_{z_{j-1}}^{\delta_j} dz \int_{\mu_{i-1}}^{\mu_i} d\mu \text{ (Boltzmann equation)} \tag{3.1}$$

is performed. Here,

$$\Delta_i = \mu_i - \mu_{i-1} , \tag{3.2}$$

$$\Delta_j = z_j - z_{j-1} , \tag{3.3}$$

$$\Delta_n = v_n - v_{n-1} . \tag{3.4}$$

To this end, the approximation

$$n(z, v, \mu) = \left(\frac{\mu - \mu_{i-1}}{\mu_0 - \mu_{i-1}} \right) n(z, v, \mu_i) + \left(\frac{\mu_i - \mu}{\mu_i - \mu_{i-1}} \right) n(z, v, \mu_{i-1}) \tag{3.5}$$

is used, and likewise for the dependences on z and v. The result of these operations is

$$\begin{aligned} & \left[d_n \, c_3 - \Gamma c_1 \right] n_{jni} + \left[\bar{d}_n \, c_3 - \Gamma c_2 \right] n_{jn-1\,i} + \\ + & \left[d_n \, c_4 - \Gamma c_1 \right] n_{j-1ni} + \left[\bar{d}_n \, c_4 - \Gamma c_2 \right] n_{j-1\;n-1i} + \\ + & \left[d_n \, c_5 + \Gamma c_7 \right] n_{jn\,i-1} + \left[\bar{d}_n \, c_5 + \Gamma c_8 \right] n_{j\;n-1\,i-1} + \\ + & \left[d_n \, c_6 + \Gamma c_7 \right] n_{j-1n\,i-1} + \left[\bar{d}_n \, c_6 + \Gamma c_8 \right] n_{j-1\,n-1\,i-1} \\ = & \; f_n \left[S_{jn} + S_{jn-1} + S_{j-1n} + S_{j-1n-1} \right] , \end{aligned}$$

(3.

$$= \frac{f_n \sigma_n N_n}{2} \sum_{i=2}^{IL+1} \Big[d_n (n_{jni} + n_{jni-1}) + \bar{d}_n \, (n_{jn-1i} + n_{nj-1i-1})$$

$$+ d_n (n_{j-1ni} + n_{j-1ni-1}) + \bar{d}_n \, (n_{j-1n-1i} + n_{j-1n-1i-1}) \Big], \qquad (3.7)$$

$$a_i = \frac{1}{3} \, [2\mu_i + \mu_{i-1}] \, , \qquad i \geq 1, \; a_0 = -1, \qquad (3.8)$$

$$\bar{a}_i = \frac{1}{3} \, [\mu_i + 2\mu_{i-1}] \, , \qquad i \geq 1, \qquad (3.9)$$

$$b_i = \frac{2}{3\Delta_i} \, [3 - \mu_i^2 - \mu_i \; \mu_{i-1} - \mu_{i-1}^2], \qquad i \geq 1, \; b_0 = 0 \, , \qquad (3.10)$$

$$c_1 = \frac{b_i}{\langle v_n \rangle} + \frac{2a_i}{\Delta_n} \quad , \qquad (3.11)$$

$$c_2 = \frac{b_i}{\langle v_n \rangle} - \frac{2\, a_i}{\Delta_n} \quad , \qquad (3.12)$$

$$c_3 = \frac{2a_i}{\Delta_j} + N\sigma \, , \qquad (3.13)$$

$$c_4 = \frac{-2\, a_i}{\Delta_j} + N\sigma \, , \qquad (3.14)$$

$$c_5 = \frac{2\, \bar{a}_i}{\Delta_j} + \; N\sigma \, , \qquad (3.15)$$

$$c_6 = \frac{-\, 2\, \bar{a}_i}{\Delta_j} + N\sigma \, , \qquad (3.16)$$

$$c_7 = \frac{b_i}{\langle v_n \rangle} - \frac{2\, \bar{a}_i}{\Delta_n} \quad , \qquad (3.17)$$

$$c_8 = \frac{b_i}{\langle v_n \rangle} + \frac{2\, \bar{a}_i}{\Delta_n} \qquad (3.18)$$

$$d_n = \frac{1}{3}\left[2 v_n + v_{n-1}\right], \tag{3.19}$$

$$\bar{d}_n = \frac{1}{3}\left[v_n + 2 v_{n-1}\right], \tag{3.20}$$

$$f_0 = 1, \tag{3.21}$$

$$f_n = 2, \qquad n \geq 1, \tag{3.22}$$

$$\langle v_n \rangle = \frac{v_n + v_{n-1}}{2}, \tag{3.23}$$

$$\Gamma = \frac{q\mathcal{E}}{m}. \tag{3.24}$$

In integrating from right to left, one solves for $n_{j-1,n,i}$ in terms of everything else In integrating from left to right, one solves for $n_{j,n,i}$ in terms of all else. Various other quantities are needed in the calculation. These are as follows:

$$\int_{z_{j-1}}^{z_j} dz\, \mathcal{E}(z)\, n(z) = \frac{\Delta_j}{6}\left\{2\mathcal{E}_j n_j + \mathcal{E}_j n_{j-1} + \mathcal{E}_{j-1} n_j + 2\mathcal{E}_{j-1} n_{j-1}\right\}, \tag{3.25}$$

$$T(z) = \frac{m}{k\,n(z)} \sum_{n=2}^{NL+1} \Delta_n \left\{\left[\frac{g_n}{36} - \frac{\bar{v} d_n}{3} + \frac{\bar{v}^2}{6}\right] n_n(z) + \right.$$

$$\left. + \left[\frac{\bar{g}_n}{36} - \frac{\bar{v}\,\bar{d}_n}{3} + \frac{\bar{v}^2}{6}\right] n_{n-1}(z)\right\} \tag{3.26}$$

where

$$g_n = 3 v_n^2 + 2 v_n v_{n-1} + v_{n-1}^2 , \tag{3.27}$$

$$\bar{g}_n = v_n^2 + 2 v_n v_{n-1} + 3 v_{n-1}^2 . \tag{3.28}$$

The electric intensity is determined from the following expressions, which are immediately derivable from those given in connection with the all integral method: For integration from left to right:

$$\begin{aligned} \mathcal{E}_j = &\left(\frac{\phi(z_\ell) - \phi(z_r)}{z_r - z_\ell}\right) + \frac{e}{2\epsilon(z_r - z_\ell)} \sum_{k=2}^{JL+1} \Delta_k \Big\{ h_{\ell r k}\left[n_{ik} - n_{ek}\right] \\ &+ \bar{h}_{\ell r k}\left[n_{ik-1} - n_{ek-1}\right]\Big\} + \\ &+ \frac{e\Delta_j}{2\epsilon} \sum_{k=2}^{j} \left[n_{ik} - n_{ek} + n_{ik-1} - n_{ek-1}\right] \end{aligned} \tag{3.29}$$

and for integration from right to left

$$\begin{aligned} \mathcal{E}_j = &\frac{\phi(z_\ell) - \phi(z_r)}{(z_r - z_\ell)} + \frac{e}{2\epsilon(z_r - z_\ell)} \sum_{k=2}^{JL+1} \Big\{ h_{r\ell k}\left[n_{ik} - n_{ek}\right] + \\ &+ \bar{h}_{r\ell k}\left[n_{ik-1} - n_{ek-1}\right]\Big\} \Delta_k - \frac{e}{2\epsilon} \sum_{k=j+1}^{JL+1} \Big[n_{ik} + \\ &- n_{ek} + n_{ik-1} - n_{ek-1}\Big] \Delta_k , \end{aligned} \tag{3.30}$$

where

where

$$h_{\ell r k} = \frac{2}{3} z_k + \frac{1}{3} z_{k-1} - z_r , \tag{3.31}$$

$$\bar{h}_{\ell r k} = \frac{1}{3} z_k + \frac{2}{3} z_{k-1} - z_r , \tag{3.32}$$

$$h_{r \ell k} = \frac{2}{3} z_k + \frac{1}{3} z_{k-1} - z_1 , \tag{3.33}$$

$$\bar{h}_{r \ell k} = \frac{1}{3} z_k + \frac{2}{3} z_{k-1} - z_1 . \tag{3.34}$$

In the calculation, it proved desirable to keep the calculation of the electric intensity up to date to the extent that its value was only one space step behind the calculation of the particle densities. (To keep the electric intensity up to date to the extent that its value was actually at the space step being computed for the particle densities involved solving an array of quadratic equations, which did not seem worth the effort.) It would be very expensive in machine time if the electric intensity were calculated completely anew for each mesh point. Fortunately, the value at the new mesh point is easily related to the value at the previously calculated mesh point. Let S_{LRT} represent the sum over all j in Eq. 3.29 and let S_{LRj} represent the sum up to j in Eq. 3.29. Then, it is easy to show that

$$S_{LRT\,new} = S_{LRT\,old} + \left[(\bar{h}j - d)(1 - \delta_{j,1}) + (hj+1 - d)(1 - \delta_{j,JL+1})\right] * \left[(n_{ij} - n_{ej})_{new} - (n_{ij} - n_{ej})_{old}\right], \quad 1 \le j \le JL + 1 \tag{3.35}$$

$$S_{LRj} = S_{LRj-1} + n_{ij} - n_{ej} + n_{ij-1} - n_{ej-1} . \tag{3.36}$$

Likewise, for integrating from right to left, let S_{RLT} represent the sum over all j in Eq. 3.30 and let S_{RLj} represent the sum down to j + 1 in Eq. 3.30. It is easy to show that

$$S_{RLT\ new} = S_{RLT\ old} + \left[h_{j-1}\,(1-\delta_{j-1,\,1}) + \bar{h}_j\,(1-\delta_{j-1,\,JL+1})\right]$$

$$* \left[(n_{ij-1} - n_{ej-1})_{new} - (n_{ij-1} - n_{ej-1})_{old}\right], \qquad 1 \le j \le JL+1 \qquad (3.37)$$

$$S_{RLj-1} = S_{RLj} - \left[n_{ij} - n_{ej} + n_{ij-1} - n_{ej-1}\right]. \qquad (3.38)$$

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APPENDIX 4

DETAILS OF THE S_n COMPUTER PROGRAM

In this appendix we discuss several of the details of the program evolved for the S_n method describing the motion of charged particles in an electric field.

A flow diagram of the main program is shown in Figure 4. 1. The logic is very primitive; the logic of the subroutines is even more elementary, so no flow diagram is presented of these subroutines. No explanation of the flow diagram is believed needed other than the remark that the S_n method requires integration in two directions according to the sign of μ and this fact must be taken into account in the logic, as it is. Figure 4. 2 is a genealogy chart of the S_n program; it is most elementary. The functions of the various subprograms are listed.in Table 4. 1.

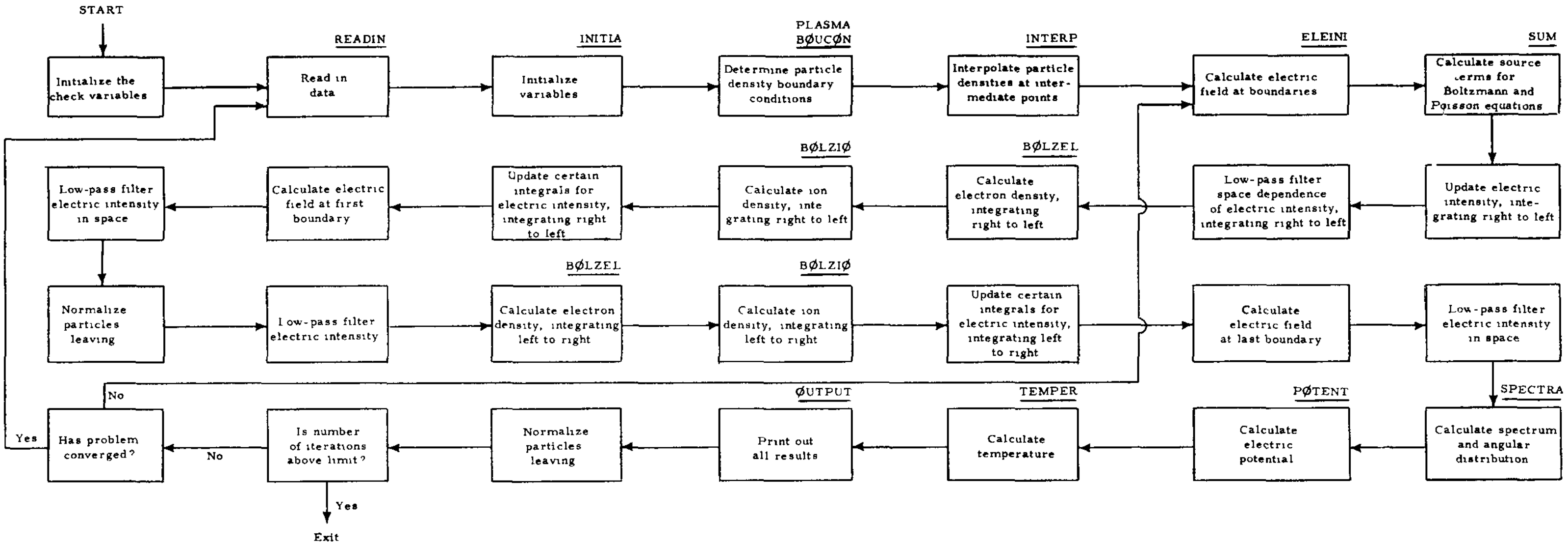

Figure 4.1 Flow Diagram of S_n Method.

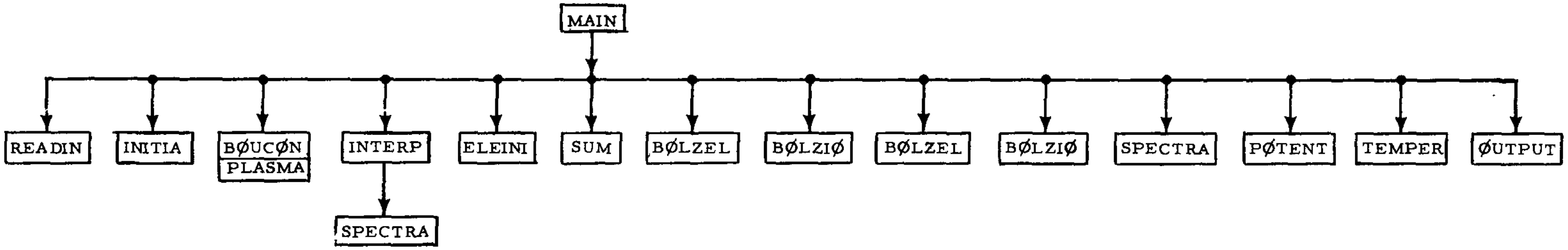

Figure 4.2 Genealogy Chart of S_n Program.

TABLE 4.1

FUNCTIONS OF VARIOUS SUBROUTINES IN S_n PROGRAM

Program Name	Function
BOLZEL	Calculates electron density from source and electric field.
BOLZIO	Calculates ion density from source and electric field.
BOUCON	Calculates boundary conditions at electrodes.
ELEINI	Calculates the bounding values of the electric field.
INITIA	Initializes all variables.
INTERP	Interpolates initial charge distribution.
MAIN	Controls everything.
OUTPUT	Writes out all results.
PLASMA	Calculates boundary conditions at plasma-sheath interface.
POTENT	Calculates the potential.
READIN	Reads in all data.
SPECTRA	Calculates the spectral and angular distribution of the electron and ion densities.
SUM	Calculates sums needed for source terms in the equations for the electron and ion densities.
TEMPER	Calculates the temperatures and drift velocities of the electrons and ions.

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APPENDIX 5

PROGRAM FOR INTEGRAL FORMULATION

```
 JØB TECØ,4137,A
 LIMIT (TIME,30),(UØ,500),(DØ,2)
 FØRTRAN SI,GØ,LS,X
C MELVILLE CLARK
C
C PRØGRAM NUMBERS ARE AS FØLLØWS:
C MAIN, 6;BØUCØN, 3;CØEFEL,25;CØEFIN, 26;DEBUG, 12;DENSIT, 2;DEPTH, 27;
C DETEJL, 16; DETEJR, 15; FLIØDE, 1; INITIA, 5;INTEGRAL, 11;
C INTERP, 14; KEPARA, 17; KET, 18; KPARN, 30; ØUTPUT, 7; P, 21;
C PLASMA, 8;PØTENT, 4;READIN, 10; RJACØB, 22; SØLREL, 23; SØURIN, 24;
C SPECTRA, 9; TEM, 29; TEMPER, 13; VDRIFT, 28; NØKEPA, 19
C
C PRØGRAM NUMBER 6
C THIS PRØGRAM USES MKS RATIØNALIZED UNITS INTERNALLY


C CØNTRØLS EVERYTHING
C IF TYPE = 1, INTEGRATE FRØM RIGHT ELECTRØDE TØ LEFT ØNE AND BACK TØ
C RIGHT ELECTRØDE. IF TYPE = 2, INTEGRATE FRØM PLASMA TØ RIGHT ELECTRØDE
C AND BACK TØ PLASMA. IF TYPE = 3, INTEGRATE FRØM PLASMA TØ LEFT
C ELECTRØDE AND BACK TØ PLASMA. IF TYPE = 4, INTEGRATE ØNLY ALØNG AXIS
C FRØM RIGHT ELECTRØDE TØ LEFT ØNE. IF TYPE = 5, INTEGRATE ØNLY ALØNG
C AXIS FRØM RIGHT ELECTRØDE TØ PLASMA. IF TYPE = 6, INTEGRATE ØNLY ALØNG
C AXIS FRØM PLASMA TØ LEFT ELECTRØDE.
C Z-AXIS IS PØSITIVE TØ THE RIGHT AND NEGATIVE TØ THE LEFT.
      IMPLICIT REAL*8 (A-H, Ø-Z)
      REAL*8 NETT,NITT
      INTEGER*4 TYPE
      GLØBAL LI, TL, PHIL, JL, TR, PHIR, JLP, LIP, IT, ITL,PØT(051,4),
     A CØDEN, ML, EPS,NL,TYPE,CSLE,CSLER,CSLEL,CNDEN,GAMMA,IMMAX,IM,
     B PØTP(051),NETT(051),NITT(051),ITIMPR,ITIMAX,IEXTRA,ITIMA,
     C ITIMI,ITIMCY
X     IF FLØATING ØVERFLØW 500,500
X500  CØNTINUE
      CALL STIMER
      CALL TTIMER(ITIMI)
C RETURN PØINT TØ EXECUTE THE NEXT JØB IN THE STACK
2     CØNTINUE
      ITALLY = 0; ITIMCY = 0
C READ IN THE INPUT DATA
      CALL READIN
      WRITE(108,403) ITIMAX,ITIMPR,IEXTRA
403   FØRMAT(' ','ITIMAX=',I4,X,'ITIMPR=',I4,X,'IEXTRA=',I4)
C CALCULATE THE INITIAL VALUES ØF ALL VARIABLES PØSSIBLE
      CALL INITIA
      IM = 1
C INTEGRATE FRØM LEFT ELECTRØDE TØ RIGHT ELECTRØDE
      IF(TYPE .EQ. 1 .ØR. TYPE .EQ. 4), LI = 1; CSLE = CSLEL;
     A CALL BØUCØN(TL,PHIL); LI = JL+1; CSLE = CSLER;
     B CALL BØUCØN(TR,PHIR); GØ TØ 8
C INTEGRATE FRØM PLASMA TØ RIGHT ELECTRØDE
      IF(TYPE .EQ. 2 .ØR. TYPE .EQ. 5), LI = JL+1;CSLE = CSLER;
     A CALL BØUCØN(TR,PHIR); JLP = 1; LIP = 2; CALL PLASMA; GØ TØ 8
C INTEGRATE FRØM LEFT ELECTRØDE TØ PLASMA
      IF(TYPE .EQ. 3 .ØR. TYPE .EQ. 6), LI = 1; CSLE = CSLEL;
     A CALL BØUCØN(TL,PHIL); JLP = JL+1; LIP = 1;CALL PLASMA; GØ TØ 8
      ØUTPUT, 'MAIN3', TYPE
8     CØNTINUE
C INTERPØLATE THE ELECTRØN AND IØN DENSITIES BETWEEN THEIR BØUNDING
C VALUES TØ GET INITIAL TRIAL VALUES AT VARIØUS PØSITIØNS
      CALL INTERP
      CALL TTIMER(ITIMA)
      GØ TØ 22
3     CØNTINUE
      CNDEN = (1.0D0 - GAMMA)/(1.0D0 - GAMMA**(IT+1))
      CØDEN = (1.0D0 - GAMMA**IT)*GAMMA/(1.0D0 - GAMMA**(IT+1))
C CALCULATE THE PARTICLE DENSITIES AT ALL PØINTS
      CALL FLIØDE
22    CØNTINUE
```

```
C CALCULATE THE SPECTRUM
        CALL SPECTRA
        IF(IM .GT. 1), GO TO 6
C CALCULATE THE ELECTRON AND ION TEMPERATURES AS A FUNCTION OF POSITION
        CALL TEMPER
C SAVE THE OLD POTENTIAL
        REPEAT 5, FOR JP = (2,JL,1)
5       POTP(JP) = POT(JP,1)
6       CONTINUE
C CALCULATE THE POTENTIAL
        CALL POTENT
        CALL TTIMER(ITIMC)
        WRITE(108,402) IM,IT,ITIMA,ITIMB,ITIMC,ITIMI,ITIMCY,ITALLY
402     FORMAT (' ','IM=',I4,X,'IT=',I4,X,'ITIMA=',I8,X,'ITIMB=',I8,X,
     A  'ITIMC=',I8,X,'ITIMI=',I8,X,'ITIMCY=',I5,X,'ITALLY=',I4)
C INNER LOOP ITERATION CONVERGENCE TEST
        REPEAT 4, FOR JP1 = (2,JL,1)
4       IF(DABS(POT(JP1,1)-POT(JP1,2)) .GT. EPS .AND. IM .LE. IMMAX),
     A  IM = IM+1; GO TO 22
        IM = 1
C COUNT THE ITERATIONS AND DO NOT EXCEED ITERATION LIMIT
        IF(IT .GT. ITL) OUTPUT, 'MAIN1',POTP, POT; GO TO 13
C MAXIMUM NUMBER OF ITERATIONS TOLERATED HAVE BEEN EXHAUSTED.. EXIT.
C MAXIMUM NUMBER OF ITERATIONS IS NOT YET EXHAUSTED.
C TEST TO DETERMINE IF CONVERGENCE HAS BEEN ACHIEVED
        DO 11 JP = 2, JL,1
11      IF(DABS(POT(JP,1) - POTP(JP)) .GT. EPS .OR. IT .LE. 1), GO TO 7
C ITERATE AGAIN. CONVERGENCE NOT ACHIEVED
C CONVERGED. UPDATE CONVERGENCE TALLY.
        ITALLY = ITALLY + 1
        IF(ITALLY .GT. IEXTRA), GO TO 13
C EXTRA CONVERGENCES HAVE BEEN DONE.
C EXTRA CONVERGENCES HAVE NOT BEEN DONE.
C PRINT OUT RESULTS. CLEAN UP DENSITY ARRAYS IN NEXT ITERATION.
        GAMMA = 0.D0; OUTPUT,GAMMA,ITALLY
1       CONTINUE
C PRINT POTENTIAL
        CALL OUTPOT
C PRINT ALL RESULTS
        CALL OUTPUT
9       CONTINUE
C KEEP GOING & GET AS MUCH DONE AS POSSIBLE BEFORE TIME IS UP.
        IT = IT + 1
        GO TO 3
7       CONTINUE
C UPDATE THE MAXIMUM CYCLE TIME.
        CALL TTIMER(ITIMB)
        ITIMCY = MAXO(ITIMCY,IABS(ITIMA-ITIMB))
        ITIMA = ITIMB
        IF(IABS(ITIMB-ITIMI) .LT. ITIMAX-(ITIMPR+ITIMCY)),GO TO 9
C PLENTY OF TIME REMAINS. BYPASS RESULT OUTPUT.
C TIME IS NEARLY UP. PRINT OUT RESULTS.
        GO TO 1
```

```
13        CONTINUE
C PRINT OUT ALL RESULTS
          CALL OUTPAT
          CALL OUTPUT
C CONTINUE READING DATA UNTIL ALL ARE EXHAUSTED
          OUTPUT,'END OF PRESENT CASE'; GO TO 2
          END
C MELVILLE CLARK
C
          BLOCK DATA
C
C INITIALIZES VARIOUS VARIABLES AND ASSERTS VALUES OF CONSTANTS
          INTEGER*4 IL/4/, ITL/10/, ML/4/,  NL/4/, TYPE/1/, JMIN/2/,
      A   IMMAX/4/
X         INTEGER Z1/1/,Z2/2/,Z3/3/,Z4/4/
          REAL*8 E/1.6021D-19/,                          EPS/.01/
          REAL*8 EPSILO/8.854D-12/,H/6.625D-34/,K/1.3804D-23/
          REAL*8 ME/9.108D-31/,MI/2.206927D-25/,NEP/0./,NIP/0./,BETA/0./
          REAL*8 PI/3.141592653589793/,VI/3.893/,TLEL/2500./,TREL/2000./
          REAL*8 CODEN/0.D0/,CNDEN/1.D0/,GAMMA/0.D0/
X         REAL*8 BIGNO/1.E74/,BBIGNO/1.E74/
          GLOBAL E,             EPS,EPSILO,H,K,ME,MI,
      A   NEP, NIP, BETA, PI, VI, TLEL, TREL,ML, NL,JMIN,IL,TYPE,ITL,
      B   CODEN,CNDEN,IMMAX,GAMMA
X         GLOBAL Z1,Z2,Z3,Z4,BIGNO,BBIGNO
          END
C MELVILLE CLARK
C
          SUBROUTINE BOUCON(TEMP,PHIW)
C
C PROGRAM NUMBER 3
C CALCULATES BOUNDARY CONDITIONS AT ELECTRODES
          IMPLICIT REAL*8 (A-H,O-Z)
          REAL*8 NE,KET,KEPARA,NI
          COMMON NE(051,09,02,02),NI(051,09,02,02)
          GLOBAL LI,CRE,IL,NL,CSLE,Q,E,IO
C ZERO EMISSION PRESCRIBED FROM EMITTER OR COLLECTOR
          REPEAT 10, FOR N = (1,NL+1,1)
          REPEAT 10, FOR I = (1,(IL+1)/2,1)
          REPEAT 10, FOR L = 1,2
          Q = -E
          TEMPEL = KET(LI,N)
          IF(TEMPEL .LE. 0.D0), NE(LI,N,I,L) = 0.D0; GO TO 1
          NE(LI,N,I,L) = CRE*TEMPEL*DEXP(-(PHIW+TEMPEL)/TEMP)
1         CONTINUE
          Q = E
          TEMPCS = KET(LI,N)
          IF(TEMPCS .LE. 0.D0), NI(LI,N,I,L) = 0.D0; GO TO 2
          NI(LI,N,I,L) = CSLE*TEMPCS*DEXP(-TEMPCS/TEMP)
2         CONTINUE
X         IF(DMIN(NE(LI,N,I,L),NI(LI,N,I,L)).LT. 0.D0 .OR.
X     A   DMAX(NE(LI,N,I,L),NI(LI,N,I,L)).GT. 1.E21) OUTPUT, 'BOUCON4',
X     B   I,LI,N,NE(LI,N,I,L), NI(LI,N,I,L),Q,N,I,KET(LI,N),CRE,TEMPEL,
```

```
X     C  DEXP(-(PHIW+TEMPEL)/TEMP),DEXP(-TEMPCS/TEMP),CSLE,TEMPCS,TEMP,
X     D  PHIW; CALL EXIT
10       CØNTINUE
X        IF FLØATING ØVERFLØW 602, 502
X502     CØNTINUE
         RETURN
X602     ØUTPUT,'ØVERFLØW IN BØLCØN',N,NL,I,IL,L,LI,TEMP,PHIW,CRE,CSLE,
X     A  TEMPCS,TEMPEL,DEXP(-(PHIW+TEMPEL)/TEMP),DEXP(-TEMPCS/TEMP);IØ=2;
X     B  CALL DEBUG('BØUCØN5'); CALL EXIT
         END
C MELVILLE CLARK
C
X        SUBRØUTINE DEBUG(NAME)
C
C PRØGRAM NUMBER 12
C DEBUGS ALL ØTHER SUBRØUTINES UPØN CALL
X        IMPLICIT REAL*8 (A-H,Ø-Z)
X        INTEGER Z1, Z2, Z3, Z4, IØ
X        REAL*8 NE,NI,NETT,NITT,K,NII,NEI,NEN,NIN
X        DIMENSIØN NAME(2)
X        CØMMØN NE(051,09,02,02),NI(051,09,02,02),NEN(051,02,02),
X     A  NIN(051,02,02),NEI(051,09,02),NII(051,09,02)
X        GLØBAL                                 TE(051),TI(051),
X     A  NETT(051),NITT(051),PØT(051),K
X        GLØBAL Z1,Z2,Z3,Z4,IØ
X        IF(IØ .EQ. 1) WRITE(108,400) (NAME(KI), KI = 1,2); GØ TØ 1
X        WRITE(108,401) (NAME(KI), KI = 1,2)
X400     FØRMAT(1H ,2A4,2X, 'INPUT')
X401     FØRMAT(1H ,2A4,2X, 'ØUTPUT')
X1       ØUTPUT,'NE MATRIX, NEI MATRIX, NETT VECTØR'
X        WRITE(108,500)((KN,(KJ,(NE(KJ,KN,1,1),NE(KJ,KN,2,1),
X     A                             NE(KJ,KN,2,2),NE(KJ,KN,1,2),
X     B  NEI(KJ,KN,1)+NEI(KJ,KN,2),NETT(KJ)),KJ=1,51),KN=1,9))
X500     FØRMAT(('0','N=',I4,X,'J=',I4,1P6E11.3/,50(8X,'J=',I4,
X     A  1P6E11.3/)))
X        ØUTPUT,'NI MATRIX, NII MATRIX, NITT VECTØR'
X        WRITE(108,500)((KN,(KJ,(NI(KJ,KN,1,1),NI(KJ,KN,2,1),
X     A                             NI(KJ,KN,2,2),NI(KJ,KN,1,2),
X     B  NII(KJ,KN,1)+NII(KJ,KN,2),NITT(KJ)),KJ=1,51),KN=1,9))
X        ØUTPUT,'NEN MATRIX, NIN MATRIX'
X        WRITE(108,502)(KJ,NEN(KJ,1,1),NEN(KJ,2,1),
X     A                NEN(KJ,2,2),NEN(KJ,1,2),NIN(KJ,1,1),NIN(KJ,2,1),
X     B                             NIN(KJ,2,2),NIN(KJ,1,2),KJ=1,51)
X502     FØRMAT('0', 1('J=',I4,X,1P08E10.2/),50(X,'J=',I4,X,1P08E10.2/))
X        ØUTPUT, 'ELECTRIC PØTENTIAL, ELECTRØN DENSITY, IØN DENSITY,',
X     A  'ELECTRØN TEMPERATURE, IØN TEMPERATURE'
X        WRITE(108,501) (KJ,PØT(KJ), NETT(KJ), NITT(KJ), TE(KJ)/K,
X     A  TI(KJ)/K, KJ=1,51)
X501     FØRMAT('1', 'J =' , I4,X,1P1E11.3,1P2D23.15,1P2E11.3/,50(X,
X     A  'J =',I4,X,1P1E11.3,1P2D23.15,1P2E11.3/))
X        RETURN
X        END
C MELVILLE CLARK
```

```
C
          SUBROUTINE DENSIT(JD, ND, ID, LD, SOUPR1, SOUPR2, COEF, NN)
C
C         PROGRAM NUMBER 2
C COMPUTES THE PARTICLE DENSITIES
          IMPLICIT REAL*8(A-H, O-Z)
          REAL*8 NN, INTEGRAL
          DIMENSION NN(051,09,02,02)
          GLOBAL NCASE,CNDEN,  JLL, JRL, LDL, LDR, J3,CODEN,BRIGNO
          EXTERNAL SOUPR1, SOUPR2
          GO TO (1,2,1,4,5,2,7,8), NCASE
C PARTICLE GOES FROM LEFT BOUNDARY TO RIGHT BOUNDARY
C PARTICLE GOES FROM LEFT BOUNDARY TO RIGHT REFLECTION POINT
1         J1 = JLL; LDL = 2; LDR = 2
3         TEMPD1 = NN(J1,ND,ID,LDR)*P(J1,JD,ND,ID) + COEF*INTEGRAL(J1,JD,
     A    SOUPR1,ND,ID)
          NN(JD,ND,ID,LDL) = CNDEN*TEMPD1 + CODEN*NN(JD,ND,ID,LDL)
X         IF(NN(JD, ND, ID, LDL) .LT.0.D0.OR. NN(JD, ND, ID, LDL) .GT.
X    A    BRIGNO),OUTPUT, 'DENSI3', NN(JD, ND, ID, LDL), J1, ND, ID, LDL,
X    B    BRIGNO,NN(J1, ND, ID, LDR), LDR, JD, CODEN,CNDEN,TEMPD1,
X    C    P(J1, JD, ND, ID), COEF,
X    D    INTEGRAL(J1, JD, SOUPR1, ND, ID),NCASE; CALL EXIT
X         IF FLOATING OVERFLOW 601, 501
X501      CONTINUE
          GO TO 100
C PARTICLE GOES FROM RIGHT TO LEFT FROM ONE BOUNDARY TO THE OTHER
2         J1 = JRL; LDR = 1; LDL = 1; GO TO 3
C PARTICLE GOES FROM LEFT BOUNDARY TO RIGHT WHERE IT IS REFLECTED
C BY THE POTENTIAL AND THEN MOVES TO THE LEFT
4         J1 = JLL; J3 = JRL; LDL = 1; LDR = 2
6         TEMPD4 = NN(J1,ND,ID,LDR)*P(J1,J3,ND,ID)*P(J3,JD,ND,ID) + COEF*
     A    (INTEGRAL(JD,J3,SOUPR1,ND,ID) + INTEGRAL(J1,J3,SOUPR2,ND,ID)*
     B    P(J3,JD,ND,ID))
          NN(JD,ND,ID,LDL) = CNDEN*TEMPD4 + CODEN*NN(JD,ND,ID,LDL)
X         IF(NN(JD, ND, ID, LDL).LT.0.D0.OR. NN(JD, ND, ID, LDL) .GT.
X    A    BRIGNO),OUTPUT, 'DENSI4', NN(JD, ND, ID, LDL), JD, ND, ID, LDL,
X    B    LDR, P(J1, J3, ND, ID), P(J3, JD, ND, ID), CNDEN,CODEN,TEMPD4,
X    C    COEF,INTEGRAL(JD,J3,SOUPR1,
X    D    ND, ID), INTEGRAL(J1, J3, SOUPR2, ND, ID), P(J3, JD, ND, ID),
X    E    J1, J3, JLL, JRL,BRIGNO,NCASE; CALL EXIT
X         IF FLOATING OVERFLOW 602, 502
X502      CONTINUE
          GO TO 100
C PARTICLE GOES FROM RIGHT BOUNDARY TO LEFT WHERE IT IS REFLECTED
C BY THE POTENTIAL AND THEN MOVES TO THE RIGHT
5         J1 = JRL; J3 = JLL; LDL = 2; LDR = 1; GO TO 6
C PARTICLE GOES TO THE RIGHT AFTER EXPERIENCING MULTIPLE REFLECTIONS
7         J1 = JRL; J3 = JLL; LDL = 2
10        TEMPD7 = (INTEGRAL(J3,JD,SOUPR1,ND,ID) +
     A    INTEGRAL(J3,J1,SOUPR2,ND,ID)*P(J3,JD,ND,ID))
          TEMPDE = P(J3,J1,ND,ID)
          IF(1.D0 - TEMPDE .LE. 0.D0),TEMPD7 = NN(JD,ND,ID,LDL);
     A    GO TO 9
```

```
         TEMPD7 = (CØEF*TEMPD7)/(1.D0 - (TEMPDE**2))
         NN(JD,ND,ID,LDL) = CNDEN*TEMPD7 + CØDEN*NN(JD,ND,ID,LDL)
9        CØNTINUE
X        IF(NN(JD, ND, ID, LDL) .LT.0.D0.ØR. NN(JD, ND, ID, LDL) .GT.
X     A  BBIGNØ),ØUTPUT, 'DENSI5', NN(JD, ND, ID, LDL), JD, ND, ID, LDL,
X     B  INTEGRAL(J3,JD,SØUPR1,ND,ID),J3,SØUPR1(JD,ND,ID),INTEGRAL(J3,J1,
X     C  SØUPR2,ND,ID),SØUPR2(JD,ND,ID),P(J3,JD,ND,ID),CØEF,
X     D  J1, TEMPDE,TEMPD7,     J1,LDL,LDR,NN(J1,ND,ID,LDL),J1,ND,ID,
X     E  NN(JD,ND,ID,LDL),CNDEN,CØDEN,CØEF,
X     F                                  J3,NN(J1,ND,ID,LDR), BBIGNØ,
X     G  P(J1,JD,ND,ID),INTEGRAL(J1,JD,SØUPR1,ND,ID),
X     H  INTEGRAL(JD,J3,SØUPR1,ND,ID),INTEGRAL(J1,J3,SØUPR2,ND,ID),NCASE;
X     I  CALL EXIT
X        IF FLØATING ØVERFLØW 603, 503
X503     CØNTINUE
100      CØNTINUE
         RETURN
C PARTICLE GØES TØ THE LEFT AFTER EXPERIENCING MULTIPLE REFLECTIØNS
8        J1 = JLL; J3 = JRL; LDL = 1; GØ TØ 10
X601     ØUTPUT, 'ØVERFLØW IN DENSIT FØR NCASE = 1,2,3, ØR 6',NCASE,JD,
X     A  ND,ID,LDL,J1,LDR,JLL,JRL,NN(JD,ND,ID,LDL),NN(J1,ND,ID,LDR),
X     B  CNDEN,CØDEN,TEMPD1,P(J1,JD,ND,ID),CØEF,
X     C  INTEGRAL(J1,JD,SØUPR1,ND,ID); CALL EXIT
X602     ØUTPUT,'ØVERFLØW IN DENSIT FØR NCASE = 4 ØR 5',NCASE,JD,ND,ID,
X     A  LDL,LDR,J1,J3,P(J1,J3,ND,ID),P(J3,JD,ND,ID),NN(JD,ND,ID,LDL),
X     B  NN(J1,ND,ID,LDR),CNDEN,CØDEN,TEMPD4,CØEF,
X     C                          INTEGRAL(JD,J3,SØUPR1,ND,ID),
X     D  INTEGRAL(J1,J3,SØUPR2,ND,ID),P(J3,JD,ND,ID); CALL EXIT
X603     ØUTPUT,'ØVERFLØW IN DENSIT FØR NCASE = 7 ØR 8',NCASE,J1,JRL,
X     A  J3,JLL,LDL,JD,ND,ID,CØEF,TEMPD7,NN(JD,ND,ID,LDL),CNDEN,CØDEN,
X     B  P(J3,J1,ND,ID),INTEGRAL(J3,JD,SØUPR1,ND,ID),P(J3,JD,ND,ID),
X     C  INTEGRAL(J3,J1,SØUPR2,ND,ID); CALL EXIT
         END
C MELVILLE CLARK
C
         FUNCTIØN DEPTH(JDP, NDP, IDP)
C
C        PRØGRAM NUMBER 27
C CØMPUTES THE ØPTICAL DEPTH
         IMPLICIT REAL*8 (A-H,Ø-Z)
         REAL*8 MU,KEP,KET
         GLØBAL BIGNØ, SIGMA,KEP(10,04)
X        IF(KET(JDP,NDP) .LT. 0.D0 .ØR. KEP(NDP,IDP) .LT. 0.D0), ØUTPUT,
X     A  'DEPTH6', JDP,IDP,NDP,KET(JDP,NDP),KEP(NDP,IDP); CALL EXIT
         TEMP =1.D0- (KEP(NDP,IDP)/KET(JDP,NDP))
X        IF(TEMP.LT.0.D0), ØUTPUT, 'DEPTH4', NDP,IDP,JDP,KEP(NDP,IDP),
X     A  KET(JDP,NDP); CALL EXIT
         MU = DABS(DSQRT(TEMP))
X        IF(MU .GT.1.D0.ØR. MU.LT.0.D0), ØUTPUT, 'DEPTH5', NDP, IDP, JDP,
X     A  KEP(NDP,IDP), KET(JDP,NDP), TEMP, MU; CALL EXIT
         DEPTH = SIGMA/MU
X        IF(DEPTH .LT.0.D0.ØR. DEPTH .GT. BIGNØ), ØUTPUT, 'DEPTH3',
X     A  SIGMA, JDP, NDP, IDP, MU, DEPTH; CALL EXIT
```

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      RETURN
      END
C MELVILLE CLARK
C
      SUBROUTINE DETEJL (JDT,NDT,IDT)
C
C     PROGRAM NUMBER 16
C     DETERMINES THE GRID POINT OF THE LEFT BOUNDARY OR LEFT
C   A REFLECTING POINT
      IMPLICIT REAL*8 (A-H, O-Z)
      REAL*8 KEPARA
      GLOBAL JLL,JRL,JL,NCASE,JMIN,ITIMB,ITIMI,ITIMAX,ITIMPR,ITIMCY
      IF(KEPARA(JLL-1,NDT,IDT).LE.0.D0), GO TO 10
C INADMISSIBLE REGION. FIND THE NEW JRL AND JLL
C ADMISSIBLE REGION.
      REPEAT 5, FOR JT4 = (JLL  ,JL+1,1)
      IF(KEPARA(JT4,NDT,IDT).LE.0.D0),JRL = JT4-1; GO TO 6
C NEW JRL IS A RIGHT REFLECTION POINT
5     CONTINUE
C NEW JRL IS THE RIGHT ELECTRODE
      JRL = JL+1
6     CONTINUE
C FIND THE NEW INADMISSIBLE REGION. FIND JLL
      REPEAT 11, FOR JT3 = (JLL-2,1, -1)
      IF(KEPARA(JT3,NDT,IDT).LE.0.D0), JLL = JT3+1; NCASE =6; GO TO 4
C INADMISSIBLE REGION AND JLL FOUND
11    CONTINUE
C NO NEW ADMISSIBLE REGION EXISTS
      NCASE = 2
      JLL = 1
      GO TO 20
10    CONTINUE
C FIND THE NEW JRL.
      REPEAT 1, FOR JT1 = (JLL-2, 2, -1)
      IF(KEPARA(JT1,NDT,IDT).GT.0.D0), JRL = JT1;GO TO 2
C THE NEW JRL HAS BEEN FOUND
1     CONTINUE
7     CONTINUE
C THE CASE NUMBER IS NOT NEEDED AND MAKES NO DIFFERENCE.
      JRL = 0; JLL = 0; GO TO 20
2     CONTINUE
C FIND THE NEW JLL
      REPEAT 3, FOR JT2 = (JT1-1, 1, -1)
      IF(KEPARA(JT2,NDT,IDT).LE.0.D0), JLL = JT2+1; NCASE = 8; GO TO 4
C THE NEW JLL HAS BEEN FOUND
3     CONTINUE
C THE LEFT BOUNDARY IS THE LEFT ELECTRODE.
      NCASE = 4
      JLL = 1
      GO TO 20
C IS THE NEW ADMISSIBLE REGION TRIVIAL  IF SO, FIND A NEW REGION.
4     CONTINUE
      IF((JRL-JMIN .LT. 1) .OR. (JRL-JMIN .LT. JLL .AND.JLL .LE. 2)),
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      A   GO TO 7
          IF(JLL .GT. JRL-JMIN),                    GO TO 10
C THE CASE IS TRIVIAL
20        CONTINUE
C THE CASE IS NOT TRIVIAL
X         IF(JRL .LT. JLL    .OR. MIN(JLL,JRL) .LT. 0 .OR. MAX (JRL,JLL)
X     A   .GT. JL+1 .OR. NCASE .LT. 1 .OR. NCASE .GT. 8), OUTPUT,
X     B   'DETERJL3', JDT,     JRL,JLL,JL,NCASE,JMIN,NDT,IDT,JT1,JT2,JT3,
X     C            KEPARA(JLL-1,NDT,IDT),KEPARA(JT3,NDT,IDT),
X     D   KEPARA(JT1,NDT,IDT), KEPARA(JT2,NDT,IDT); CALL EXIT
          IF(IABS(ITIMB-ITIMI) .LT. ITIMAX-(ITIMPR+ITIMCY)),GO TO 8
          WRITE(108,400) JDT,NDT,IDT,NCASE,JLL,JRL
400       FORMAT(' ','JDT=',I4,'NDT=',I4,'IDT=',I4,'NCASE=',I4,'JLL=',I4,
      A   'JRL=',I4)
8         CONTINUE
          RETURN
          END
C MELVILLE CLARK
C
          SUBROUTINE DETERJR(JDT, NDT, IDT)
C
C         PROGRAM NUMBER 15
C DETERMINES THE GRID POINT OF THE RIGHT BOUNDARY OR RIGHT REFLECTION
C POINT
          IMPLICIT REAL*8(A-H, O-Z)
          REAL*8 KEPARA
          GLOBAL  JRL,JLL,NCASE,JL,JMIN,ITIMB,ITIMI,ITIMAX,ITIMPR,ITIMCY
          IF(KEPARA(JRL+1, NDT, IDT).LE.0.D0), GO TO 10
C THE NEW REGION IS INADMISSIBLE.
C THE NEW REGION IS ADMISSIBLE.
          REPEAT 5, FOR JT4 = (JRL   ,1,-1)
          IF(KEPARA(JT4,NDT,IDT).LE.0.D0), JLL = JT4+1; GO TO 6
C THE NEW JLL IS A LEFT REFLECTION POINT
5         CONTINUE
C THE NEW JLL IS THE LEFT ELECTRODE.
          JLL = 1
6         CONTINUE
C FIND THE NEW INADMISSIBLE REGION AND JRL.
          REPEAT 11, FOR JT3 = (JRL+2,JL+1,1)
          IF(KEPARA(JT3, NDT, IDT).LE.0.D0), JRL = JT3-1; NCASE = 3;
      A   GO TO 4
C THE NEW INADMISSIBLE REGION AND JRL HAVE BEEN FOUND
11        CONTINUE
C NO NEW INADMISSIBLE REGION EXISTS.
          NCASE = 1
          JRL = JL + 1
          GO TO 20
10        CONTINUE
C FIND THE NEW LEFT REFLECTING BOUNDARY.
          REPEAT 1, FOR JT1 = (JRL+2, JL   ,1)
          IF(KEPARA(JT1, NDT, IDT).GT.0.D0), JLL = JT1;           GO TO 2
C THE NEW LEFT REFLECTING BOUNDARY AND JLL HAVE BEEN FOUND.
1         CONTINUE
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```
7         CONTINUE
C THE CASE NUMBER IS NOT NEEDED AND MAKES NO DIFFERENCE.
          JRL = JL+2; JLL = JL+2; GO TO 20
2         CONTINUE
C FIND THE NEW RIGHT BOUNDARY.
          REPEAT 3, FOR JT2 = (JT1 + 1, JL + 1, 1)
          IF(KEPARA(JT2, NDT, IDT).LE.0.D0 ), JRL = JT2-1; NCASE = 7;
      A   GO TO 4
C THE NEW RIGHT REFLECTING BOUNDARY AND JRL HAVE BEEN FOUND.
3         CONTINUE
C THE RIGHT BOUNDARY IS THE RIGHT ELECTRODE.
          NCASE = 5
          JRL = JL+1
          GO TO 20
C IS THE NEW ADMISSIBLE REGION TRIVIAL  IF SO, FIND A NEW REGION.
4         CONTINUE
          IF((JLL+JMIN .GT. JL+1) .OR. (JLL+JMIN .GT. JRL .AND. JRL .GE.
      A   JL)), GO TO 7
          IF(JRL .LT. JLL+JMIN),                       GO TO 10
C THE CASE IS TRIVIAL
C THE CASE IS NOT TRIVIAL
20        CONTINUE
X         IF(JRL .LT. JLL    .OR. MIN(JLL, JRL) .LT. 1 .OR. MAX(JRL, JLL)
X     A   .GT. JL+2 .OR. NCASE .LT. 1 .OR. NCASE .GT. 8), OUTPUT,
X     B   'DETE JR3', JDT,NDT,        JRL, JLL, JL, NCASE, JMIN, JT1,
X     C   JT2, JT3, IDT, KEPARA(JRL+1, NDT, IDT), KEPARA(JT3, NDT, IDT),
X     D   KEPARA(JT1, NDT, IDT), KEPARA(JT2, NDT, IDT); CALL EXIT
          IF(IABS(ITIMB-ITIMI) .LT. ITIMAX-(ITIMPR+ITIMCY)),GO TO 8
          WRITE(108,400) JDT,NDT,IDT,NCASE,JLL,JRL
400       FORMAT(' ','JDT=',I4,'NDT=',I4,'IDT=',I4,'NCASE=',I4,'JLL=',I4,
      A   'JRL=',I4)
8         CONTINUE
          RETURN
          END
C MELVILLE CLARK
C
          SUBROUTINE ELIODE
C
C PROGRAM NUMBER 1
C CONTROLS THE CALCULATION OF PARTICLE DENSITIES
          IMPLICIT REAL*8 (A-H,O-Z)
          REAL*8 NE,NI,ISOPR1,ISOPR2
          COMMON NE(051,09,02,02),NI(051,09,02,02)
          GLOBAL  E,Q,SIGMAE,SIGMAI,IL,JL,NL,JRL,JLL,J3, SIGMA,CODEN,
      A                                                  COEFEL,S2MIOP
          EXTERNAL         ISOPR1,ISOPR2,ESOPR1,ESOPR2
          ESOPR1(JI1,NI1,II1) = SOUREL(JI1,NI1,II1)*P(JI1,J,NI1,II1)
          ESOPR2(JI2,NI2,II2) = SOUREL(JI2,NI2,II2)*P(JI2,J3,NI2,II2)
          ISOPR1(JI3,NI3,II3) = SOURIN(JI3,NI3,II3)*P(JI3,J,NI3,II3)
          ISOPR2(JI4,NI4,II4) = SOURIN(JI4,NI4,II4)*P(JI4,J3,NI4,II4)
C CALCULATE ELECTRON DENSITIES FOR ELECTRONS MOVING TO THE RIGHT
          SIGMA = SIGMAE; Q = -E; L = 2
          REPEAT 1, FOR N = (NL+1, 1, -1)
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        REPEAT 2, FOR I = (1,(IL+1)/2,1)
        JRL = 0
        CALL DETEJR(J,N,I)
        REPEAT 3, FOR J = (2, JL+1, 1)
        IF(J .LT. JLL), GO TO 15
        IF(J .LE. JRL), GO TO 31
C FIND THE NEW RIGHT BOUNDARY AND JRL
        CALL DETEJR(J,N,I)
C SET THE PARTICLE DENSITY EQUAL TO ZERO BETWEEN THE OLD RIGHT BOUNDARY
C AND THE NEW LEFT BOUNDARY
15      CONTINUE
        REPEAT 16, FOR JE1 = (J   ,JLL-1,1)
        NE(JE1,N,I,L) = CODEN*NE(JE1,N,I,L)
16      CONTINUE
        J = MAX(JLL,2)
31      CONTINUE
        IF(JLL  .GT. JL+1), GO TO 3
        CALL DENSIT(J,N,I,L,FSOPR1,FSOPR2,COEFEL,NF)
3       CONTINUE
2       CONTINUE
1       CONTINUE
X       IF FLOATING OVERFLOW 601, 501
X501    CONTINUE
C CALCULATE ELECTRON DENSITIES FOR ELECTRONS MOVING TO THE LEFT
        L = 1
        REPEAT 4, FOR N = (NL+1, 1, -1)
        REPEAT 5, FOR I = (1,(IL+1)/2,1)
        JLL = JL + 2
        CALL DETEJL(J,N,I)
        REPEAT 6, FOR J = (JL   , 1, -1)
        IF(J .GT. JRL), GO TO 14
        IF(J .GE. JLL), GO TO 33
C FIND THE NEW LEFT BOUNDARY AND JLL
        CALL DETEJL(J,N,I)
C SET THE PARTICLE DENSITY EQUAL TO ZERO BETWEEN THE OLD LEFT BOUNDARY
C AND THE NEW RIGHT BOUNDARY
14      CONTINUE
        REPEAT 13, FOR JE2 = (J,JRL+1,-1)
        NE(JE2,N,I,L) = CODEN*NE(JE2,N,I,L)
13      CONTINUE
        J = MIN(JRL,JL)
33      CONTINUE
        IF(JRL  .LT. 1), GO TO 6
        CALL DENSIT(J,N,I,L,FSOPR1,FSOPR2,COEFEL,NF)
6       CONTINUE
5       CONTINUE
4       CONTINUE
X       IF FLOATING OVERFLOW 602, 502
X502    CONTINUE
C CALCULATE ION DENSITIES FOR IONS MOVING TO THE RIGHT
        SIGMA = SIGMAI; Q = F; L = 2
        REPEAT 7, FOR N = (NL+1, 1, -1)
        REPEAT 8, FOR I = (1,(IL+1)/2,1)
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          JRL = 0
          CALL DETEJR(J,N,I)
          REPEAT 9, FØR J = (2, JL+1, 1)
          IF(J .LT. JLL), GØ TØ 17
          IF(J .LE. JRL), GØ TØ 41
C FIND THE NEW RIGHT BØUNDARY AND JRL
          CALL DETEJR(J,N,I)
C SET THE PARTICLE DENSITY EQUAL TØ ZERØ BETWEEN THE ØLD RIGHT BØUNDARY
C AND THE NEW LEFT BØUNDARY
17        CØNTINUE
          REPEAT 26, FØR JE3 = (J  ,JLL-1,1)
          NI(JE3,N,I,L) = CØDEN*NI(JE3,N,I,L)
26        CØNTINUE
          J = MAX(JLL,2)
41        CØNTINUE
          IF(JLL .GT. JL+1), GØ TØ 9
          CALL DENSIT(J,N,I,L,ISØPR1,ISØPR2,S2MIØP,NI)
9         CØNTINUE
8         CØNTINUE
7         CØNTINUE
X         IF FLØATING ØVERFLØW 603, 503
X503      CØNTINUE
C CALCULATE IØN DENSITIES FØR IØNS MØVING TØ THE LEFT
          L = 1
          REPEAT 10, FØR N = (NL+1, 1, -1)
          REPEAT 11, FØR I = (1,(IL+1)/2,1)
          JLL = JL + 2
          CALL DETEJL(J,N,I)
          REPEAT 12, FØR J = (JL  , 1, -1)
          IF(J .GT. JRL), GØ TØ 18
          IF(J .GE. JLL), GØ TØ 43
C FIND THE NEW LEFT BØUNDARY AND JLL
          CALL DETEJL(J,N,I)
C SET THE PARTICLE DENSITY EQUAL TØ ZERØ BETWEEN THE ØLD LEFT BØUNDARY
C AND THE NEW RIGHT BØUNDARY
18        CØNTINUE
          REPEAT 53, FØR JE4 = (J,JRL+1,-1)
          NI(JE4,N,I,L) = CØDEN*NI(JE4,N,I,L)
53        CØNTINUE
          J = MIN(JRL,JL)
43        CØNTINUE
          IF(JRL .LT. 1), GØ TØ 12
          CALL DENSIT(J,N,I,L,ISØPR1,ISØPR2,S2MIØP,NI)
12        CØNTINUE
11        CØNTINUE
10        CØNTINUE
X         IF FLØATING ØVERFLØW 604, 504
X504      CØNTINUE
          RETURN
X601      ØUTPUT,'ØVERFLØW IN ELIØDF AFTER STATEMENT 1'; CALL EXIT
X602      ØUTPUT,'ØVERFLØW IN ELIØDF AFTER STATEMENT 4'; CALL EXIT
X603      ØUTPUT,'ØVERFLØW IN ELIØDF AFTER STATEMENT 7'; CALL EXIT
X604      ØUTPUT,'ØVERFLØW IN ELIØDF AFTER STATEMENT 10'
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      END
C MELVILLE CLARK
C
      SUBROUTINE INITIA
C
C PRØGRAM NUMBER 5
C INITIALIZES ALL VARIABLES
      IMPLICIT REAL*8 (A-H, Ø-Z)
      INTEGER TYPE
      REAL*8 KEP,K,ME,MI,NCS,NEP,NIP,MBDIST
      GLØBAL PI,SR8ME, R2SRPI,ME,MI,SR8MI,R2ME,    VL,VR,IL,JL,NL,
     A       FNL,DELPØS,DEL1,DEL2,K,TG,TI ,TLEL,TPLE,TR,TREL,Z(051),NCS,
     B PG,DELMU,FJL,FIL,SIGMAE,SIGMAI,C1MB(011),TI(051),BETA,CKF,PHIL,
     C EN(10),      KEP(10,04),TYPE, TE(051),PHIR,CRE,      F,EPSILØ,
     D NEP,NIP,TEMRES,ML,PØT(051,4),   SPACIN,RENCRE,RENCRI,ITL,EPS,
     E VI,H,CSLEL,CSLER,R2MI,S2MEØP,S2MIØP,SR2ME,SR2MI,S2Ø9ME,S2Ø9MI,
     F CØEFEL,PØTP(051),IT,RS2ME,RS2MI
      MBDIST(ENERGY,TEMPE) = S4ØPI*DSQRT(ENERGY/TEMPE)*DEXP(-ENERGY/
     A TEMPE)/TEMPE
      FIL = IL
      FJL = JL
      FNL = NL
      DELPØS = SPACIN/FJL
      PG = (3.2663988D10/DSQRT(TEMRES))*DEXP(-8910./TEMRES)
      NCS = PG/(K*TG)
      CKF = 1.5D0/F
      CØEFEL = 1.D0/2.D0
      CRE = (8.D0*PI/H)*((ME/H)**2)
      DELMU = 2.D0/FIL
      DEL1 = DELPØS/3.D0
      DEL2 = DELPØS/2.D0
      EN(1) = EMIN
      IT = 0
      REPEAT 5, FØR M = (1,ML,1)
      PØT(1,M) = 0.D0
      PØT(JL+1,M) = VR -VL
5     CØNTINUE
      PØTP(1) = 0.D0
      PØTP(JL+1) = VR-VL
      R2ME = 1.D0/(2.D0*ME)
      R2MI = 1.D0/(2.D0*MI)
      RS2ME = DSQRT(R2ME)
      RS2MI = DSQRT(R2MI)
      R2SRPI = 1.D0/(2.D0*DSQRT(PI))
      SIGMAE = NCS*SIGMAE
      SIGMAI = NCS*SIGMAI
      SR8ME = DSQRT(8.D0*ME)
      SR8MI = DSQRT(8.D0*MI)
      S2MEØP = DSQRT(2.D0*ME/PI)
      S2MIØP = DSQRT(2.D0*MI/PI)
      S2Ø9ME = DSQRT(2.D0/(9.D0*ME))
      S2Ø9MI = DSQRT(2.D0/(9.D0*MI))
      S4ØPI = DSQRT(4.D0/PI)
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          TG = K*TG
          TL = K*TL
          TLEL = K*TLEL
          TPLE = K*TPLE
          TR = K*TR
          TREL = K*TREL
          CSLEL = PG*DSQRT(2.D0*MI/(PI*TG))/((TL**2)*(1.D0+2.D0*DEXP(E*(VI
       A  -PHIL)/TL)))
          CSLER = PG*DSQRT(2.D0*MI/(PI*TG))/((TR**2)*(1.D0+2.D0*DEXP(E*(VI
       A  -PHIR)/TR)))
          PHIL = E*PHIL
          PHIR = E*PHIR
          Z(1) = 0.D0
X         IF(DMIN(FIL,FJL,FNL,DELPAS,PG,NCS,RS2ME, DELMU,DELEN,DEL1,DEL2,
X      A  EN(1),IT,SIGMAF,SIGMAI,RS2MI,          R2SRPI,TG,TL,TLEL,TPLE,
X      B  CSLEL,CSLER,S2MEOP,SR8ME,SR8MI,S2MIOP,S2O9ME,S2O9MI,R2ME,R2MI,
X      C  TR,TREL,Z(1),CKE).LT.0.D0.OR.DMAX(FIL,FJL,FNL).GT.1000..OR.
X      D  DELPAS .GT. SPACIN .OR. NCS .GT. 1.E29 .OR. R2ME.GT.6.E29.OR.
X      E  DELEN .GT. EMAX .OR. DEL1 .GT. DELPAS .OR. DEL2 .GT.
X      F  DELPAS.OR.EN(1).GT.EMAX.OR.IT.GT.ITL.OR.R2MI.GT.4.E26.OR.S2O9ME
X      G  .GT.8.E14.OR.RS2MI.GT.2.E13.OR.SR8ME.GT.3.E-15.OR.SR8MI.GT.
X      H  2.E-11.OR.S2MIOP.GT.6.E-12.OR.S2MEOP.GT.8.E-16
X      I  .OR. DMAX(TG,TL,TLEL,   TPLE,TR, TREL) .GT. 2.E-19 .OR. Z(1)
X      J  .GT. SPACIN .OR. RS2ME .GT. 8.E14 .OR. RS2MI .GT. 2.E13),OUTPUT,
X      K  'INIT16',IL,JL,NL,SPACIN,FJL,FIL,FNL,PG,
X      L  TEMRES,NCS,TG,K,        PI,DELMU,DELEN,EMAX,EMIN,DEL1,DEL2,CKE,
X      M  DELPAS,EN(1),SIGMAF,SIGMAI,       ME,       R2SRPI,TL,TLEL,
X      N  TPLE,TR,TREL,Z(1),IT,ITL,CSLEL,CSLER,R2ME,R2MI,S2O9ME,S2O9MI,
X      O  SR8ME,SR8MI,S2MIOP,S2MEOP,MI; CALL EXIT
          REPEAT 19, FOR J = (2,JL,1)
          REPEAT 19, FOR M = (1,ML ,1)
          POT(J,M) = 0.D0
19        CONTINUE
X         REPEAT 10, FOR J = (1,JL+1,1)
X         REPEAT 10, FOR M = (1,ML, 1)
X         IF(DABS(POT(J,M)).GT.10.),OUTPUT,'INIT8',J,POT(J,M);CALL EXIT
X10       CONTINUE
          REPEAT 16, FOR M = (1,ML,1)
          C1MB(M) =1.D0- BETA**M
X         IF(C1MB(M) .LT.0.D0.OR. C1MB(M).GT.1.D0), OUTPUT, 'INIT10', ML,
X      A  BETA,C1MB(M),M; CALL EXIT
16        CONTINUE
          RENCRE = SIGMAF/4.D0
          RENCRI = SIGMAI/(2.D0*(2.D0**0.5D0))
C CALCULATE THE CONSTANTS FOR INTEGRATION OVER SPACE VARIABLES
          DELEN = DMIN(TG,TPLE)/25.D0
          ENER = 0.D0; N = 0; FINAL = 2.D0/(FNL+2.0D0)
2         CONTINUE
          N = N + 1
          SUM1 = 0.D0
1         CONTINUE
          ENER = ENER + DELEN
          SUM1 = SUM1 + (MBDIST(ENER,TPLE) + MBDIST(ENER,TG))*DELEN
```

```
          IF(SUM1 .LE. FINAL), GØ TØ 1
          EN(N) = ENER
          IF(N .LT. NL+1), GØ TØ 2
          EN(NL+2) = 2.D0*FINAL/(MBDIST(ENER,TPLE) + MBDIST(ENER,TG)) +
     A    EN(NL+1)
          WRITE(108,401)
401       FØRMAT ('(',         'ENERGY GRØUPS')
          WRITE(108,400)         (N,EN(N),N=1,NL+2)
400       FØRMAT(' ',          10(I3,X,1PE11.3))
          REPEAT  6, FØR N = (1,NL+2,1)
          KEP(N,1) = 0.D0
          REPEAT 12, FØR I = (2,(IL/2)+1,1)
          KEP(N,I) = (1.D0 - (1.D0 - (I-1)*DELMU)**2)*EN(N)
X         IF(KEP(N,I) .LT. 0.D0), ØUTPUT,'INIT9',KEP(N,I),N,I,DELMU,EN(N);
X    A    CALL EXIT
12        CØNTINUE
X         IF(KEP(N,1) .LT. 0.D0), ØUTPUT,'INIT8',KEP(N,1),N; CALL EXIT
6         CØNTINUE
C CALCULATE THE CØNSTANTS FØR INTEGRATIØN ØVER SPEEDS WITH WHICH A
C PARTICLE MØVES
          DØ 14 J = 2, JL+1,1
          Z(J) = Z(J-1) + DELPØS
X         IF(Z(J).LT.0.D0.ØR.Z(J).GT.SPACIN*(1.D0+EPS)),ØUTPUT,'INITIA5',
X    A    DELPØS,JL,J,Z(J),SPACIN,Z(JL+1); CALL EXIT
14        CØNTINUE
C CØMPUTE THE TEMPERATURES ØF IØNS AND ELECTRØNS AT ALL SPACE PØINTS
          IF(TYPE.EQ.1.ØR.TYPE.EQ.4),TE(1)=TLEL;TDIFFEL=TREL-TLEL;
     A    TE(JL+1)  = TREL; TI(1)=TL;TDIFIØ=TR-TL; TI(JL+1)=
     B    TR; GØ TØ 17
          IF(TYPE .EQ. 2 .ØR. TYPE .EQ. 5), TE(1) = TPLE;
     A    TDIFFEL = TREL-TPLE;  TE(JL+1) = TREL;  TI(1) = TG;
     B    TDIFIØ = TR-TG;  TI(JL+1) = TR; GØ TØ 17
          IF(TYPE .EQ. 3 .ØR. TYPE .EQ. 6), TE(1) = TLEL;
     A    TDIFFEL = TPLE-TLEL;  TE(JL+1) = TPLE;  TI(1) = TL;
     B    TDIFIØ = TG-TL;  TI(JL+1) = TG
17        CØNTINUE
          DØ 15 J = 2, JL,1
          TE(J) = TE(1) + TDIFFEL*Z(J)/SPACIN
          TI(J) = TI(1) + TDIFIØ*Z(J)/SPACIN
X         IF( TE(J) .LE.  TI(J) .ØR.  TE(J) .LT. DMIN(TREL,TPLE,TLEL)
X    A    .ØR.  TE(J) .GT. DMAX(TREL,TPLE,TLEL) .ØR.  TI(J) .LT. DMIN
X    B    (TR,TG,TL) .ØR.  TI(J) .GT. DMAX(TR,TG,TL))ØUTPUT, 'INITIA6',
X    C    TR,TG,TL,TLEL,TPLE,TREL,TDIFFEL,TDIFIØ, TE(J), TI(J),J,JL,Z(J),
X    D    SPACIN; CALL EXIT
15        CØNTINUE
          IF(NIP.LE.0.D0) NIP = NEP
X         IF FLØATING ØVERFLØW 601, 501
X501      CØNTINUE
          RETURN
X601      ØUTPUT,'ØVERFLØW IN INITIA',IL,FIL,JL,FJL,FNL,NL,EMAX,EMIN,E,
X    A    DELPØS,SPACIN,PG,TEMRES,NCS,TG,K,        PI,CKE,CRE,MF,H,DELMU,
X    B    DELEN,DEL1,DEL2,EN,IT,M,ML,VR,VL,SIGMAE,S2Ø9ME,S2Ø9MI,R2ME,R2MI,
X    C    SIGMAI,SR8ME,SR8MI,  R2SRPI,TL,TLEL,TPLE,TR,TREL,CSLEL,VI,PHIL,
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X     D  COLFR,PHIR,    Z,J,POT,C1MB,BETA,RENCRE,RENCRI,KEP,EPS,TYPE,
X     E  TE(1),TDIFFE,TE(JL+1),TI(1),TI(JL+1),TDIFIO,         NIP,NEP;
X     F  CALL EXIT
         END
C MELVILLE CLARK
C
         FUNCTION INTEGRAL (LAI,LBI,QUANTI, NIZ,II)
C
C        PROGRAM NUMBER 11
C INTEGRATES OVER Z BY SIMPSON'S RULE
         IMPLICIT REAL*8 (A-H,O-Z)
         REAL *8 INTEGRAL
         GLOBAL DEL1,DEL2
         EXTERNAL QUANTI
C MAKE LA THE SMALLEST AND LB THE LARGEST LIMITS
         IF(LAI .GT. LBI), LA = LBI; LB = LAI; GO TO 2
         LA = LAI; LB = LBI
2        CONTINUE
         INTEGRAL = 0.D0; JI = LA-2
C CALCULATE AS MUCH OF THE INTEGRAL AS POSSIBLE BY SIMPSON'S RULE
         REPEAT 1, FOR JT = (LA,(LB-2),2)
         JI = JT
1        INTEGRAL = INTEGRAL+DEL1*(QUANTI(JT,NIZ,II) + 4.D0*
      A  QUANTI(JT+1,NIZ,II) + QUANTI(JT+2,NIZ,II))
C CALCULATE THE FINAL STEP IF NECESSARY
         IF(MOD((LB-LA), 2) .GT. 0), INTEGRAL = INTEGRAL+DEL2*
      A  (QUANTI(JI+2,NIZ,II) + QUANTI(JI+3,NIZ,II))
X        IF FLOATING OVERFLOW 601, 501
X501     CONTINUE
         RETURN
X601     OUTPUT,'OVERFLOW IN INTEGRAL'; CALL EXIT
         END
C MELVILLE CLARK
C
         SUBROUTINE INTERP
C
C PROGRAM NUMBER 14
C INTERPOLATES INITIAL CHARGE DISTRIBUTION
         IMPLICIT REAL*8 (A-H, O-Z)
         REAL*8 NE,NI
         COMMON NE(051,09,02,02),NI(051,09,02,02)
         GLOBAL                                    SPACIN,IL,NL,Z(051),
      A  JL,POT(051,4),IO
C INTERPOLATE OVER ALL TOTAL ENERGIES, AND OVER ALL PERPENDICULAR
C KINETIC ENERGIES
         REPEAT 11, FOR N = (1,NL+1,1)
         REPEAT 11, FOR I = (1,(IL+1)/2,1)
         REPEAT 11, FOR L = 1,2
         DIFFE = (NE(JL+1,N,I,L) - NE(1,N,I,L))/SPACIN
         DIFFI = (NI(JL+1,N,I,L) - NI(1,N,I,L))/SPACIN
C INTERPOLATE BETWEEN BOUNDARY VALUES
         REPEAT 11, FOR J = (2,JL,1)
         NE(J,N,I,L) = NE(1,N,I,L) + DIFFE*Z(J)
```

```
          NI(J,N,I,L) = NI(1,N,I,L) + DIFFI*Z(J)
X         IF(NE(J,N,I,L) .LE.0.D0.OR. NI(J,N,I,L).LE.0.D0) OUTPUT,
X     A   'INTERP3', NE(J,N,I,L),NI(J,N,I,L),I,J,N,SPACIN,DIFFE,DIFFI,IL,
X     B   JL,NL,Z(J),L,NE(JL+1,N,I,L),NI(JL+1,N,I,L),NE(1,N,I,L),
X     C   NI(1,N,I,L); CALL EXIT
11        CONTINUE
          REPEAT 10, FOR J = (2,JL,1)
          POT(J,1) = POT(JL+1,1)*Z(J)/SPACIN
X         IF(DABS(POT(J,1)) .GT. 10.),OUTPUT,'INTER4',POT(J,1),J,Z(J),
X     A   SPACIN,POT(JL+1,1),JL; CALL EXIT
10        CONTINUE
X         IF FLOATING OVERFLOW 603, 503
X503      CONTINUE
          RETURN
X603      OUTPUT,'OVERFLOW IN INTERP',NL,IL,L,I,N,SPACIN,DIFFE,DIFFI,Z,JL;
X     A   IO=2; CALL DEBUG('INTERP' ); CALL EXIT
          END
C MELVILLE CLARK
C
          FUNCTION KEPARA(JV, NV, IV)
C
C         PROGRAM NUMBER 17
C CALCULATES THE COMPONENT OF THE KINETIC ENERGY RESULTING FROM THE
C     A   PERPENDICULAR COMPONENT OF THE VELOCITY
          IMPLICIT REAL*8 (A-H,O-Z)
          REAL*8 KEP, KET, KEPARA
          GLOBAL KEP(10,04),BIGNO
          KEPARA = KET(JV, NV)-KEP(NV, IV)
X         IF FLOATING OVERFLOW 601, 501
X501      CONTINUE
X         IF(DABS(KEPARA) .GT. BIGNO), OUTPUT, 'KEPARA3', KET(JV, NV),
X     A   KEPARA, JV, NV, KEP(NV, IV),IV; CALL EXIT
          RETURN
X601      OUTPUT,'OVERFLOW IN KEPARA',KET(JV,NV),JV,NV,KEP(NV,IV),IV ;
X     A   GO TO 501
          END
C MELVILLE CLARK
C
          FUNCTION KET(JK, NK)
C
C         PROGRAM NUMBER 18
C CALCULATES THE TOTAL KINETIC ENERGY
          IMPLICIT REAL*8(A-H, O-Z)
          REAL*8 KET
          GLOBAL POT(051,04),      Q, EN(10),BIGNO
          KET = EN(NK)-Q*POT(JK,1)
X         IF(DABS(KET)                .GT. BIGNO), OUTPUT, 'KET3', NK,
X     A   EN(NK), Q, KET,POT(JK,1),            JK; CALL EXIT
X         IF FLOATING OVERFLOW 601, 501
X501      CONTINUE
          RETURN
X601      OUTPUT,'OVERFLOW IN KET',EN(NK),NK,Q,POT(JK,1),JK;GO TO 501
          END
```

```
C MELVILLE CLARK
C
          FUNCTIØN KPARN(JKP,NKP,IKP,NA)
C
C PRØGRAM NUMBER 30
C CALCULATES PARTICLE FLUX ALØNG AXIS
          IMPLICIT REAL*8 (A-H,Ø-Z)
          REAL*8 NA,KEPARA,KPARN,KPARN1
          DIMENSIØN NA(051,09,02,02)
          GLØBAL BIGNØ
          KPARN1 = KEPARA(JKP,NKP,IKP)
          IF(KPARN1 .LE. 0.D0), KPARN = 0.D0; GØ TØ 1
          KPARN = (NA(JKP,NKP,IKP,2) - NA(JKP,NKP,IKP,1))*DSQRT(KPARN1)
1         CØNTINUE
X         IF(DABS(KPARN) .GT. BIGNØ), ØUTPUT, 'KPARN3', KPARN,JKP,NKP,IKP,
X     A   KEPARA(JKP,NKP,IKP), NA(JKP,NKP,IKP,2), NA(JKP,NKP,IKP,1),
X     B   KPARN1; CALL EXIT
X         IF FLØATING ØVERFLØW 601, 501
X501      CØNTINUE
          RETURN
X601      ØUTPUT,'ØVERFLØW IN KPARN',KPARN,KPARN1,
X     A   NA(JKP,NKP,IKP,2),NA(JKP,NKP,IKP,1),JKP,NKP,IKP; GØ TØ 501
          END
C MELVILLE CLARK
C
          FUNCTIØN MU(JM,NM,IMU,LM)
C
C CALCULATES THE DIRECTIØN CØSINE
C PRØGRAM NUMBER 20
          IMPLICIT REAL*8 (A-H,Ø-Z)
          REAL*8 KEP,MU,KET
          GLØBAL KEP(10,04)
          TEMM = KEP(NM,IMU)/KET(JM,NM)
          IF(TEMM .LT. 0.D0 .ØR. TEMM .GT. 1.D0), MU = 0.D0; GØ TØ 1
X         IF(DABS(TEMM) .GT. 1.D0),ØUTPUT,'MU5',KEP(NM,IMU),KET(JM,NM),
X     A   TEMM,JM,NM,IMU,LM; CALL EXIT
          MU = DSQRT(1.D0 - TEMM)
1         CØNTINUE
          IF(LM .EQ. 1), MU = - MU
X         IF(DABS(MU) .GT. 1.D0), ØUTPUT,'MU3',MU,TEMM,KEP(NM,IMU),
X     A   JM,NM,IMU,LM,KET(JM,NM); CALL EXIT
X         IF FLØATING ØVERFLØW 601, 501
X501      CØNTINUE
          RETURN
X601      ØUTPUT,'MU4',KET(JM,NM),                        TEMM,MU,JM,NM,IMU,LM;
X     A   CALL EXIT
          END
C MELVILLE CLARK
C
          FUNCTIØN NØKEPA(JNØ,NNØ,INØ,LNØ,NFLIØ)
C PRØGRAM NUMBER 19
C CALCULATES INTEGRAND FØR TEMPERATURE CALCULATIØN
          IMPLICIT REAL*8 (A-H,Ø-Z)
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          REAL*8 NELIO,NOKEPA,KET
          DIMENSION NELIO(051,09,02,02)
          GLOBAL BIGNO
          NOKEPA = NELIO(JNO,NNO,INO,LNO)*KET(JNO,NNO)
1         CONTINUE
X         IF FLOATING OVERFLOW 601, 501
X501      CONTINUE
X         IF(DABS(NOKEPA) .GT. BIGNO),OUTPUT,'NOKEPA3',NOKEPA,KET(JNO,NNO)
X     A ,NELIO(JNO,NNO,INO,LNO),NNO,JNO,INO,LNO; CALL EXIT
          RETURN
X601      OUTPUT,'OVERFLOW IN NOKEPA',NOKEPA,KET(JNO,NNO),
X     A   NELIO(JNO,NNO,INO,LNO),JNO,NNO,INO,LNO; CALL EXIT
          END
C MELVILLE CLARK
C
          SUBROUTINE OUTPOT
C
C WRITES POTENTIAL OUT
          IMPLICIT REAL*8 (A-H,O-Z)
          REAL*8 NETT,NITT
          GLOBAL POT(051,04),POTP(051),ML,NETT(051),NITT(051),JL
          WRITE(108,401)
          WRITE(108,400)(J,POTP(J),(POT(J,M),M=1,ML),NETT(J),NITT(J),
      A   NITT(J)-NETT(J),J=1,JL+1)
400       FORMAT (' ','J= ',I4,1P8E11.3/,50(X,'J= ',I4,1P8E11.3/))
401       FORMAT ('0',T10,'POTP(J)',T21,'POT(J,1)',T32,'POT(J,2)',T43,
      A   'POT(J,3)',T54,'POT(J,4)',T65,'NETT(J)',T76,'NITT(J)',T87,
      B   'NET CHARGE')
          RETURN
          END
C MELVILLE CLARK
C
          SUBROUTINE OUTPUT
C
C PROGRAM NUMBER 7
C WRITES OUT ALL RESULTS
          IMPLICIT REAL*8 (A-H, O-Z)
          REAL*8 NEN,NIN,NE,NI,KEP,NEI,NII,NETT,NITT,KEI,KEE,JEJ,JIJ
          DIMENSION KEE(051), KEI(051)
          COMMON NE(051,09,02,02),NI(051,09,02,02),NEN(051,02,02),
      A   NIN(051,02,02),NEI(051,09,02),NII(051,09,02)
          GLOBAL DELPOS,KEP(10,04),EPSILO,E,POT(051,4),NL,IL,JL,IO,
      B   TE(051), TI(051),CKE,JIJ(051),JEJ(051),Z(051),NETT(051),
      C   NITT(051), IT,           BBIGNO
C CALCULATE THE KINETIC ENERGY OF ELECTRONS AND IONS AS A FUNCTION OF
C POSITION
          DO 14 J = 1, JL+1,1
          KEE(J) = CKE*TE(J)
          KEI(J) = CKE*TI(J)
X         IF(DMAX(DABS(KEE(J)),DABS(KEI(J))).GT.BBIGNO) OUTPUT, 'OUTPUT5',
X     A     J,JL ,KEE(J),KEI(J),       N,NL ,                        TI(J),
X     B   TE(J),CKE; CALL EXIT
14        CONTINUE
```

```
C PUBLISH ALL RESULTS
X         CALL DEBUG('OUTPUT6')
          WRITE (108,104) IT
104       FORMAT (1H0,T1,'RESULTS ARE AS FOLLOWS: THE ITERATION NUMBER IS'
     A    ,I4)
          WRITE (108,100)
100       FORMAT (1H1,T5,'POSITION',T19,'POTENTIAL',T31,'ELECTRIC FIELD',
     A    T47,'ELECTRON',T60,'ION DENSITY',T75,'ELECTRON',T88,'ION ',
     B    'CURRENT',T103,'ELECTRON',T116,'ION KINETIC'/T47,'DENSITY',T75,
     C    'CURRENT',T101,'KINETIC ENERGY',T119,'ENERGY')
          WRITE (108,101) (Z(J),POT(J,1),(POT(J,1)-POT(J+1,1))/DELPOS,
     A    NETT(J),NITT(J),JEJ(J),JIJ(J),KEE(J),KEI(J),J=1,JL+1)
101       FORMAT (X,1PE14.6,T16,1PE14.6,T30,1PE14.6,T44,1PE14.6,T58,
     A    1PE14.6,T72,1PE14.6,T86,1PE14.6,T100,1PE14.6,T114,1PE14.6)
          WRITE (108,102)
102       FORMAT (1H0,T5,'POSITION',T50,'ELECTRON SPEED SPECTRUM')
          WRITE(108,106)(Z(J),(NEI(J,N,1)+NEI(J,N,2),N=1,NL+1),J=1,JL+1)
          WRITE(108,107)
107       FORMAT('0',X,'POSITION',T52,'ION SPEED SPECTRUM')
          WRITE(108,106)(Z(J),(NII(J,N,1)+NII(J,N,2),N=1,NL+1),J=1,JL+1)
106       FORMAT(' ',1P10E11.3)
          WRITE (108,103)
103       FORMAT (1H0,T5,'POSITION',T29,'ELECTRON ANGULAR DISTRIBUTION',
     A    T88,'ION ANGULAR DISTRIBUTION')
          WRITE(108,105)(Z(J),NEN(J,1,1),NEN(J,2,1),
     A    NEN(J,2,2),NEN(J,1,2),NIN(J,1,1),NIN(J,2,1),
     B                 NIN(J,2,2),NIN(J,1,2),J=1,JL+1)
105       FORMAT(X,1P09E9.2)
X         IF FLOATING OVERFLOW 607, 507
X507      CONTINUE
          RETURN
X607      OUTPUT,'OVERFLOW IN OUTPUT',J,JL,I,IL,L,N,NL,    CKE ;
X    A    CALL EXIT
          END
C MELVILLE CLARK
C
          FUNCTION P(JAL,JBL,NP, IP)
C
C         PROGRAM NUMBER 21
C CALCULATES THE PROBABILITY OF NOT SCATTERING BETWEEN TWO POINTS
          IMPLICIT REAL*8 (A-H,O-Z)
          GLOBAL DEL1, DEL2,BIGNO
          IF(JAL .LT. JBL), JA = JBL; JB = JAL; GO TO 2
          JA = JAL; JB = JBL
2         CONTINUE
          SUM = 0.D0; JIP = JA-2
          REPEAT 1, FOR JTP = (JA,(JB-2),2)
          JIP = JTP
1         SUM=SUM+DEL1*(DEPTH(JTP,NP,IP)+4.D0*DEPTH(JTP+1,NP,IP)+
     A    DEPTH(JTP+2,NP,IP))
          IF(MOD((JB-JA),2) .GT. 0 ), SUM = SUM + DEL2*(DEPTH(JIP+2,NP,IP)
     A    + DEPTH(JIP+3,NP,IP))
X         IF(SUM .GT. BIGNO .OR.SUM.LT.0.D0), OUTPUT,'P4',DEL1,SUM,JTP,
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```
X    A   DEPTH(JIP,NP,IP),DEPTH(JIP+1,NP,IP),                      JA,JB,
X    B   NP,IP,JIP
         P = DEXP(-SUM)
X        IF(P .LT.0.D0.OR. P.GT.1.D0),OUTPUT,'P3',P,SUM,JTP,JIP,DEL1,
X    A   JA,JB,DEPTH(JIP,NP,IP),DEPTH(JTP,NP,IP),NP,IP,DEL2,
X    B   DEPTH(JIP+1,NP,IP),DEPTH(JTP+1,NP,IP),DEPTH(JTP+2,NP,IP);
X    C   CALL EXIT
         RETURN
         END
C MELVILLE CLARK
C
         SUBROUTINE PLASMA
C
C        PROGRAM NUMBER 8
C CALCULATES THE BOUNDARY CONDITION IN THE PLASMA
         IMPLICIT REAL*8 (A-H, O-Z)
         REAL *8 NE, NI, NEP, NIP,KET,NETT,NITT,NEN,NIN,KET2,KET3,NEI,NII
         COMMON NE(051,09,02,02),NI(051,09,02,02),NEN(051,02,02),
     A   NIN(051,02,02),NEI(051,09,02),NII(051,09,02)
         GLOBAL JLP, NEP,NIP,
     A   E, TI(051),TE(051),
     B          POT(051,4),                  Q,NL,IL,NETT(051),NITT(051),
     C   S2MEOP,S2MIOP,SR8ME,SR8MI,RS2ME,RS2MI,BIGNO,BBIGNO,IO
         REPEAT 1, FOR NP = (1, NL + 1, 1)
         REPEAT 2, FOR IP = (1,(IL+1)/2,1)
C CALCULATE THE ELECTRON DIRECTIONAL DENSITY
         Q = -E
         KET2 = KET(JLP,NP)
         IF(                       KET2 .LT. 0.D0), NE(JLP,NP,IP,1) =
     A   0.D0; GO TO 31
         NE(JLP,NP,IP,1) = S2MEOP*NEP*KET2*DEXP(-KET2/TE(JLP))/(TE(JLP)**
     A   1.5D0)
31       CONTINUE
         NE(JLP,NP,IP,2) = NE(JLP,NP,IP,1)
4        CONTINUE
C CALCULATE THE ION DIRECTIONAL DENSITY
         Q = E
         KET3 = KET(JLP,NP)
         IF(                       KET3 .LT. 0.D0), NI(JLP,NP,IP,1) =
     A   0.D0; GO TO 32
         NI(JLP,NP,IP,1) = S2MIOP*NIP*KET3*DEXP(-KET3/TI(JLP))/(TI(JLP)**
     A   1.5D0)
32       CONTINUE
         NI(JLP,NP,IP,2) = NI(JLP,NP,IP,1)
5        CONTINUE
X        IF(DMIN(NE(JLP, NP, IP, 1),  NI(JLP, NP, IP, 1)) .LT.0.D0.OR.
X    A   DMAX(NE(JLP, NP, IP, LP), NI(JLP, NP, IP, LP)).GT.BBIGNO) ,
X    B   OUTPUT, 'PLASMA3', NE(JLP, NP, IP, 1),  NI(JLP, NP, IP, 1),Q,E,
X    C   JLP, NP, IP, NEP, NIP,          E,POT(JLP,1), TE(JLP), TI(JLP),
X    D                              KET(JLP,NP),NETT(JLP),NITT(JLP),
X    E   KET2,KET3; CALL EXIT
2        CONTINUE
1        CONTINUE
```

```
C RENORMALIZATION OF SOURCE IN PLASMA
C CALCULATE THE TOTAL ELECTRON AND ION DENSITY
          Q = -E
          CALL SPEED(JLP,NE,NEI,NETT,RS2ME)
          Q = E
          CALL SPEED(JLP,NI,NII,NITT,RS2MI)
          RE = NEP/NETT(JLP); RI = NIP/NITT(JLP)
          WRITE(108,400) RE,RI
400       FORMAT (' ','RE=',1PE11.3,2X,'RI=',1PE11.3)
          REPEAT 8, FOR NP = (1,NL+1,1)
          REPEAT 9, FOR IP = (1,(IL+1)/2,1)
          REPEAT 10, FOR LP = 1,2
          NE(JLP,NP,IP,LP) = NE(JLP,NP,IP,LP)*RE
          NI(JLP,NP,IP,LP) = NI(JLP,NP,IP,LP)*RI
10        CONTINUE
9         CONTINUE
8         CONTINUE
X         IF FLOATING OVERFLOW 602, 502
X502      CONTINUE
          RETURN
X602      OUTPUT,'OVERFLOW IN PLASMA',    ML,IP,E,Q,KET2,NEP,TE(JLP),
X     A   S2MEOP,S2MIOP,KET3,          NIP,TI(JLP),L,N,IL,I,     RE,RI,LP,NP,
X     C                              VSPED0,VSPED1,RS2ME,
X     D   IO;IO = 2; CALL DEBUG('PLASMA6'); CALL EXIT
          END
C MELVILLE CLARK
C
          SUBROUTINE  POTENT
C
C         PROGRAM NUMBER 4
C CALCULATES THE POTENTIAL
          IMPLICIT REAL*8 (A-H,O-Z)
          REAL*8 INTEGRAL, INTEGR1, INTEGR2, NITT, NETT
          GLOBAL NETT(051), ML,        EPSILO,        JL,E,C1MR(011),BETA,
     A    IO,     IT,         NITT(051),SPACIN,Z(051),POT(051,04),BIGNO
          EXTERNAL INTEGR1, INTEGR2
          INTEGR1(JIR,NIR,IIP) = (Z(JIR) - SPACIN)*(NITT(JIR) - NETT(JIR))
          INTEGR2(JIQ,NIQ,IIQ) = (Z(JIQ) - Z(JPO))*(NITT(JIQ) - NETT(JIQ))
          JPOT = 1; NPOT = 1; IPOT = 1
          REPEAT 1, FOR JPO = (2, JL   , 1)
          REPEAT 2, FOR M = (MAX(2,MIN(ML,IT+1)),2,-1)
          POT(JPO,M) = POT(JPO,M-1)
2         CONTINUE
          POT(JPO,1) = (Z(JPO)/SPACIN)*POT(JL+1,1)-((Z(JPO)/SPACIN)-1.D0)
     A    *POT(1,1)-E*((Z(JPO)/SPACIN)*INTEGRAL(JPOT,JL+1,INTEGR1,NPOT,
     B    IPOT) - INTEGRAL(JPOT,JPO,INTEGR2,NPOT,IPOT))/EPSILO
X         IF(DABS(POT(JPO,1)).GT.BIGNO)OUTPUT,'POTEN3',POT(JPO,1),JPO,
X     A   Z(JPO), SPACIN, POT(JL+1,1),JL,POT(1,1),  INTEGR1( JIR,NIR,IIP),
X     B   INTEGR2(JIQ,NIQ,IIQ),E,JIR,EPSILO,NETT,NITT,     NIR,IIP,JIQ,NIQ,
X     C   IIQ,INTEGRAL(JPOT,JL+1,INTEGR1,NPOT,IPOT),INTEGRAL(JPOT,JPO,
X     D   INTEGR2,NPOT,IPOT); CALL EXIT
1         CONTINUE
C LOW-PASS FILTERING OF POTENTIAL
```

```
          REPEAT 5, FOR J = (2,JL,1)
          MLL = 1
          REPEAT 3, FOR M = (2,ML,1)
          IF(IT-M .LT. -1), GO TO 4
          PAT(J,1) = PAT(J,1) +(BETA**(M-1))*PAT(J,M)
3         MLL = M
4         CONTINUE
          PAT(J,1) = (C1MB(1)/C1MB(MLL))*PAT(J,1)
X         IF(DABS(PAT(J,1)).GT.BIGNO), OUTPUT, 'PATEN5', PAT(J,1),J,BIGNO,
X      A  C1MB(1),ML,C1MB(MLL),MLL,IT,M,BETA,JL;IO=2;CALL DEBUG
X      B  ('PATEN5'); CALL EXIT
5         CONTINUE
X         IF FLOATING OVERFLOW 605, 505
X505      CONTINUE
          RETURN
X605      OUTPUT,'OVERFLOW IN PATENT',C1MB(1),C1MB(MLL),PAT,IT,ML,BETA,7,
X      A  SPACIN,JL,E,JIR,INTEGR1(JIR,NIR,IIR),INTEGR2(JIQ,NIQ,IIQ),
X      B  NETT(JIR),NITT(JIR),INTEGRAL(JPAT,JL+1,INTEGR1,NPAT,IPAT),
X      C  INTEGRAL(JPAT,JPO,INTEGR2,NPAT,IPAT),EPSILO,JPO,MLL,JPAT,NPAT,
X      D  IPAT,         M; CALL EXIT
          END
C MELVILLE CLARK
C
          SUBROUTINE READIN
C
C PROGRAM NUMBER 10
C READS IN ALL DATA
          IMPLICIT REAL*8 (A-H, O-Z)
          INTEGER TYPE, CASE
          REAL*8 NEP, NIP
          GLOBAL                EPS,IL,JL,ML, NEP,NIP,NL,PHIR,PHIL,SIGMAE,
       A  SIGMAI,SPACIN,TL,TR,TEMRES,TPLF,TG,TYPE,VL,VR,VI,ITL,
       B                 TLEL,TREL,BETA,GAMMA,JMIN, CASE,IMMAX,BBIGNO,BIGNO,
       C  ITIMPR,ITIMAX,IEXTRA
          NAMELIST CASE,             EPS,IL,JL,NEP,NIP,NL,PHIR,PHIL,
       A  SIGMAE,SIGMAI,SPACIN,TL,ML, TR,TG,TYPE,VL,VR,VI,ITL,TPLF,
       B          BETA,TLEL,TREL,TEMRES,JMIN,BIGNO,BBIGNO,GAMMA,IMMAX,
       C  ITIMPR,ITIMAX,IEXTRA
C READ IN ALL DATA
          INPUT
C WRITE OUT ALL DATA
          OUTPUT, 'INPUT DATA', CASE
          OUTPUT,               EPS,IL,JL,ML, NEP,NIP,NL,PHIR,PHIL,SIGMAE,
       A  SIGMAI,SPACIN,TL,TR,TEMRES,TPLF,TG,TYPE,VL,VR,VI,ITL,
       B                 TLEL,TREL,BETA,BIGNO,JMIN,BBIGNO,GAMMA,IMMAX,
       C  ITIMPR,ITIMAX,IEXTRA
C CHECK THE INPUT DATA
X         IF(NL .LT. 1 .OR. JL .LT. 1 .OR. IL .LT. 1
X      A                                        .OR. EPS .LT.0.D0.OR. EPS
X      B  .GT.1.D0.OR. ITL .LT. 0 .OR. BIGNO .LE.0.D0.OR. NEP .LT.0.D0.OR.
X      C  NIP .LT.0.D0.OR. PHIR .LT. -10. .OR. PHIR .GT. 10. .OR. PHIL
X      D  .LT. -10. .OR. PHIL .GT. 10. .OR. SIGMAE .LT.0.D0.OR. SIGMAI
X      E  .LT.0.D0.OR. SPACIN .LE.0.D0.OR. SPACIN .GT. .01 .OR. TG .GT.
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```
X     F  DMAX(TL,TR) .GE. TG .LT. DMIN(TL,TR) .OR. TYPE .LT. 0 .OR. TRLF
X     G  .GT. 1. E4 .OR. TLLF .LT. 700. .OR. TEMRES .LT. 200. .OR. TEMRES
X     H  . T. 3000. .OR. DMIN(VL,VR) .LT. -10. .OR. DMAX(VL,VR) .GT. 1 .
X     I  .OR. VI .LT. .01 .OR. VI .GT. 20. .OR.
X                     DMAX(TLFL,TRFL) .GT. 1.E4 .OR. DMIN(TRFL,TLFL) .LT.
X     K  600. .OR. BETA .GT.1.D0.OR. ML  .GT. 4     .OR. ML  .LT. 0 .OR.
X     L  JMIN .LT. 0 .OR. JMIN .GT. JL+1  .OR. GAMMA .LT. 0.D0 .OR.
X     M  GAMMA .GE. 1.D0 .OR. IMMAX .LT. 0) OUTPUT,'READIN3',
X     N  EPS,TL,ITL,JL,NEP,NIP,NL,PHIR,BETA,PHIL,SIGMAE,SIGMAI,SPACIN,
X     O  T EL,TLFL,TEMRES,TG,TR,TL,TRLF,               TYPE,VL,VR,VI,ML,
X     P       JMIN,BIGNO,GAMMA,IMMAX; CALL EXIT
         RETURN
         END
C MELVILLE CLARK
C
         FUNCTION RJACOB (JJ,  NJ, IJ)
C
C        PROGRAM NUMBER 22
C CALCULATES THE RECIPROCAL OF THE JACOBIAN OF THE TRANSFORMATION
         IMPLICIT REAL*8 (A-H, O-Z)
         REAL*8 KEPARA,KET
         GLOBAL OBIGNO
         IF(KET(JJ,NJ) .LT. 0.D0 .OR. KEPARA(JJ,NJ,IJ) .LT. 0.D0),
      A  RJACOB = OBIGNO; GO TO 1
         RJACOB = (KET(JJ,NJ)*DSQRT(KEPARA(JJ,NJ,IJ)))
1        CONTINUE
X        IF(RJACOB .LT.0.D0.OR. RJACOB .GT. 2.*OBIGNO),OUTPUT,'RJACOB3',
X     A  RJACOB, KEPARA(JJ, NJ, IJ), JJ, NJ, KET(JJ, NJ),OBIGNO, IJ;
X     B  CALL EXIT
X        IF FLOATING OVERFLOW 601, 501
X501     CONTINUE
         RETURN
X601     OUTPUT,'OVERFLOW IN RJACOB'; CALL EXIT
         END
C MELVILLE CLARK
C
         FUNCTION SOUREL (JSE, NSE, ISE)
C
C        PROGRAM NUMBER 23
C CALCULATES THE SOURCE FOR ELECTRONS
         IMPLICIT REAL*8 (A-H, O-Z)
         REAL*8 KET, NEI,KEPARA,NE,NI,NEN,NIN,NII
         COMMON NE(051,09,02,02),NI(051,09,02,02),NEN(051,02,02),
      A  NIN(051,02,02),NEI(051,09,02),NII(051,09,02)
         GLOBAL SIGMAE,BIGNO
X        IF(KET(JSE,NSE) .LT. 0.D0 .OR. KEPARA(JSE,NSE,ISE) .LT. 0.D0),
X     A  OUTPUT, 'SOURE4',JSE,NSE,ISE,KET(JSE,NSE),KEPARA(JSE,NSE,ISE);
X     B  CALL EXIT
         SOUREL = SIGMAE*(NEI(JSE,NSE,1) + NEI(JSE,NSE,2))*
      A  DSQRT(KET(JSE,NSE)/KEPARA(JSE,NSE,ISE))
X        IF(SOUREL .LT.0.D0.OR. SOUREL .GT. BIGNO), OUTPUT, 'SOUREL3',
X     A  SOUREL,SIGMAE,                JSE,NSE,NEI(JSE,NSE,1),
X     B  NEI(JSE,NSE,2),KEPARA(JSE,NSE,ISE),ISE; CALL EXIT
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X        IF FLOATING OVERFLOW 601, 501
X501     CONTINUE
         RETURN
X601     OUTPUT,'OVERFLOW IN SOUREL'; CALL EXIT
         END
C MELVILLE CLARK
C
         FUNCTION SOURIN(JSI, NSI, ISI)
C
C        PROGRAM NUMBER 24
C CALCULATES THE SOURCE FOR IONS
         IMPLICIT REAL*8(A-H, O-Z)
         REAL*8 NITT,KETOTI,KEPARA,KET
         GLOBAL TI(051), SIGMAI, E, NITT(051),BIGNO
X        IF(KET(JSI,NSI) .LT. 0.D0 .OR. KEPARA(JSI,NSI,ISI) .LT. 0.D0),
X     A  OUTPUT,'SOURIE', JSI,NSI,ISI,KET(JSI,NSI),KEPARA(JSI,NSI,ISI);
X     B  CALL EXIT
C CALCULATE THE RATIO OF THE TOTAL KINETIC ENERGY TO THE TEMPERATURE
         IF( TI(JSI) .LE. 0.D0), SOURIN = 0.D0; GO TO 1
         KETOTI = KET(JSI,NSI)/TI(JSI)
X        IF(KETOTI.LT.0.D0.OR. KETOTI .GT. BIGNO), OUTPUT, 'SOURIN4',
X     A  KETOTI,JSI,NSI,TI(JSI),KET(JSI,NSI); CALL EXIT
         SOURIN = SIGMAI*(KETOTI**1.5D0)*NITT(JSI)*
      A  DEXP(-KETOTI)/DSQRT(KEPARA(JSI,NSI,ISI))
1        CONTINUE
X        IF(SOURIN .LT.0.D0.OR. SOURIN .GT. BIGNO), OUTPUT, 'SOURIN3',
X     A  SOURIN, KEPARA (JSI, NSI, ISI), JSI, NSI, ISI, SIGMAI,
X     B  KETOTI,NITT(JSI); CALL EXIT
X        IF FLOATING OVERFLOW 601, 501
X501     CONTINUE
         RETURN
X601     OUTPUT,'OVERFLOW IN SOURIN'; CALL EXIT
         END
C MELVILLE CLARK
C
         SUBROUTINE SPECTRA
C
C PROGRAM NUMBER 9
C CALCULATE THE SPECTRAL DISTRIBUTION OF ELECTRON DENSITY AND ION
C DENSITY
         IMPLICIT REAL*8 (A-H, O-Z)
         REAL*8      NEI,NII,NE,NI,NETT,NITT,NEP,NIP,NEN,NIN
         COMMON NE(051,09,02,02),NI(051,09,02,02),NEN(051,02,02),
      A  NIN(051,02,02),NEI(051,09,02),NII(051,09,02)
         GLOBAL NEP,Q,JL,IL,NL,IO,NIP,EN(10),    NETT(051),NITT(051),E,
      A  S2RME,S2RMI,POT(051,04),RS2ME,RS2MI,BIGNO
C CALCULATE THE SPATIAL DISTRIBUTION OF ELECTRON DENSITY AND ION DENSITY
         Q = -E
         REPEAT 16, FOR J = (1,JL+1,1)
         CALL SPEED(J,NE,NEI,NETT,RS2ME)
16       CONTINUE
         Q = E
         REPEAT 26, FOR J = (1,JL+1,1)
```

```
          CALL SPEED(J,NI,NII,NITT,RS2MI)
26        CONTINUE
C CALCULATE THE ANGULAR DISTRIBUTION AT ALL POINTS OF SPACE
          REPEAT 17, FOR J = (1,JL+1,1)
          REPEAT 17, FOR I = (1,(IL+1)/2,1)
          REPEAT 17, FOR L = 1,2
          NEN(J,I,L) = 0.D0
          NIN(J,I,L) = 0.D0
          REPEAT 11, FOR N = (2,NL+1,1)
          Q = -E
          NEN(J,I,L) = NEN(J,I,L) +(NE(J,N,I,L) + NE(J,N-1,I,L))*
     A    (EN(N) - EN(N-1))/(SR8ME*RJACOB(J,N,I))
          Q = E
          NIN(J,I,L) = NIN(J,I,L) +(NI(J,N,I,L) + NI(J,N-1,I,L))*
     A    (EN(N) - EN(N-1))/(SR8MI*RJACOB(J,N,I))
X         IF(DMIN(NEN(J,I,L), NIN(J,I,L)) .LT.0.D0.OR. DMAX(NEN(J,I,L),
X    A    NIN(J,I,L)).GT.BIGNO),OUTPUT,'SPECR5',NEN(J,I,L),SR8ME,SR8MI,
X    B    NIN(J,I,L),J,I,L, NE(J,N,I,L), NI(J,N,I,L), N,NL,IL,JL,EN(N),
X    C    EN(N-1); CALL EXIT
11        CONTINUE
          NEN(J,I,L) = NEN(J,I,L)/2.D0
          NIN(J,I,L) = NIN(J,I,L)/2.D0
17        CONTINUE
X         IF FLOATING OVERFLOW 604, 504
X504      CONTINUE
          RETURN
X604      OUTPUT,'OVERFLOW IN SPECTRA', J,JL,L,N,NL,IL,I,BIGNO,EN,SR8ME,
X    A    SR8MI,VSPED0,VSPED1,RS2ME,RS2MI,Q,E;
X    B    IB = 2; CALL DEBUG('SPECTRA5'); CALL EXIT
          END
C MELVILLE CLARK
C
          SUBROUTINE SPEED(JS,NS,NSI,NSTT,RS2M)
C
C PROGRAM CALCULATES THE SPEED SPECTRUM.
          IMPLICIT REAL*8 (A-H,O-Z)
          REAL*8 NS,NSI,NSTT,KET,MU
          DIMENSION NS(051,09,02,02),NSI(051,09,02),NSTT(051)
          GLOBAL NL,IL,BIGNO
          NSTT(JS ) = 0.D0
          REPEAT 13, FOR N = (1,NL+1,1)
          REPEAT 6, FOR L = 1,2
          NSI(JS ,N,L) = 0.D0
C SUM     OVER ALL PERPENDICULAR KINETIC ENERGIES
          REPEAT 12, FOR I = (2,(IL+1)/2,1)
          NSI(JS ,N,L) = NSI(JS ,N,L) + (NS(JS ,N,I,L) + NS(JS ,N,I-1,L))*
     A    DABS(MU(JS ,N,I,L) - MU(JS ,N,I-1,L))
X         IF(NSI(JS ,N,L) .LT. 0.D0 .OR. NSI(JS ,N,L) .GT. BIGNO),OUTPUT,
X    A    'SPED1',NSI(JS ,N,L), JS ,N,L,NS(JS ,N,I,L),NS(JS ,N,I-1,L),
X    B    MU(JS ,N,I,L),MU(JS ,N,I-1,L); CALL EXIT
12        CONTINUE
          NSI(JS ,N,L) = NSI(JS ,N,L)/2.D0
          NSI(JS ,N,L) = NSI(JS ,N,L) + NS(JS ,N,(IL+1)/2,L)*
```

```
      A   DABS(MU(JS ,N,(IL/2)+1,L) - MU(JS ,N,(IL+1)/2,L))
X         IF(NSI(JS ,N,L) .LT. 0.D0 .ØR. NSI(JS ,N,L) .GT. BIGNØ),ØUTPUT,
X     A   'SPED2',NSI(JS ,N,L),JS ,N,L,NS(JS ,N,(IL+1)/2,L),(IL+1)/2,
X     B   MU(JS ,N,(IL/2)+1,L),MU(JS ,N,(IL+1)/2,L ),(IL+1)/2,(IL/2)+1;
X     C   CALL EXIT
6         CØNTINUE
13        CØNTINUE
          REPEAT 3, FØR N = (2,NL+1,1)
          REPEAT 11, FØR L = 1,2
          VSPED0 = KET(JS ,N); VSPED1 = KET(JS ,N-1)
          IF(VSPED0 .LT. 0.D0), VSPED0 = 0.D0
          IF(VSPED1 .LT. 0.D0), VSPED1 = 0.D0
          NSTT(JS ) = NSTT(JS ) +(NSI(JS ,N,L)+NSI(JS ,N-1,L))*
      A   (DSQRT(VSPED0) - DSQRT(VSPED1))*RS2M
X         IF(NSTT(JS).LT. 0.D0 .ØR. NSTT(JS).GT. BIGNØ),ØUTPUT,'SPED3',
X     A   VSPED0,KET(JS ,N),JS ,N,VSPED1,KET(JS ,N-1),NSTT(JS ),
X     B   NSI(JS ,N,L),L,RS2M ,NSI(JS ,N-1,L); CALL EXIT
11        CØNTINUE
3         CØNTINUE
          VSPED0 = KET(JS,1); VSPED1 = KET(JS,NL+1); VSPED2 = KET(JS,NL+2)
          IF(VSPED0 .LT. 0.D0), VSPED0 = 0.D0
          IF(VSPED1 .LT. 0.D0), VSPED1 = 0.D0
          IF(VSPED2 .LT. 0.D0), VSPED2 = 0.D0
          REPEAT 7, FØR L=1,2
          NSTT(JS ) = NSTT(JS ) + (NSI(JS ,1,L)*DSQRT(VSPED0)+
      A   NSI(JS ,NL+1,L)*(DSQRT(VSPED2)- DSQRT(VSPED1)))*RS2M
7         CØNTINUE
          RETURN
          END
C MELVILLE CLARK
C
          FUNCTIØN TEM(JTE,NT,NTTT,VTJ)
C
C         PRØGRAM NUMBER 29
C         CALCULATES THE TEMPERATURE
          IMPLICIT REAL*8 (A-H, Ø-Z)
          REAL*8 NT,NTTT,MU, MASS,KEP,NØKEPA,KET
          DIMENSIØN NT(051,09,02,02),VTJ(051),NTTT(051)
          DIMENSIØN NT(051,09,02,02),VTJ(051),NTTT(051)
          DIMENSIØN NT(051,09,02,02),VTJ(051),NTTT(051)
          GLØBAL NL,MASS,        KEP(10,04),IL      ,S289M,BIGNØ
          TEM = 0.D0
          NTEM = 1
          REPEAT 16, FØR N = (2,NL+1,1)
          N0 = N; N1 = N-1
1         CØNTINUE
          TEMI = 0.D0
          REPEAT 17, FØR L = 1,2
          REPEAT 15, FØR I = (2,(IL+1)/2,1)
          TEMI = TEMI + DABS(MU(JTE,N,I,L)-MU(JTE,N,I-1,L))*
      A   (NØKEPA(JTE,N,I,L,NT) + NØKEPA(JTE,N,I-1,L,NT))
X         IF FLØATING ØVERFLØW 501,501
X501      CØNTINUE
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```
X          IF(DABS(TEM) .GT. BIGNØ),ØUTPUT,'TEM3',TEM,MU(JTE,N,I,L),
X       A  NØKEPA(JTE,N,I,L,NT),                            N,I,L,TEMI,
X       B  NØKEPA(JTE,N,I-1,L,NT),                          JTE,NL,(IL+1)/2;
X       C  CALL EXIT
15         CØNTINUE
17         CØNTINUE
           TEMI = TEMI/2.D0
           REPEAT 14, FØR L = 1,2
           TEMI = TEMI + DABS(MU(JTE,N,(IL/2)+1,L) - MU(JTE,N,(IL+1)/2,L))*
        A  NØKEPA(JTE,N,(IL+1)/2,L,NT)
X          IF FLØATING ØVERFLØW 503, 503
X503       CØNTINUE
X          IF(DABS(TEMI).GT. BIGNØ), ØUTPUT,'TEM4',N,MU(JTE,N,(IL/2)+1,L),
X       A  (IL/2)+1,(IL +1)/2,TEMI,MU(JTE,N,(IL+1)/2,L),
X       B  NØKEPA(JTE,N,(IL+1)/2,L,NT);
X       C  CALL EXIT
14         CØNTINUE
           GØ TØ (5,3,4,5),NTEM
5          CØNTINUE
           TEM0 = KET(JTE,N0); TEM1 = KET(JTE,N1)
           IF(TEM0 .LT. 0.D0), TEM0 = 0.D0
           IF(TEM1 .LT. 0.D0), TEM1 = 0.D0
           TEM = TEM + TEMI*(DSQRT(TEM0) - DSQRT(TEM1))
           GØ TØ (16,8,8,7),NTEM
16         CØNTINUE
           NTEM = 4
           REPEAT 7, FØR N=(1,NL,1)
           N0 = N+1; N1 = N
           GØ TØ 1
7          CØNTINUE
           NTEM = 2; N = 1; GØ TØ 1
3          CØNTINUE
           TE0 = TEMI; NTEM = 3; N = NL+1; GØ TØ 1
4          CØNTINUE
           TE1 = TEMI
           TEM0 = KET(JTE,1); TEM1 = KET(JTE,NL+1); TEM2 = KET(JTE,NL+2)
           IF(TEM0 .LT. 0.D0), TEM0 = 0.D0
           IF(TEM1 .LT. 0.D0), TEM1 = 0.D0
           IF(TEM2 .LT. 0.D0), TEM2 = 0.D0
           TEM = TEM + (TE0*DSQRT(TEM0) + TE1*(DSQRT(TEM2) - DSQRT(TEM1)))
           IF(NTTT(JTE) .EQ. 0.D0), TEM = 0.D0; GØ TØ 2
           TEM = (TEM*S2Ø9M)/NTTT(JTE)       - MASS*(VTJ(JTE)**2)/3.D0
X          IF FLØATING ØVERFLØW 602, 502
X502       CØNTINUE
2          CØNTINUE
           RETURN
X601       ØUTPUT,'ØVERFLØW IN TEM JUST BEFØRE STATEMENT 15',TEM,
X       A                NØKEPA(JTE,N,I,L,NT),NØKEPA(JTE,N-1,I,L,NT),JTE,N,I,
X       B  NØKEPA(JTE,N,I-1,L,NT),NØKEPA(JTE,N-1,I-1,L,NT),L,TEMI,
X       C  MU(JTE,N,I,L),MU(JTE,N,I-1,L),MU(JTE,N-1,I,L),MU(JTE,N-1,I-1,L);
X       D  CALL EXIT
X602       ØUTPUT,'ØVERFLØW IN TEM',TEM,TEMI,KET(JTE,N),KET(JTE,N-1),S2Ø9M,
X       A  NØKEPA(JTE,N,I,L,NT),NØKEPA(JTE,N-1,I,L,NT),JTE,N,I,IL,
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X     B   NOKEPA(JTE,N,I-1,L,NT),NOKEPA(JTE,N-1,I-1,L,NT),
X     C   NITT(JTE),VIJ(JTE),MASS,NL,L; CALL EXIT
X603      OUTPUT,'OVERFLOW IN TEM AFTER TEM CALCULATION',TEM,TEMI,
X     A   MU(JTE,N,(IL/2)+1,L),ML(JTE,N,(IL+1)/2,L),MU(JTE,N-1,(IL/2)+1,L)
X     B   ,ML(JTE,N-1,(IL+1)/2,L), NOKEPA(JTE,N,(IL+1)/2,L,NT),JTE,
X     C   NOKEPA(JTE,N-1,(IL+1)/2,L,NT),(IL+1)/2,N,IL;
X     D   CALL EXIT
X8        OUTPUT,'TEM5',NTEM,JTE,N,I,L,NO,N1,NL,IL,TEMO,TEM1,TEC,TE1,TEMI,
X     A   TEM2,TEM
          END
C MELVILLE CLARK
C
          SUBROUTINE TEMPER
C
C PROGRAM 13
C CALCULATES THE TEMPERATURE
          IMPLICIT REAL*8 (A-H, O-Z)
          REAL*8 NE,NETT,NI,NITT,          JEJ,JIJ,K,MASS,ME,MI
          COMMON NE(051,09,02,02),NI(051,09,02,02)
          GLOBAL Q,E,VEJ(051),                    NETT(051),JL, TE(051),NL,
        A TI(051),K,MASS,ME,MI,S289M,S289ME,S289MI,
        B CODEN,CNDEN,VIJ(051),
        C JIJ(051),                    NITT(051),        JEJ(051)
C CALCULATE THE DRIFT VELOCITY OF ELECTRONS AND IONS AS A FUNCTION OF
C POSITION
          Q = -E; MASS = ME
          REPEAT 15, FOR J = (1,JL+1,1)
          VEJ(J) = VDRIFT(J,NE,NETT)
X         IF FLOATING OVERFLOW  601, 501
X501      CONTINUE
15        CONTINUE
          Q = E; MASS = MI
          REPEAT 16, FOR J = (1,JL+1,1)
          VIJ(J) = VDRIFT(J,NI,NITT)
C CALCULATE THE ELECTRIC CURRENT OF ELECTRONS AND IONS AS A FUNCTION OF
C POSITION
          JEJ(J) =-E*VEJ(J)*NETT(J)
          JIJ(J) = E*VIJ(J)*NITT(J)
X         IF FLOATING OVERFLOW 602, 502
X502      CONTINUE
16        CONTINUE
C CALCULATE THE ELECTRON TEMPERATURE AND ION TEMPERATURE AT ALL SPATIAL
C POINTS
          Q = -E; MASS = ME; S289M = S289ME
          REPEAT 11, FOR J = (1,JL+1,1)
          IF(NETT(J) .LE. 0.D0),TE(J) = 0.D0; GO TO 21
          TE(J) = TEM(J,NE ,NETT,VEJ)
21        CONTINUE
X         IF FLOATING OVERFLOW 603, 503
X503      CONTINUE
11        CONTINUE
          Q = E; MASS = MI; S289M = S289MI
          REPEAT 13, FOR J = (1,JL+1,1)
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      IF(NITT(J) .LE. 0.D0), TI(J) = 0.D0; GO TO 22
      TI(J) = TEM(J,NI ,NITT,VIJ)
22    CONTINUE
X     IF FLOATING OVERFLOW 604, 504
X504  CONTINUE
13    CONTINUE
      RETURN
X601  OUTPUT,'OVERFLOW IN TEMPER AFTER STATEMENT 15',J,VEJ(J),NETT(J),
X    A MASS,Q,E,JL; GO TO 501
X602  OUTPUT,'OVERFLOW IN TEMPER  AFTER STATEMENT 16',J,VIJ(J),
X    A NITT(J),E,JEJ(J),JIJ(J),VEJ(J),NETT(J),G,MASS,ME,MI; GO TO 502
X603  OUTPUT,'OVERFLOW IN TEMPER AFTER STATEMENT 11',TE(J),J,NETT(J),
X    A VEJ(J),Q,E,MASS,S2OOME,S2OOM; GO TO 503
X604  OUTPUT,'OVERFLOW IN TEMPER AFTER STATEMENT 13',TI(J),NITT(J),J,
X    A VIJ(J),Q,E,MASS,MI,S2OOMI,S2OOM; GO TO 504
      END
C MELVILLE CLARK
C
      FUNCTION VDRIFT (JV,NV,NVTT)
C
C     PROGRAM NUMBER 28
C     CALCULATES DRIFT VELOCITY
      IMPLICIT REAL*8 (A-H, O-Z)
      REAL*8 MASS,MU,KET,KPARN,NV,NVTT
      DIMENSION NV(051,09,02,02),NVTT(051)
      GLOBAL             MASS,IL,NL,BIGNO
      LV = 1
      VDRIFT = 0.D0
      NDRIFT = 1
      REPEAT 16, FOR N = (2,NL+1,1)
      NO = N; N1 = N-1
1     CONTINUE
      VDRIFT = 0.D0
      REPEAT 15, FOR I = (2,(IL+1)/2,1)
      VDRIFT = VDRIFT + (KPARN(JV,N,I,NV)+KPARN(JV,N,I-1,NV))*
     A DABS(MU(JV,N,I,LV) - MU(JV,N,I-1,LV))
X     IF FLOATING OVERFLOW 601, 501
X501  CONTINUE
X     IF(DABS(VDRIFT ) .GT. BIGNO), OUTPUT, 'VDRIFT4', VDRIFT,
X    A JV,                   KPARN(JV,N,I,NV),
X    B KPARN(JV,N,I-1,NV),                        LV,N,I,IL,NL,
X    C MU(JV,N,I,LV),MU(JV,N,I-1,LV);
X    D CALL EXIT
15    CONTINUE
      VDRIFT = VDRIFT/2.D0
      VDRIFT = VDRIFT + KPARN(JV,N,(IL+1)/2,NV)*
     A DABS(MU(JV,N,(IL/2)+1,LV) - MU(JV,N,(IL +1)/2,LV))
X     IF FLOATING OVERFLOW 603, 503
X503  CONTINUE
X     IF(DABS(VDRIFT ) .GT. BIGNO), OUTPUT, 'VDRIFT3',
X    B VDRIFT ,N,BIGNO,IL,MU(JV,N,(IL/2)+1,LV),MU(JV,N,(IL+1)/2,LV),
X    D KPARN(JV,N,(IL+1)/2,NV),                       JV,NVTT(JV);
X    E                          CALL EXIT
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          GO TO (5,3,4,5),NDRIFT
5         CONTINUE
          VDRIF0 = KET(JV,N0); VDRIF1 = KET(JV,N1)
          IF(VDRIF0 .LT. 0.D0), VDRIF0 = 0.D0
          IF(VDRIF1 .LT. 0.D0), VDRIF1 = 0.D0
          VDRIFT = VDRIFT + VDRIFI*(DSQRT(VDRIF0) - DSQRT(VDRIF1))
          GO TO (16,8,8,7),NDRIFT
16        CONTINUE
          NDRIFT = 4
          REPEAT 7, FOR N = (1,NL,1)
          N0 = N+1; N1 = N
          GO TO 1
7         CONTINUE
          NDRIFT = 2; N = 1; GO TO 1
3         CONTINUE
          VDRI0 = VDRIFT
          NDRIFT = 3; N = NL+1; GO TO 1
4         CONTINUE
          VDRI1 = VDRIFT
          VDRIF0 = KET(JV,1); VDRIF1 = KET(JV,NL+1); VDRIF2 = KET(JV,NL+2)
          IF(VDRIF0 .LT. 0.D0), VDRIF0 = 0.D0
          IF(VDRIF1 .LT. 0.D0), VDRIF1 = 0.D0
          IF(VDRIF2 .LT. 0.D0), VDRIF2 = 0.D0
          VDRIFT = VDRIFT + (VDRI0*DSQRT(VDRIF0) + VDRI1*(DSQRT(VDRIF2) -
      A   DSQRT(VDRIF1)))
          IF(NVTT(JV) .EQ. 0.D0), VDRIFT = 0.D0; GO TO 2
          VDRIFT = VDRIFT/(NVTT(JV)*MASS)
X         IF FLOATING OVERFLOW 602, 502
X502      CONTINUE
2         CONTINUE
          RETURN
X601      OUTPUT,'OVERFLOW IN VDRIFT BEFORE STATEMENT 15',VDRIFT,
X     A   N,I,                  KPARN(JV,N,I,NV),JV, KPARN(JV,N-1,I,NV),
X     B   KPARN(JV,N,I-1,NV),KPARN(JV,N-1,I-1,NV),MU(JV,N,I,LV),
X     C   MU(JV,N,I-1,LV),MU(JV,N-1,I,LV),MU(JV,N-1,I-1,LV); GO TO 501
X602      OUTPUT,'OVERFLOW IN VDRIFT AFTER STATEMENT 16',VDRIFT,MASS,
X     A   NVTT(JV),JV; GO TO 502
X603      OUTPUT,'OVERFLOW IN VDRIFT ',VDRIFT,                   N,(IL/2)+1,
X     A                       (IL+1)/2,KPARN(JV,N,(IL+1)/2,NV),JV,
X     B   KPARN(JV,N-1,(IL+1)/2,NV)                          ; GO TO 503
X3        OUTPUT,'VDRIFS',NDRIFT,IL,NL,JV,N,I,N0,N1,VDRIF0,VDRIF1,VDRI0,
X     A   VDRI1,VDRIF2,VDRIFT
          END
 METASYM SI,LO,GO
           SYSTEM    SIG5
           SYSTEM    BPM
           DEF       STIMER
           DEF       TTIMER
STIMER     M:STIMER  (SEC,1000000)
           B         *15
TTIMER     M:TTIMER  SEC
           LW,2      *15
           STW,8     *2
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        NT,15        1
                     *15
         ,ND
LMA  (CO),        (JASAT,(F4LIB)),(LMN,CLARK1),(PERM)
 IN  (LMN,CLARK1)
 ATA
CASE=12,                          EPS=.02,ITL=30, JL=50, NEP=1.1E19,
NIP=1.1E1 , NI=4, PHIL=2.708, PHIR=1.711, SIGMAE= 0.000,
SIGMAI=0.000,    SPACIN=5.E-6, TEMPES=614., TYPE=2, IL=4,
THIF = 2300.,                     TREF   = 2000., TLEL   = 2500., BETA = .77,
 C  =  - . 37, NL  = -1.922, VI  = 3.893, TR = 910.,TL = 1920.,TG = 1415.,
 L   =  +,             JAIT=1, SIGMA = 1.E56,GAMMA = .75,  IMMAX = 20,
ITIMP =100, TEXT A=1,  ITIMAX=1000*


EN
FIN
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