

ON THE TRANSPORT OF NEUTRAL HYDROGEN ATOMS IN A HYDROGEN PLASMA

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Abstract—The F_N method is used to solve in a concise and accurate manner a linear model of the Boltzmann equation appropriate to the transport of neutral hydrogen atoms in a hydrogen plasma. Half-space and finite-slab boundary conditions are considered and numerical results are reported.

1. INTRODUCTION

THE UNDERSTANDING of neutral hydrogen atom transport in a hydrogen plasma is important in the context of present-day fusion research. SAKHAROV (1961) was the first to point out that neutral hydrogen atoms could penetrate deeply into a hot plasma by repeated charge exchange. Because the plasma scale length can be comparable to the mean-free-path of the neutrals, an accurate analysis of this problem must be based on a kinetic treatment rather than low-order moments (fluid) equations. Early kinetic models have been discussed by ZUBAREV and KLIMOV (1961) and KONSTANTINOV and PEREL (1961) who obtained analytical solutions by assuming special forms for the hydrogen ion distribution. DNE-STROVSKII *et al.* (1972) also considered a special ion distribution function and used an integral form of the Boltzmann equation to obtain some basic results. REHKER and WOBIG (1973) also used an integral form of the Boltzmann equation and a Maxwellian ion distribution function to deduce results for a half space with either perfect specular or diffuse (thermal) reflection at the boundary. In addition HACKMANN *et al.* (1978) reported results for a problem involving a spatially-dependent ion temperature and for a time-dependent problem. The method of elementary solutions (CASE, 1960; CERCIGNANI, 1962) has been used recently by CONNOR (1977) to study a half-space version of this problem for the case of a spatially constant ion temperature. BURRELL (1978) and BURRELL and CHU (1979) reconsidered the constant ion-temperature problem, for both a half space and finite slabs, and reported results for the special case of perfect specular reflection at the boundaries. We note that additional work concerning other models and alternative methods of solution has been reported by GREENSPAN (1974), HOGAN and CLARKE (1974), PARSONS and MEDLEY (1974), CLARKE and SIGMAR (1975), IZVOZCHIKOV and PETROV (1976) and DÜCHS *et al.* (1977).

We have concluded that to date computational results reported in the literature have been presented in graphical form (and usually on a log scale). While such a presentation may be adequate for the qualitative study of physical laws and/or for correlation with experimental data, we believe there is a place for accurate numerical results for an extended class of half-space and finite-slab problems. Therefore, we use here the F_N method to develop numerical results, which we believe to be of reference quality, for the desired particle distribution function basic to neutral hydrogen transport in a plasma slab for several combinations of partial specular and diffuse reflection.

The F_N method initially introduced and used efficiently in the context of neutron-transport theory (SIEWERT and BENOIST, 1979; GRANDJEAN and SIEWERT, 1979) has also proved to be a particularly efficient method of solving basic transport problems in the fields of radiative transfer (SIEWERT, 1978; DEVAUX and SIEWERT, 1980) and rarefied gas dynamics (SIEWERT *et al.*, 1980). The method, though approximate, can yield very accurate numerical results with modest computational effort. The method, which is easy to use and which can accommodate a broad class of boundary conditions, can be summarized in the following way. First a system of singular integral equations (and constraints if appropriate) for the exit distributions at the boundaries is established. The exit distributions are then approximated by a finite expansion in terms of a set of basis functions, and the coefficients in the expansion are found by requiring that the set of integral equations be satisfied at certain (collocation) points. Once the boundary distributions are established, similar ideas can be used, as discussed in Section 3, to find the desired distribution function at any location in the slab.

2. THE KINETIC EQUATION AND BOUNDARY CONDITIONS

As discussed, for example, by BURRELL and CHU (1979), at sufficiently low temperatures (< 5 keV) the dominant interactions for hydrogen neutrals in a hydrogen plasma are ionization by electron impact and charge exchange. If we assume that the neutral density is sufficiently low that neutral-neutral interactions can be neglected, the appropriate steady-state transport equation is

$$\begin{aligned} \mathbf{v} \cdot \nabla f_0(\mathbf{r}, \mathbf{v}) + f_0(\mathbf{r}, \mathbf{v}) \int |\mathbf{v} - \mathbf{v}'| [\sigma_e(|\mathbf{v} - \mathbf{v}'|) f_e(\mathbf{r}, \mathbf{v}') + \sigma_x(|\mathbf{v} - \mathbf{v}'|) f_i(\mathbf{r}, \mathbf{v}')] d\mathbf{v}' \\ = f_i(\mathbf{r}, \mathbf{v}) \int |\mathbf{v} - \mathbf{v}'| \sigma_x(|\mathbf{v} - \mathbf{v}'|) f_0(\mathbf{r}, \mathbf{v}') d\mathbf{v}'. \end{aligned} \quad (1)$$

Here $f_0(\mathbf{r}, \mathbf{v})$, $f_e(\mathbf{r}, \mathbf{v})$ and $f_i(\mathbf{r}, \mathbf{v})$ are, respectively, the neutral, electron and ion distribution functions. Also, $\sigma_e(v)$ and $\sigma_x(v)$ are the cross sections for electron ionization and charge exchange (RIVIERE, 1971). We can simplify (1) by using the experimental evidence (FREEMAN and JONES, 1974) that the charge exchange cross section is, to a very good approximation, inversely proportional to speed. In addition and due to the mass difference between electrons and neutrals, the ionization rate is essentially independent of the neutral velocity [i.e., \mathbf{v} can be neglected compared to \mathbf{v}' in the ionization term in (1)]. We thus write (1) as

$$\mathbf{v} \cdot \nabla f_0(\mathbf{r}, \mathbf{v}) + N_i(\mathbf{r})(\langle \sigma_x v \rangle + \langle \sigma_e v \rangle) f_0(\mathbf{r}, \mathbf{v}) = N_i(\mathbf{r}) \langle \sigma_x v \rangle f_n(\mathbf{r}, \mathbf{v}) \int f_0(\mathbf{r}, \mathbf{v}') d\mathbf{v}', \quad (2)$$

where $f_n(\mathbf{r}, \mathbf{v})$ is a spatially normalized ion distribution

$$f_n(\mathbf{r}, \mathbf{v}) = f_i(\mathbf{r}, \mathbf{v})/N_i(\mathbf{r}). \quad (3)$$

Here $N_i(\mathbf{r})$ is the ion density, taken as equal to the electron density by imposing charge neutrality, and the $\langle \cdot \cdot \cdot \rangle$ notation implies an average over the appropriate electron or ion distribution. (By assumption $\sigma_x v$ is a constant, and the averaging notation is superfluous in this case.)

If we specialize the problem to one of planar geometry, we can integrate (2) over v_x and v_y to obtain

$$v_z \frac{\partial}{\partial z} g_0(z, v_z) + N_i(z) (\langle \sigma_x v \rangle + \langle \sigma_e v \rangle) g_0(z, v_z) = N_i(z) \langle \sigma_x v \rangle g_n(z, v_z) \int_{-\infty}^{\infty} g_0(z, v'_z) dv'_z, \quad (4)$$

where we have defined, for $\alpha = 0$ or $\alpha = n$,

$$g_\alpha(z, v_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_\alpha(\mathbf{r}, \mathbf{v}) dv_x dv_y. \quad (5)$$

Finally it is convenient to rewrite (4) in terms of dimensionless variables. We let

$$u = v_z/\bar{v}, \quad (6)$$

where \bar{v} is a characteristic speed, introduce the optical variable

$$\tau = (\bar{v})^{-1} \int_0^z N_i(z') (\langle \sigma_x v \rangle + \langle \sigma_e v \rangle) dz', \quad (7)$$

let

$$\psi(\tau, u) \rightarrow g_0(z, v_z) \quad (8)$$

and rewrite (4), for $u \in (-\infty, \infty)$, as

$$u \frac{\partial}{\partial \tau} \psi(\tau, u) + \psi(\tau, u) = c(\tau, u) \int_{-\infty}^{\infty} \psi(\tau, u') du' \quad (9)$$

where

$$c(\tau, u) = \left[\frac{\langle \sigma_x v \rangle}{\langle \sigma_x v \rangle + \langle \sigma_e v \rangle} \right] F(\tau, u) \quad (10)$$

and

$$F(\tau, u) \rightarrow \bar{v} g_n(z, v_z). \quad (11)$$

An especially important example of (10) and (11) corresponds to a local Max-

wellian for the ion distribution, i.e.

$$F(\tau, u) = \bar{v}[\pi^{1/2}v_i(\tau)]^{-1} \exp[-u^2\bar{v}^2/v_i^2(\tau)], \tag{12}$$

where the thermal speed $v_i(\tau)$ is related to the local ion temperature $T_i(\tau)$ by the usual expression

$$v_i(\tau) = \left[\frac{2kT_i(\tau)}{m_i} \right]^{1/2}. \tag{13}$$

The case analyzed by CONNOR (1977), BURRELL (1978) and BURRELL and CHU (1979) corresponds to assuming $T_i(\tau)$ independent of τ . If we choose $\bar{v} = v_i$ (i.e. in this case it is natural to set the characteristic speed \bar{v} equal to the spatially independent speed v_i) then we can write (9) as

$$u \frac{\partial}{\partial \tau} \psi(\tau, u) + \psi(\tau, u) = c\pi^{-1/2}e^{-u^2} \int_{-\infty}^{\infty} \psi(\tau, u') du' \tag{14}$$

where $c \in [0,1]$ is given by the spatially constant value

$$c = \frac{\langle \sigma_x v \rangle}{\langle \sigma_x v \rangle + \langle \sigma_e v \rangle} \tag{15}$$

To complete the specification of this kinetic problem we now consider the boundary conditions. We assume the plasma slab occupies $0 \leq z \leq z_0$. At $z = 0$ we take $\gamma_-(\mathbf{v})$ as a known incident distribution of neutrals, and we assume that a fraction ρ^s of the neutrals is specularly reflected and that a fraction ρ^d is diffusely reflected with some known distribution $h_-(\mathbf{v})$, with $0 \leq \rho^s + \rho^d \leq 1$. The boundary condition on $f_0(\mathbf{r}, \mathbf{v})$ at $z = 0$ is then, for $v_z > 0$,

$$f_0(\mathbf{r}, \mathbf{v})|_{z=0} = \gamma_-(\mathbf{v}) + \rho^s f_0(\mathbf{r}, \mathbf{v}, r)|_{z=0} + \rho^d h_-(\mathbf{v}) j_-, \tag{16}$$

where \mathbf{v}, r stands for $(v_x, v_y, -v_z)$, the function $h_-(\mathbf{v})$ is normalized to a unit right-directed flux, i.e.,

$$\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_0^{\infty} dv_z v_z h_-(\mathbf{v}) = 1, \tag{17}$$

and j_- is the flux of left-directed neutrals at $z = 0$, i.e.,

$$j_- = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_0^{\infty} dv_z v_z f_0(\mathbf{r}, \mathbf{v}, r)|_{z=0}. \tag{18}$$

In terms of the variable $\psi(\tau, u)$, (16) yields, for $u > 0$, the boundary condition

$$\psi(0, u) = \Gamma_-(u) + \rho^s \psi(0, -u) + \rho^d H_-(u) J_-. \tag{19}$$

Here we have defined

$$\Gamma_-(u) = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \gamma_-(\mathbf{v}), \quad (20)$$

$$H_-(u) = \bar{v}^2 \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y h_-(\mathbf{v}), \quad (21)$$

$$J_- = j_-(\bar{v})^{-2} = \int_0^{\infty} \psi(0, -u) u \, du. \quad (22)$$

It follows from (17) and (21) that the function $H_-(u)$ is normalized according to

$$\int_0^{\infty} H_-(u) u \, du = 1. \quad (23)$$

A completely analogous boundary condition holds at $z = z_0$, which we take to correspond to $\tau = \tau_0$. We have, for $u < 0$,

$$\psi(\tau_0, u) = \Gamma_+(u) + \rho_+^s \psi(\tau_0, -u) + \rho_+^d H_+(u) J_+, \quad (24)$$

where $\Gamma_+(u)$ and $H_+(u)$ are specified functions and J_+ is, aside from a factor of \bar{v}^2 , the right-directed flux of neutrals at $\tau = \tau_0$, i.e.,

$$J_+ = \int_0^{\infty} \psi(\tau_0, u) u \, du. \quad (25)$$

For diffuse reflection characterized by a Maxwellian of characteristic speed w , we have as a special case

$$H_-(u) = H_+(u) = 2(\bar{v}/w)^2 \exp[-(u\bar{v}/w)^2]. \quad (26)$$

We proceed now to develop the F_N method to solve the problem here formulated.

3. THE F_N METHOD FOR HALF-SPACE AND FINITE-SLAB APPLICATIONS

We note that CONNOR (1977) has used exact analysis based on the method of elementary solutions to develop a Fredholm integral equation that in principle could be solved numerically to yield the desired solution of (14) constrained to meet boundary conditions appropriate to a semi-infinite half space. We prefer here to use the F_N method (SIEWERT and BENOIST, 1979; GRANDJEAN and SIEWERT, 1979) to establish concise and accurate approximate solutions that can be readily evaluated numerically. In order to facilitate the correlation of this work with a previously reported solution (SIEWERT *et al.*, 1980), by the F_N method, of a related problem concerning Poiseuille flow in a plane channel we let

$$Y(\tau, u) = e^{u^2} \psi(\tau, u) \quad (27)$$

and consider, for $\tau \in [0, \tau_0]$ and $c \in [0, 1)$,

$$u \frac{\partial}{\partial \tau} Y(\tau, u) + Y(\tau, u) = c\pi^{-1/2} \int_{-\infty}^{\infty} Y(\tau, \mu) e^{-\mu^2} d\mu. \tag{28}$$

For a half-space we impose the boundary conditions

$$Y(0, u) = F(u) + \rho^s Y(0, -u) + \rho^d G(u) \int_0^{\infty} Y(0, -\mu) e^{-\mu^2} d\mu, \tag{29a}$$

for $u > 0$, and, for all u ,

$$\lim_{\tau \rightarrow \infty} Y(\tau, u) = 0; \tag{29b}$$

whereas for finite slab applications we consider, for $u > 0$,

$$Y(0, u) = F_-(u) + \rho_-^s Y(0, -u) + \rho_-^d G_-(u) \int_0^{\infty} Y(0, -\mu) e^{-\mu^2} d\mu \tag{30a}$$

and

$$Y(\tau_0, -u) = F_+(u) + \rho_+^s Y(\tau_0, u) + \rho_+^d G_+(u) \int_0^{\infty} Y(\tau_0, \mu) e^{-\mu^2} d\mu. \tag{30b}$$

Here, in general, $F(u)$ and $G(u)$ are considered given and ρ^s and ρ^d are reflection coefficients.

We first investigate the case of a half-space and express $Y(\tau, u)$ in terms of the elementary solutions reported by CONNOR (1977), i.e.

$$Y(\tau, u) = \int_0^{\infty} A(\eta) \phi(\eta, u) e^{-\tau \eta} d\eta \tag{31}$$

where

$$\phi(\eta, u) = c\pi^{-1/2} \eta P v \left(\frac{1}{\eta - u} \right) + e^{\eta^2} \lambda(\eta) \delta(\eta - u), \tag{32}$$

$$\lambda(\eta) = 1 + c\pi^{-1/2} \eta P \int_{-\infty}^{\infty} e^{-\mu^2} \frac{d\mu}{\mu - \eta} \tag{33}$$

and $A(\eta)$ is an expansion coefficient to be determined. We note that the generalized functions $\phi(\eta, u)$ are normalized such that

$$\int_{-\infty}^{\infty} \phi(\eta, u) e^{-u^2} du = 1 \tag{34}$$

and that they obey the orthogonality condition (CERCIGNANI, 1969)

$$\int_{-\infty}^{\infty} \phi(\eta, u)\phi(\eta', u)e^{-u^2} u \, du = 0, \quad \eta \neq \eta'. \tag{35}$$

It is thus apparent from (31) and (35) that

$$\int_{-\infty}^{\infty} \phi(\eta, u)Y(\tau, -u)e^{-u^2} u \, du = 0, \quad \eta \in [0, \infty), \tag{36}$$

which for $\tau = 0$ yields

$$\int_0^{\infty} \phi(\eta, u)Y(0, -u)e^{-u^2} u \, du = \int_0^{\infty} \phi(-\eta, u)Y(0, u)e^{-u^2} u \, du. \tag{37}$$

If we now substitute the boundary condition given by (29a) into (37) we find, for $\eta \in [0, \infty)$,

$$\int_0^{\infty} \phi(\eta, u)Y(0, -u)e^{-u^2} u \, du - \int_0^{\infty} \phi(-\eta, u)[\rho^s Y(0, -u) + \rho^d JG(u)] e^{-u^2} u \, du = R(\eta) \tag{38}$$

where

$$J = \int_0^{\infty} Y(0, -u) e^{-u^2} u \, du \tag{39}$$

and the known term is

$$R(\eta) = \int_0^{\infty} \phi(-\eta, u)F(u) e^{-u^2} u \, du. \tag{40}$$

The fact that (31) yields, for $u \geq 0$,

$$Y(0, -u) = c\pi^{-1/2} \int_0^{\infty} \eta A(\eta) \frac{d\eta}{\eta + u} \tag{41}$$

suggests the approximation (GARCIA and SIEWERT, 1981)

$$Y(0, -u) = \sum_{\alpha=0}^N a_{\alpha} \eta_{\alpha} \left(\frac{1}{\eta_{\alpha} + u} \right) \tag{42}$$

where the basis points $\{\eta_{\alpha}\}$ are to be selected and the constants $\{a_{\alpha}\}$ are to be determined. If we substitute (42) into (38) we find

$$\sum_{\alpha=0}^N a_{\alpha} \Gamma_{\alpha}(\eta) = R(\eta) \tag{43}$$

where

$$\Gamma_{\alpha}(\eta) = M_{\alpha}(\eta) + \rho^s T_{\alpha}(\eta) - \rho^d c\pi^{-1/2} \eta \eta_{\alpha} W(\eta_{\alpha}) V(\eta), \tag{44}$$

$$M_\alpha(\eta) = \eta_\alpha \eta \left(\frac{1}{\eta_\alpha + \eta} \right) \{1 - c + c\pi^{-1/2} [W(\eta_\alpha) + W(\eta)]\}, \tag{45}$$

$$T_\alpha(\eta) = c\pi^{-1/2} \eta_\alpha \eta \left(\frac{1}{\eta_\alpha - \eta} \right) [W(\eta_\alpha) - W(\eta)], \tag{46}$$

$$W(\eta) = \int_0^\infty e^{-u^2} u \frac{du}{u + \eta} \tag{47}$$

and

$$V(\eta) = \int_0^\infty e^{-u^2} G(u) u \frac{du}{u + \eta}. \tag{48}$$

It is clear that we can now consider (43) at $N + 1$ selected values of $\eta \in [0, \infty)$ to generate the $N + 1$ linear algebraic equations

$$\sum_{\alpha=0}^N a_\alpha \Gamma_\alpha(\eta_\beta) = R(\eta_\beta), \quad \beta = 0, 1, 2, \dots, N, \tag{49}$$

that can be solved to yield the desired constants $\{a_\alpha\}$. In the following section of this work we discuss our choices of basis and collocation points and tabulate, for selected test cases, the partial flux

$$O^* = \int_0^\infty Y(0, -u) e^{-u^2} u \, du. \tag{50}$$

It is clear that the partial flux

$$I^* = \int_0^\infty Y(0, u) e^{-u^2} u \, du \tag{51}$$

can be expressed in terms of O^* ; we find

$$I^* = \int_0^\infty F(u) e^{-u^2} u \, du + (\rho^s + \rho^d) O^*. \tag{52}$$

If we presume now that (49) has been solved to yield the constants $\{a_\alpha\}$ then, for $u > 0$,

$$Y(0, u) = F(u) + \rho^s \sum_{\alpha=0}^N a_\alpha \eta_\alpha \left(\frac{1}{\eta_\alpha + u} \right) + \rho^d G(u) \sum_{\alpha=0}^N a_\alpha \eta_\alpha W(\eta_\alpha) \tag{53a}$$

and

$$Y(0, -u) = \sum_{\alpha=0}^N a_\alpha \eta_\alpha \left(\frac{1}{\eta_\alpha + u} \right) \tag{53b}$$

establish the desired solution at the boundary. At this point we could set $\tau = 0$ in

(31) and solve the resulting equation, for all u , to find $A(\eta)$ and thereby to find $Y(\tau, u)$ for all τ and u . We prefer, however, to use the F_N method in the manner discussed by DEVAUX *et al.* (1982) to find the interior distribution. Since

$$\int_{-\infty}^{\infty} \phi(\eta, u)\phi(\eta', u)e^{-u^2}u \, du = N(\eta)\delta(\eta - \eta') \tag{54}$$

where

$$N(\eta) = \eta[\lambda^2(\eta) e^{\eta^2} + \pi c^2 \eta^2 e^{-\eta^2}] \tag{55}$$

we can multiply (31) by $u\phi(\eta, u) \exp(-u^2)$ and integrate to find, for $\eta \in [0, \infty)$,

$$\int_{-\infty}^{\infty} \phi(\eta, u)Y(\tau, u)e^{-u^2}u \, du = A(\eta)N(\eta)e^{-\tau\eta} \tag{56}$$

which yields, for $\tau = 0$,

$$\int_{-\infty}^{\infty} \phi(\eta, u)Y(0, u)e^{-u^2}u \, du = A(\eta)N(\eta). \tag{57}$$

We thus can eliminate $A(\eta)N(\eta)$ between (56) and (57) to find an equation to be used with (36) for deducing $Y(\tau, u)$ for all τ and u once $Y(0, u)$ is known. We write these two equations, for $\eta \in [0, \infty)$, as

$$\int_{-\infty}^{\infty} \phi(\eta, u)Y(\tau, u)e^{-u^2}u \, du = e^{-\tau\eta} \int_{-\infty}^{\infty} \phi(\eta, u)Y(0, u)e^{-u^2}u \, du \tag{58a}$$

and

$$\int_{-\infty}^{\infty} \phi(\eta, u)Y(\tau, -u)e^{-u^2}u \, du = 0. \tag{58b}$$

Denoting two sets of appropriate basis functions by $L_\alpha(u)$ and $R_\alpha(u)$, we can now substitute the approximations, for $u > 0$,

$$Y(\tau, -u) = \sum_{\alpha=0}^N c_\alpha(\tau)L_\alpha(u) \tag{59a}$$

and

$$Y(\tau, u) = \sum_{\alpha=0}^N d_\alpha(\tau)R_\alpha(u) \tag{59b}$$

into (58) and solve the resulting equations at selected values of η to find the desired $c_\alpha(\tau)$ and $d_\alpha(\tau)$.

Let us consider now the case of a finite slab. In order to be brief, we focus our

attention on a symmetric problem; therefore, we drop the subscripts appearing in (30) and write

$$Y(\tau, u) = \int_0^\infty A(\eta)[\phi(\eta, u)e^{-\tau/\eta} + \phi(-\eta, u)e^{-(\tau_0-\tau)/\eta}] d\eta \tag{60}$$

where $A(\eta)$ is to be determined so that, for $u > 0$,

$$Y(0, u) = F(u) + \rho^s Y(0, -u) + \rho^d G(u) \int_0^\infty Y(0, -\mu) e^{-\mu^2} \mu d\mu. \tag{61}$$

We can readily deduce from (60) that, for $\eta \in [0, \infty)$,

$$\int_{-\infty}^\infty Y(\tau, -u)[e^{-(\tau_0-\tau)/\eta}\phi(-\eta, u) + e^{-\tau/\eta}\phi(\eta, u)] e^{-u^2} u du = 0 \tag{62}$$

which for $\tau = 0$ yields

$$\int_0^\infty Y(0, -u)[\phi(\eta, u) + e^{-\tau_0/\eta}\phi(-\eta, u)] e^{-u^2} u du = \int_0^\infty Y(0, u)[\phi(-\eta, u) + e^{-\tau_0/\eta}\phi(\eta, u)] e^{-u^2} u du. \tag{63}$$

If we now introduce the approximation

$$Y(0, -u) = T(u)[F(u) + \rho^d JG(u)]e^{-\tau_0/u} + c\pi^{-1/2} \sum_{\alpha=0}^N a_\alpha P_\alpha\left(\frac{2u}{U} - 1\right), \quad u > 0, \tag{64a}$$

into (61) we find

$$Y(0, u) = T(u)[F(u) + \rho^d JG(u)] + \rho^s c\pi^{-1/2} \sum_{\alpha=0}^N a_\alpha P_\alpha\left(\frac{2u}{U} - 1\right), \quad u > 0. \tag{64b}$$

Here

$$T(u) = (1 - (\rho^s)^2 e^{-2\tau_0/u})^{-1}(1 + \rho^s e^{-\tau_0/u}) \tag{65}$$

and an approximate value of

$$J = \int_0^\infty Y(0, -u) e^{-u^2} u du \tag{66}$$

can be found after we multiply (64a) by $u \exp(-u^2)$ and integrate. We find

$$J = (1 - \rho^d R)^{-1}(Q + c\pi^{-1/2} \sum_{\alpha=0}^N a_\alpha K_\alpha) \tag{67}$$

where

$$K_\alpha = \int_0^\infty P_\alpha \left(\frac{2u}{U} - 1 \right) e^{-u^2} u \, du, \tag{68}$$

$$Q = \int_0^\infty T(u)F(u) e^{-(u^2+\tau_0/u)} u \, du \tag{69}$$

and

$$R = \int_0^\infty T(u)G(u) e^{-(u^2+\tau_0/u)} u \, du. \tag{70}$$

In (64) we use a Legendre basis that is orthogonal for $u \in [0, U]$ to avoid, in subsequent systems of linear algebraic equations, the inversion of ill-conditioned matrices that occur for large N , with the use (SIEWERT *et al.*, 1980) of the simple basis functions u^α . In the next section we explain how we select the parameter U used in (64). We observe that the approximation given by (64a), with J given by (67), becomes exact for $c = 0$. We also note that (64) can be used even if $F(u)$ and $G(u)$ contain delta functionals. If we now substitute (64) and (67) into (63) and evaluate the resulting equation at $N + 1$ values of η , say $\{\eta_\beta\}$, we find the system of linear algebraic equations

$$\sum_{\alpha=0}^N a_\alpha Y_\alpha(\eta_\beta) = \Xi(\eta_\beta), \quad \beta = 0, 1, 2, \dots, N, \tag{71}$$

that can be solved to yield the desired constants $\{a_\alpha\}$. Here the known terms are

$$\begin{aligned} \Xi(\eta_\beta) = \pi^{1/2} \int_0^\infty T(u) [S(\eta_\beta, u; \tau_0) + C(\eta_\beta, u; \tau_0)] [F(u) \\ + \rho^d (1 - \rho^d R)^{-1} QG(u)] e^{-u^2} u \, du \end{aligned} \tag{72}$$

where

$$S(\eta, u; \tau) = \left(\frac{1 - e^{-\tau\eta} e^{-\tau u}}{\eta + u} \right) \tag{73}$$

and

$$C(\eta, u; \tau) = \left(\frac{e^{-\tau\eta} - e^{-\tau u}}{\eta - u} \right). \tag{74}$$

In addition, we find we can express the matrix elements in (71) as

$$\begin{aligned} Y_\alpha(\eta_\beta) = B_\alpha(\eta_\beta) + c e^{-\tau_0/\eta_\beta} A_\alpha(\eta_\beta) - \rho^s [c A_\alpha(\eta_\beta) + e^{-\tau_0/\eta_\beta} B_\alpha(\eta_\beta)] \\ - \rho^d c (1 - \rho^d R)^{-1} D(\eta_\beta) K_\alpha \end{aligned} \tag{75}$$

where

$$A_\alpha(\eta) = \frac{\pi^{1/2}}{c\eta} \int_0^\infty \phi(-\eta, u) P_\alpha\left(\frac{2u}{U} - 1\right) e^{-u^2} u \, du, \tag{76}$$

$$B_\alpha(\eta) = \frac{\pi^{1/2}}{\eta} \int_0^\infty \phi(\eta, u) P_\alpha\left(\frac{2u}{U} - 1\right) e^{-u^2} u \, du, \tag{77}$$

and

$$D(\eta) = \int_0^\infty T(u)[S(\eta, u; \tau_0) + C(\eta, u; \tau_0)]G(u) e^{-u^2} u \, du. \tag{78}$$

In the Appendix we discuss how recursive relations can be used efficiently to compute K_α , $A_\alpha(\eta)$ and $B_\alpha(\eta)$. We presume now that the constants $\{a_\alpha\}$ have been deduced so that (64) and (67) establish $Y(0, u)$ for all u . We thus seek to deduce an approximate solution $Y(\tau, u)$ for all τ and u . If we multiply (60), after we change u to $-u$, by $u\phi(\eta, u) \exp(-u^2)$ and integrate we find, for $\eta \in [0, \infty)$,

$$\int_{-\infty}^\infty \phi(\eta, u) Y(\tau, -u) e^{-u^2} u \, du = A(\eta)N(\eta) e^{-(\tau_0-\tau)/\eta}. \tag{79}$$

In a similar manner (60) yields, for $\eta \in [0, \infty)$,

$$\int_{-\infty}^\infty \phi(\eta, u) Y(\tau, u) e^{-u^2} u \, du = A(\eta)N(\eta) e^{-\tau/\eta}. \tag{80}$$

The unknown $A(\eta)N(\eta)$ can be eliminated from (79) by, for example, considering again that equation for $\tau = \tau_0$. In the same way $A(\eta)N(\eta)$ can be eliminated from (80) by evaluating that same equation at $\tau = 0$. In this way we develop, after invoking the fact that $Y(\tau_0, u) = Y(0, -u)$, the equations, for $\eta \in [0, \infty)$,

$$\int_{-\infty}^\infty \phi(\eta, u) Y(\tau, u) e^{-u^2} u \, du = e^{-\tau/\eta} \int_{-\infty}^\infty \phi(\eta, u) Y(0, u) e^{-u^2} u \, du \tag{81a}$$

and

$$\int_{-\infty}^\infty \phi(\eta, u) Y(\tau, -u) e^{-u^2} u \, du = e^{-(\tau_0-\tau)/\eta} \int_{-\infty}^\infty \phi(\eta, u) Y(0, u) e^{-u^2} u \, du \tag{81b}$$

that are the desired generalizations of (58). We now write, for $u > 0$,

$$Y(\tau, -u) = T(u)[F(u) + \rho^d JG(u)] e^{-(\tau_0-\tau)/u} + c\pi^{-1/2} \sum_{\alpha=0}^N c_\alpha(\tau) P_\alpha\left(\frac{2u}{U} - 1\right) \tag{82a}$$

and

$$Y(\tau, u) = T(u)[F(u) + \rho^d JG(u)] e^{-\tau u} + c\pi^{-1/2} \sum_{\alpha=0}^N d_\alpha(\tau) P_\alpha\left(\frac{2u}{U} - 1\right) \quad (82b)$$

where the coefficients $\{c_\alpha(\tau)\}$ and $\{d_\alpha(\tau)\}$ are to be determined. On substituting (82) into (81) and considering the resulting equations at $N + 1$ values of η , say $\{\eta_\beta\}$, we find the system of linear algebraic equations

$$\sum_{\alpha=0}^N [c_\alpha(\tau) c A_\alpha(\eta_\beta) - d_\alpha(\tau) B_\alpha(\eta_\beta)] = e^{-\tau \eta_\beta} \sum_{\alpha=0}^N a_\alpha [c A_\alpha(\eta_\beta) - \rho^s B_\alpha(\eta_\beta)] - \Omega(\eta_\beta) \quad (83a)$$

$$\sum_{\alpha=0}^N [c_\alpha(\tau) B_\alpha(\eta_\beta) - d_\alpha(\tau) c A_\alpha(\eta_\beta)] = -e^{-(\tau_0 - \tau) \eta_\beta} \sum_{\alpha=0}^N a_\alpha [c A_\alpha(\eta_\beta) - \rho^s B_\alpha(\eta_\beta)] + \Phi(\eta_\beta) \quad (83b)$$

to be solved. Here

$$\Omega(\eta) = \pi^{1/2} \int_0^\infty T(u)[e^{-(\tau_0 - \tau)u} S(\eta, u; \tau) + C(\eta, u; \tau)][F(u) + \rho^d JG(u)] e^{-u^2} u \, du \quad (84)$$

and

$$\Phi(\eta) = \pi^{1/2} \int_0^\infty T(u)[e^{-\tau u} S(\eta, u; \tau_0 - \tau) + C(\eta, u; \tau_0 - \tau)][F(u) + \rho^d JG(u)] e^{-u^2} u \, du. \quad (85)$$

We observe that the functions $A_\alpha(\eta_\beta)$ and $B_\alpha(\eta_\beta)$ appearing in (83) are the same as used in (71), and thus $\Omega(\eta_\beta)$ and $\Phi(\eta_\beta)$ are the only new quantities to be evaluated. Finally we note that the matrix of coefficients in (83) is independent of τ . The solution of these equations for many values of τ can thus be achieved at modest computational cost. In the following section we discuss our numerical results for $\psi(\tau, u)$ and the partial flux

$$O^* = \int_0^\infty Y(0, -u) e^{-u^2} u \, du. \quad (86)$$

Here we also find

$$I^* = \int_0^\infty Y(0, u) e^{-u^2} u \, du = \int_0^\infty F(u) e^{-u^2} u \, du + (\rho^s + \rho^d) O^*. \quad (87)$$

4. NUMERICAL RESULTS

In solving (49) for the constants $\{a_\alpha\}$ required in (53) to establish the

boundary distribution for the half space we have used the following scheme for selecting the collocation and basis points:

$$\eta_\alpha = \left(\frac{\xi_\alpha}{1 - \xi_\alpha} \right), \quad \alpha = 0, 1, 2, \dots, N, \tag{88}$$

where ξ_α are the zeros of the Chebyshev polynomial of the first kind $T_{N+1}(2x - 1)$, i.e.,

$$\xi_\alpha = \frac{1}{2} + \frac{1}{2} \cos \left(\frac{2\alpha + 1}{2N + 2} \pi \right). \tag{89}$$

In order to generate numerical results for a half-space problem, we consider initially in (29a) the explicit forms:

$$F(u) = \frac{1}{u_0} \exp(u_0^2) \delta(u - u_0) \tag{90}$$

and

$$G(u) = (2a) \exp[-(a - 1)u^2]. \tag{91}$$

We report in Table 1, for several test cases, converged F_N results for the partial flux O^* which were deduced with $N < 30$. We also consider a half-space problem with $G(u)$ given by (91) and

$$F(u) = (2b) \exp[-(b - 1)u^2]. \tag{92}$$

Converged F_N results ($N < 20$) are reported in Table 2.

Turning our attention to the slab problem, we first would like to explain how we select the parameter U used in (64). We note that the distribution function $\psi(\tau, \pm u)$, $u \in [0, \infty)$, is in general very small for $u \approx 5$ and, in fact, becomes negligible for increasing u . Thus by choosing $U = 12$ in (64) we aim to represent $\psi(\tau, \pm u)$ efficiently on $[0, 12]$ by using a set of basis functions which is orthogonal on $[0, 12]$. Of course this particular choice of U is not essential; in fact, we have found that $U = 8$ or 10 works as well and yields the same converged results.

TABLE 1.—THE PARTIAL FLUX O^* FOR $u_0 = 20$ AND $a = 2$

c	$\rho^s = 0.0$ $\rho^d = 1.0$	$\rho^s = 0.2$ $\rho^d = 0.8$	$\rho^s = 0.5$ $\rho^d = 0.5$	$\rho^s = 0.8$ $\rho^d = 0.2$	$\rho^s = 1.0$ $\rho^d = 0.0$
0.1	0.00150433	0.00150331	0.00150177	0.00150024	0.00149922
0.6	0.0205588	0.0204342	0.0202471	0.0200600	0.0199351
0.9	0.123119	0.121266	0.118509	0.115778	0.113971
0.95	0.254887	0.250047	0.242888	0.235847	0.231216
0.99	7.74354	7.50295	7.15595	6.82451	6.61163

TABLE 2.—THE PARTIAL FLUX O^* FOR $b = 10$ AND $a = 2$

c	$\rho^s = 0.0$ $\rho^d = 1.0$	$\rho^s = 0.2$ $\rho^d = 0.8$	$\rho^s = 0.5$ $\rho^d = 0.5$	$\rho^s = 0.8$ $\rho^d = 0.2$	$\rho^s = 1.0$ $\rho^d = 0.0$
0.1	0.0322111	0.0322089	0.0322055	0.0322021	0.0321999
0.6	0.330242	0.329614	0.328676	0.327743	0.327123
0.9	1.14504	1.13483	1.11965	1.10466	1.09476
0.95	1.78900	1.76541	1.73056	1.69634	1.67387
0.99	14.6382	14.2063	13.5835	12.9886	12.6066

We show in Table 3, for several test cases, converged F_N results for O^* obtained with $N < 30$ when we used the explicit forms for $F(u)$ and $G(u)$ given, respectively, by (90) and (91) in (61). In Table 4 we report analogous converged results ($N < 35$) obtained when we used the forms for $F(u)$ and $G(u)$ given, respectively, by (92) and (91) in (61).

In solving (71) for the constants $\{a_\alpha\}$ required to establish the results reported in Tables 3 and 4 we have used for $c < 0.9$ the collocation scheme:

$$\eta_\alpha = U\xi_\alpha, \quad \alpha = 0, 1, 2, \dots, N, \tag{93}$$

where the ξ_α are given by (89).

However, for $c \geq 0.9$, we have found that an alternative collocation scheme is needed to obtain accurate results. The reason the above scheme fails for $c \geq 0.9$ can be related to the influence of

$$\nu_0 = \frac{1}{\sqrt{2(1-c)}}, \tag{94}$$

TABLE 3.—THE PARTIAL FLUX O^* FOR $\rho^s = 0.2$, $\rho^d = 0.5$, $u_0 = 20$ AND $a = 2$

c	$\tau_0 = 1$	$\tau_0 = 5$	$\tau_0 = 10$	$\tau_0 = 20$
0.1	1.3428	0.93854	0.70136	0.40410
0.6	1.6683	1.0845	0.81058	0.47423
0.9	2.4449	1.5505	1.1456	0.69608
0.95	2.7853	1.9168	1.4261	0.88660
0.99	3.3190	3.2646	3.1801	2.9529

TABLE 4.—THE PARTIAL FLUX O^* FOR $\rho^s = 0.2$, $\rho^d = 0.5$, $b = 10$ AND $a = 2$

c	$\tau_0 = 1$	$\tau_0 = 5$	$\tau_0 = 10$	$\tau_0 = 20$
0.1	0.10534	0.032465	0.031994	0.031978
0.6	0.64475	0.31685	0.30612	0.30564
0.9	1.9033	1.0188	0.89374	0.87624
0.95	2.4517	1.5097	1.2630	1.1994
0.99	3.3103	3.2457	3.1735	3.0492

as discussed by CONNOR (1977) in the context of the method of elementary solutions. Therefore, for $c \geq 0.9$ we use a modified scheme that includes a finite number of points in the vicinity of ν_0 :

$$\eta_0 = \nu_0, \tag{95}$$

$$\eta_{2\beta-1} = \nu_0(1 + \beta/50), \quad \beta = 1, 2, \dots, 5, \tag{96}$$

$$\eta_{2\beta} = \nu_0(1 - \beta/50), \quad \beta = 1, 2, \dots, 5, \tag{97}$$

plus

$$\eta_\alpha = U\xi_{\alpha-11}, \quad \alpha = 11, 12, \dots, N. \tag{98}$$

In Table 5 we show converged F_N results for the neutral distribution $\psi^*(\tau, u)$ at selected values of τ and u for one of the cases studied in Table 3. The asterisk in $\psi^*(\tau, u)$ indicates that the delta-function contribution due to $F(u)$ is ignored when computing the boundary distribution by (64) and the interior distribution by (82). In Table 6 we show the neutral distribution $\psi(\tau, u)$ for one of the cases studied in Table 4. In addition, we list in Table 7 converged F_N results for the neutral distribution $\psi(\tau, u)$ for a special case with $F(u)$ given by (92), perfect specular reflection and no diffuse reflection at the boundaries. Our results for this case exhibit a behavior similar to those reported by BURRELL (1978). We would like to point out that for this type of problem once $\psi(\tau, u)$ is known, one can immediately obtain the complete neutral distribution $f_0(\tau, \nu)$ with the use of a

TABLE 5.—THE NEUTRAL DISTRIBUTION $\psi^*(\tau, u)$ FOR $c = 0.6$, $\tau_0 = 20$, $\rho^s = 0.2$, $\rho^d = 0.5$, $u_0 = 20$ AND $a = 2$

u	$\tau = 0$	$\tau = \tau_0/8$	$\tau = \tau_0/4$	$\tau = 3\tau_0/8$	$\tau = \tau_0/2$
-5.0	0.1160(-11) [†]	0.82159(-12)	0.78603(-12)	0.77993(-12)	0.78301(-12)
-4.0	0.1002(-7)	0.67389(-8)	0.64131(-8)	0.63826(-8)	0.64697(-8)
-3.0	0.1201(-4)	0.74834(-5)	0.70396(-5)	0.69917(-5)	0.71234(-5)
-2.0	0.2036(-2)	0.11328(-2)	0.10452(-2)	0.10289(-2)	0.10435(-2)
-1.0	0.5168(-1)	0.23621(-1)	0.21155(-1)	0.20567(-1)	0.20541(-1)
-0.8	0.7960(-1)	0.34237(-1)	0.30408(-1)	0.29491(-1)	0.29386(-1)
-0.6	0.1150	0.45899(-1)	0.40364(-1)	0.39049(-1)	0.38839(-1)
-0.4	0.1571	0.56957(-1)	0.49489(-1)	0.47743(-1)	0.47406(-1)
-0.2	0.2068	0.65495(-1)	0.56048(-1)	0.53900(-1)	0.53429(-1)
-0.0	0.2919	0.69933(-1)	0.58649(-1)	0.56190(-1)	0.55602(-1)
0.0	0.1007(+1)	0.69933(-1)	0.58649(-1)	0.56190(-1)	0.55602(-1)
0.2	0.9169	0.69661(-1)	0.56728(-1)	0.54094(-1)	0.53429(-1)
0.4	0.7201	0.66585(-1)	0.50770(-1)	0.48095(-1)	0.47406(-1)
0.6	0.4847	0.63695(-1)	0.42235(-1)	0.39505(-1)	0.38839(-1)
0.8	0.2796	0.55885(-1)	0.32941(-1)	0.30013(-1)	0.29386(-1)
1.0	0.1387	0.41882(-1)	0.23968(-1)	0.21128(-1)	0.20541(-1)
2.0	0.7254(-3)	0.15240(-2)	0.12420(-2)	0.10999(-2)	0.10435(-2)
3.0	0.2416(-5)	0.83780(-5)	0.79639(-5)	0.74392(-5)	0.71234(-5)
4.0	0.2005(-8)	0.66861(-8)	0.68279(-8)	0.66385(-8)	0.64697(-8)
5.0	0.2320(-12)	0.73495(-12)	0.78582(-12)	0.78851(-12)	0.78301(-12)

[†]Read as 0.1160×10^{-11}

TABLE 6.—THE NEUTRAL DISTRIBUTION $\psi(\tau, u)$ FOR $c = 0.6$, $\tau_0 = 20$, $\rho^s = 0.2$, $\rho^d = 0.5$, $b = 10$ AND $a = 2$

u	$\tau = 0$	$\tau = \tau_0/8$	$\tau = \tau_0/4$	$\tau = 3\tau_0/8$	$\tau = \tau_0/2$
-5.0	0.1939(-11) [†]	0.18173(-12)	0.15988(-12)	0.24169(-12)	0.39348(-12)
-4.0	0.1879(-7)	0.12895(-8)	0.86548(-9)	0.13757(-8)	0.25153(-8)
-3.0	0.2611(-4)	0.13628(-5)	0.52229(-6)	0.79506(-6)	0.17378(-5)
-2.0	0.5374(-2)	0.23801(-3)	0.44797(-4)	0.35006(-4)	0.95315(-4)
-1.0	0.1795	0.68148(-2)	0.10382(-2)	0.23711(-3)	0.24745(-3)
-0.8	0.2982	0.10722(-1)	0.16151(-2)	0.34717(-3)	0.26430(-3)
-0.6	0.4713	0.15738(-1)	0.23412(-2)	0.48524(-3)	0.29798(-3)
-0.4	0.7212	0.21613(-1)	0.31660(-2)	0.63831(-3)	0.33294(-3)
-0.2	0.1118(+1)	0.27906(-1)	0.40046(-2)	0.78809(-3)	0.35780(-3)
-0.0	0.2345(+1)	0.34170(-1)	0.47569(-2)	0.91409(-3)	0.36675(-3)
0.0	0.2108(+2)	0.34170(-1)	0.47569(-2)	0.91409(-3)	0.36675(-3)
0.2	0.1419(+2)	0.40646(-1)	0.53445(-2)	0.99959(-3)	0.35780(-3)
0.4	0.4626(+1)	0.59015(-1)	0.57961(-2)	0.10385(-2)	0.33294(-3)
0.6	0.9383	0.72556(-1)	0.65392(-2)	0.10501(-2)	0.29798(-3)
0.8	0.2628	0.67177(-1)	0.74385(-2)	0.10957(-2)	0.26430(-3)
1.0	0.1195	0.54609(-1)	0.77572(-2)	0.11894(-2)	0.24745(-3)
2.0	0.1280(-2)	0.29422(-2)	0.99665(-3)	0.31066(-3)	0.95315(-4)
3.0	0.5232(-5)	0.17976(-4)	0.86901(-5)	0.39186(-5)	0.17378(-5)
4.0	0.3758(-8)	0.14575(-7)	0.84821(-8)	0.46496(-8)	0.25153(-8)
5.0	0.3877(-12)	0.15997(-11)	0.10428(-11)	0.64413(-12)	0.39348(-12)

[†]Read as 0.1939×10^{-11}

TABLE 7.—THE NEUTRAL DISTRIBUTION $\psi(\tau, u)$ FOR $c = 0.2$, $\tau_0 = 20$, $\rho^s = 1.0$, $\rho^d = 0.0$ AND $b = 100$

u	$\tau = 0$	$\tau = \tau_0/8$	$\tau = \tau_0/4$	$\tau = 3\tau_0/8$	$\tau = \tau_0/2$
-5.0	0.3922(-12) [†]	0.27122(-13)	0.40345(-13)	0.65955(-13)	0.10863(-12)
-4.0	0.3846(-8)	0.12935(-9)	0.19329(-9)	0.35492(-9)	0.66181(-9)
-3.0	0.5486(-5)	0.72455(-7)	0.84590(-7)	0.18416(-6)	0.42165(-6)
-2.0	0.1189(-2)	0.78152(-5)	0.24478(-5)	0.54074(-5)	0.18253(-4)
-1.0	0.4482(-1)	0.21762(-3)	0.27035(-4)	0.58688(-5)	0.10205(-4)
-0.8	0.7811(-1)	0.34453(-3)	0.42195(-4)	0.80996(-5)	0.67580(-5)
-0.6	0.1321	0.50956(-3)	0.61479(-4)	0.11311(-4)	0.67757(-5)
-0.4	0.2248	0.70660(-3)	0.83681(-4)	0.14937(-4)	0.74836(-5)
-0.2	0.4250	0.92395(-3)	0.10674(-3)	0.18533(-4)	0.80138(-5)
-0.0	0.2068(+1)	0.11514(-2)	0.12828(-3)	0.21635(-4)	0.82061(-5)
0.0	0.2021(+3)	0.11514(-2)	0.12828(-3)	0.21635(-4)	0.82061(-5)
0.2	0.4088(+1)	0.14235(-2)	0.14664(-3)	0.23878(-4)	0.80138(-5)
0.4	0.2248	0.28346(-2)	0.16542(-3)	0.25183(-4)	0.74836(-5)
0.6	0.1321	0.65712(-2)	0.25803(-3)	0.27252(-4)	0.67757(-5)
0.8	0.7811(-1)	0.91692(-2)	0.53449(-3)	0.42501(-4)	0.67580(-5)
1.0	0.4482(-1)	0.90818(-2)	0.84264(-3)	0.82924(-4)	0.10205(-4)
2.0	0.1189(-2)	0.74601(-3)	0.21841(-3)	0.63208(-4)	0.18253(-4)
3.0	0.5486(-5)	0.50462(-5)	0.22199(-5)	0.96837(-6)	0.42165(-6)
4.0	0.3846(-8)	0.42628(-8)	0.23026(-8)	0.12353(-8)	0.66181(-9)
5.0	0.3922(-12)	0.48205(-12)	0.29461(-12)	0.17899(-12)	0.10863(-12)

[†]Read as 0.3922×10^{-12}

scaling factor which depends of course on v_x and v_y . Finally, we note that all our numerical results are correct, we believe, to within ± 1 in the last figure shown.

In reporting the numerical results shown in Tables 5, 6 and 7 we used

$$B_\alpha(\eta) = B_0(\eta)P_\alpha\left(\frac{2\eta}{U} - 1\right) - cG_\alpha(\eta), \tag{99}$$

where the $G_\alpha(\eta)$, with $G_0(\eta) = 0$, are given by

$$(\alpha + 1)G_{\alpha+1}(\eta) - (2\alpha + 1)\left(\frac{2\eta}{U} - 1\right)G_\alpha(\eta) + \alpha G_{\alpha-1}(\eta) = \frac{2}{U}(2\alpha + 1)K_\alpha, \tag{100}$$

to deduce from (71) for $u \in [0, \infty)$ the following alternative expressions which proved to be improvements over the usual (64) in the computation of the boundary distributions, especially as $u \rightarrow 0$:

$$Y(0, -u) = T(u)[F(u) + \rho^d JG(u)] e^{-\tau_0 u} + \frac{c}{\pi} Y(u) \tag{101a}$$

and

$$Y(0, u) = T(u)[F(u) + \rho^d JG(u)] + \rho^s \frac{c}{\pi} Y(u). \tag{101b}$$

Here

$$Y(u) = (1 - \rho^s e^{-\tau_0 u})^{-1} \left\{ \Xi(u) + c \sum_{\alpha=0}^N a_\alpha [\rho^d (1 - \rho^d R)^{-1} D(u) K_\alpha - [e^{-\tau_0 u} - \rho^s] A_\alpha(u)] \right\} + c \sum_{\alpha=0}^N a_\alpha \left[[\pi^{1/2} - A_0(u)] P_\alpha\left(\frac{2u}{U} - 1\right) + G_\alpha(u) \right]. \tag{102}$$

One additional comment is needed regarding the convergence of our method for slab problems. While for integrated quantities such as O^* the F_N method converges to 5 significant figures with $N < 35$, we have found that higher N is necessary to obtain accurate neutral distributions. For example, to obtain the results shown in Table 6 we used $N = 60$. We note also that the convergence in the calculation of neutral distributions is slowest at the boundaries and this explains why we have reported boundary distributions with fewer significant figures than interior distributions.

Since the elementary solutions appropriate to a class of spatially varying ion temperatures have recently been established (POMRANING, 1981), we intend, in our continuing study, to use the F_N method to develop numerical results for this important generalization of the present work.

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APPENDIX

Recursive relations

In order to compute accurately the constants K_α defined by (68), we use elementary properties of the Legendre polynomials to deduce, for $\alpha \geq 0$,

$$\left(\frac{\alpha+3}{2\alpha+7}\right)K_{\alpha+4} + K_{\alpha+3} + \left[\left(\frac{\alpha+2}{2\alpha+3}\right) - \left(\frac{\alpha+3}{2\alpha+7}\right) - \frac{2}{U^2}(2\alpha+5)\right]K_{\alpha+2} - K_{\alpha+1} - \left(\frac{\alpha+2}{2\alpha+3}\right)K_\alpha = 0. \quad (\text{A.1})$$

(A.1), with given values of K_0 , K_1 , K_2 and K_3 , defines an initial value problem. We have found that forward recursion is unstable here, and thus we use the method discussed by OLIVER (1968) to compute the required K_α , for α up to a fixed L . First we select M and replace the initial value

problem by a convenient boundary value problem defined by (A.1) with

$$K_0 = \frac{1}{2}, K_1 = \frac{1}{2} \left(\frac{\pi^{1/2}}{U} - 1 \right), K_{L+M+1} = K_{L+M+2} = 0, \tag{A.2, A.3, A.4}$$

and solve the resulting $L + M - 1$ linear algebraic equations for K_2, K_3, \dots, K_{L+M} by Gaussian elimination. We repeat this procedure for different M until we obtain K_α with the desired accuracy for α up to L . Indeed by using a double-precision Gauss elimination routine and an IBM 370/165 machine we were able to compute K_α accurate to 14 significant figures for α up to 185, with $M = 15$.

In regard to the functions $A_\alpha(\eta)$ defined by (76) we find for $\alpha \geq 0$

$$(\alpha + 1)A_{\alpha+1}(\eta) + (2\alpha + 1) \left(\frac{2\eta}{U} + 1 \right) A_\alpha(\eta) + \alpha A_{\alpha-1}(\eta) = \frac{2}{U} (2\alpha + 1) K_\alpha \tag{A.5}$$

with

$$A_0(\eta) = \int_0^\infty e^{-u^2} u \frac{du}{u + \eta}. \tag{A.6}$$

Due to the fact that the generation of $A_\alpha(\eta)$ for $\eta > 0$ is unstable when using (A.5) in the forward direction, we use a combination of (A.5) and the corresponding homogeneous equation, both in the backward direction, to compute $A_\alpha(\eta)$ accurately for α up to N . First we take $A_{N+M+1}^*(\eta) = A_{N+M}^*(\eta) = 0$ for some M and use (A.5) backwards to generate $A_{N+M-1}^*(\eta), A_{N+M-2}^*(\eta), \dots, A_{N+1}^*(\eta)$. We then increase M and repeat the procedure until convergence in $A_{N+1}^*(\eta)$ is achieved. Next we set, for some M , $A_{N+M+1}^{**}(\eta) = 0, A_{N+M}^{**}(\eta) = \epsilon$, and use the homogeneous version of (A.5) backwards to generate $A_{N+M-1}^{**}(\eta), A_{N+M-2}^{**}(\eta), \dots, A_{N+1}^{**}(\eta)$. By increasing M and repeating this procedure, convergence in the ratio $A_{N+1}^{**}(\eta)/A_{N+2}^{**}(\eta)$ is finally achieved. We then propose for $\alpha = 0, 1, 2, \dots, N$:

$$A_\alpha(\eta) = k(\eta) A_\alpha^{**}(\eta) + A_\alpha^*(\eta). \tag{A.7}$$

Once we have completed the generation of $A_\alpha^*(\eta)$ and $A_\alpha^{**}(\eta)$ down to $\alpha = 0$, we can compute the normalization factor from

$$k(\eta) = \left[A_1^{**}(\eta) + \left(\frac{2\eta}{U} + 1 \right) A_0^{**}(\eta) \right]^{-1} \left[\frac{2}{U} K_0 - A_1^*(\eta) - \left(\frac{2\eta}{U} + 1 \right) A_0^*(\eta) \right] \tag{A.8}$$

and find the desired $A_\alpha(\eta)$ by using (A.7). For $\eta > 1$, however, we discovered that the convergence of $A_{N+1}^*(\eta)$ becomes progressively slow; therefore we use the Christoffel-Darboux formula (HOCHSTRASSER, 1964) for the Legendre polynomials to deduce the alternative recursion relation

$$P_\alpha \left(\frac{2\eta}{U} + 1 \right) A_{\alpha+1}(\eta) + P_{\alpha+1} \left(\frac{2\eta}{U} + 1 \right) A_\alpha(\eta) = \frac{2}{U} \left(\frac{1}{\alpha + 1} \right) \sum_{\beta=0}^{\alpha} (2\beta + 1) (-1)^{\alpha+\beta} K_\beta P_\beta \left(\frac{2\eta}{U} + 1 \right). \tag{A.9}$$

(A.9) was used backwards in the manner suggested by MILLER (1952) to generate the required $A_\alpha(\eta)$ for $\eta > 1$. We note that by computing K_α as outlined in the beginning of the Appendix we were able to compute $A_\alpha(\eta)$ accurate to at least 13 significant figures for $\eta > 0$ and α up to 100. In addition, the use (obligatory in this case) of the recursive relations given by (A.5) and (A.9) in the backward direction yields $A_0(\eta)$ automatically, i.e., no numerical integration is needed to compute $A_0(\eta)$.

The functions $B_\alpha(\eta)$ defined by (77) may in turn be expressed for $\alpha \geq 0$ by

$$(\alpha + 1)B_{\alpha+1}(\eta) - (2\alpha + 1) \left(\frac{2\eta}{U} - 1 \right) B_\alpha(\eta) + \alpha B_{\alpha-1}(\eta) = -\frac{2c}{U} (2\alpha + 1) K_\alpha \tag{A.10}$$

with

$$B_0(\eta) = \pi^{1/2} (1 - c) + cA_0(\eta). \tag{A.11}$$

(A.10) can be used efficiently in the forward direction to generate the required $B_\alpha(\eta)$ for $\eta > 0$.