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ELENDIF: A TIME-DEPENDENT BOLTZMANN SOLVER FOR PARTIALLY IONIZED PLASMAS

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ELENDIF calculates the time evolution of the electron energy distribution function in a mixture of partially ionized gases with or without an applied electric field. The code can treat inelastic and superelastic processes, electron–electron and electron–ion collisions, photon–electron (free–free) processes, attachment and recombination, ionization including a distribution of secondary electrons, and an external source of electrons (e.g. an electron beam). The code also computes the mean electron energy, drift velocity, diffusion coefficient, rate coefficients and energy flow rates for the processes being included in the calculation.

PROGRAM SUMMARY

Title of program: ELENDIF77

Catalogue number: ABLX

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: Cray X-MP; *Installation*: Lawrence Livermore National Laboratory; *Operating system*: NLTSS

Computer: DEC Vax 8650; *Installation*: Joint Institute for Laboratory Astrophysics, Lawrence Berkeley Laboratory; *Operating system*: VMS

Computer: Sun 3/280; *Installation*: Lawrence Livermore National Laboratory; *Operating system*: UNIX

Computer: Apple Macintosh II; *Operating system*: Mac OS

Computer: IBM PC Compatibles; *Operating system*: DOS

Programming language used: FORTRAN 77

No. of lines in combined program and test deck: 3596

Keywords: Boltzmann equation, electron distribution, transport coefficients, laser physics, plasma physics, gas discharges

Nature of physical problem
ELENDIF calculates the time evolution of the electron energy distribution function in a mixture of partially ionized gases with or without an applied electric field. The code can treat inelastic and superelastic processes, electron–electron and electron–ion collisions, photon–electron (free–free) processes, attachment and recombination, ionization including a distribution of secondary electrons, and an external source of electrons

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(e.g. an electron beam). The code also computes the mean electron energy, drift velocity, diffusion coefficient, rate coefficients and energy flow rates for the processes being included in the calculation.

Method of solution
ELENDIF solves the time-dependent Boltzmann transport equation in terms of the electron number density [1]. By finite-differencing the electron energy axis, the Boltzmann equation is transformed into a finite set of coupled differential equations for the electron number density at each energy grid as a function of time. The matrix of densities is then evolved forward in time using a combination of explicit and implicit methods. The electron energy distribution is then convolved with the cross sections to provide the transport coefficients, collisional rates and energy flow rates.

Restrictions on the complexity of the problem
It is assumed in the formulation of ELENDIF that the two-term spherical harmonic expansion of the electron distribution function is adequate.

Typical running time
On the Vax 8650 the code takes 0.11 seconds per timestep if the effects of electron–electron collisions are ignored, and 0.46 seconds per timestep if electron–electron collisions are included.

Reference
[1] D. Rockwood, Phys. Rev. A 8 (1973) 2348.

LONG WRITE-UP

1. Introduction

ELENDIF calculates the electron energy distribution function in a mixture of partially ionized gases which may or may not be under the influence of an external electric field. This is done by solving a form of the Boltzmann transport equation. This problem has a long history. The approach used here, that of expressing the distribution function as a sum of a spherically symmetric term and a small directional term as described below, dates back to the work of Lorenz [1] on electron transport in metals. This approach was applied to electrons in partially ionized gases by Allis in the 1930's [2] and further developed by Holstein in 1946 [3]. The application of this formalism, with greatly enhanced utility due to the use of computers and numerical mathematics, to atoms and molecules with inelastic channels for electron energy loss was pioneered by Phelps and his collaborators in the 1960's [4–7]. They solved the Boltzmann equation as part of the process of obtaining electron impact cross sections by modeling the transport properties of electron swarms in gases. More recently Rockwood [8] and Elliot and Greene [9] have developed a finite difference formulation of the Boltzmann equation that is general enough to easily accomodate many different kinds of collision processes as well as time dependence in the model. ELENDIF is based on their formulation.

ELENDIF solves a time dependent form of the Boltzmann equation that is derived from the full transport equation using the first two terms of a spherical harmonic expansion for the velocity distribution function. The development of the code was initiated at Wayne State University in 1972 as part of research in modeling energy transfer processes in CO electric discharge lasers [10,11]. Due to the large cross sections for vibrational excitation by electrons in a discharge, the electron energy distribution is very highly non-Maxwell–Boltzmann [12]. The evolution of the code continued at the Joint Institute for Laboratory Astrophysics [13] and at the Lawrence Livermore National Laboratory. Special problems occuring in the study of discharges [14,15], excimer lasers [16,17] and laser-produced plasmas [18] necessitated the inclusion of additional physical processes such as electron–electron and electron–ion collisions, inverse bremsstrahlung, and processes such as ionization and attachment that alter the electron density. Older versions of the code have been distributed to many academic and research institutions.

Because its development has been associated with a number of diverse applications, ELENDIF possesses come capabilities which have not been included in the Boltzmann codes [19,20] previously published in Computer Physics Communications. The code can compute the time evolution of the distribution function and treat inelastic and superelastic processes, photon–electron (free–free) processes,

attachment and recombination, ionization including a distribution of secondaries, and an external source of electrons such as might be due to ionization by an electron beam. A constant field is assumed, although it is not difficult to modify the program to treat a time-varying field. The program is applicable to a wide variety of problems within the limitations of the approximations used to reduce the Boltzmann equation to a manageable form. The most severe of these is the two term spherical harmonic approximation. In treating certain classes of molecules, such as polar molecules having rotational cross sections that are very large in comparison with the elastic cross section, or molecules such as CH_4 which has a vibrational cross section that overlaps a Ramsauer minimum in the elastic cross section, the two term expansion is known to be inaccurate [21]. The greatest accuracy is obtained in such situations by a multi-term expansion [21–23] or by a Monte Carlo simulation [24].

For many kinds of problems ELENDIF is self-contained. In some instances, the user may want to define an initial non-Maxwellian distribution, define the distribution of secondary electrons due to ionization, include an energy dependent recombination cross section, or define the energy distribution of an external source of electrons. We have provided the shells of such subprograms in ELENDIF and the appropriate subprogram calls so that users can tailor aspects of the model to their specific applications. All of the other processes mentioned above are programmed into ELENDIF and dealt with via the appropriate flags and cross section lists in the input file.

2. The Boltzmann equation

The general form of the Boltzmann transport equation is

$$\left(\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla_{\mathrm{r}} + \frac{e\boldsymbol{E}}{m}\cdot\nabla_{\mathrm{v}}\right) f(\boldsymbol{r}, \boldsymbol{v}, t) = \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}}, \tag{1}$$

where $f(\boldsymbol{r}, \boldsymbol{v}, t)$ is the distribution function for electrons at time t and spatial location $\boldsymbol{r}$ with velocity $\boldsymbol{v}$. In the present formulation it is assumed that the electric field is independent of space and time, and the problem at hand is spatially uniform, so $f(\boldsymbol{r}, \boldsymbol{v}, t) \rightarrow f(\boldsymbol{v}, t)$. The function $f(\boldsymbol{v}, t)$ is also expressed in terms of the two-term spherical harmonic expansion [3]

$$f(\boldsymbol{v}) = f_0(v) + \frac{\boldsymbol{v}}{v}\cdot\boldsymbol{f}_1(v). \tag{2}$$

With these assumptions and including only momentum transfer, inelastic and superelastic processes, the Bolzmann equation can be expressed in terms of the electron number density $n(\epsilon)$ as [8,9]

$$\frac{\partial n}{\partial t} = -\frac{\partial J_{\mathrm{f}}}{\partial \epsilon} - \frac{\partial J_{\mathrm{el}}}{\partial \epsilon} + \sum_{s,j} N_s^0 \left[R_{sj}(\epsilon+\epsilon_{sj}) n(\epsilon+\epsilon_{sj}) - R_{sj}(\epsilon) n(\epsilon)\right] - \sum_{s,j} N_s^j \left[R_{sj}^*(\epsilon) n(\epsilon) - R_{sj}^*(\epsilon-\epsilon_{sj}) n(\epsilon-\epsilon_{sj})\right], \tag{3}$$

where

$$J_{\mathrm{f}} = \frac{2Ne^2(E/N)^2\epsilon}{3m(2\epsilon/m)^{1/2}\sum_s \delta_s \sigma_s(\epsilon)}\left(\frac{n}{2\epsilon} - \frac{\partial n}{\partial \epsilon}\right), \tag{4}$$

$$J_{\mathrm{el}} = -N\left(\frac{2\epsilon}{m}\right)^{1/2}\sum_s \delta_s \frac{2m}{M_2}\sigma_e(\epsilon)\left[n\left(\frac{kT}{2} - \epsilon\right) - kT\epsilon\frac{\partial n}{\partial \epsilon}\right], \tag{5}$$

$$R_{sj}(\epsilon) = \left(\frac{2}{m}\right)^{1/2}\left[\epsilon^{1/2}\sigma_{sj}(\epsilon)\right], \tag{6}$$

$$R^*_{sj}(\epsilon) = \left(\frac{2}{m}\right)^{1/2}\left[\frac{(\epsilon+\epsilon_{sj})}{\epsilon^{1/2}}\sigma_{sj}(\epsilon+\epsilon_{sj})\right], \tag{7}$$

$$n(\epsilon) = n_e f_0(\epsilon)\epsilon^{1/2}, \quad \text{such that } \int_0^\infty n(\epsilon)\,d\epsilon = n_e. \tag{8}$$

Here N = total number density = $\Sigma_s(N_s^0 + \Sigma_j N_s^j)$, with the index s denoting the species and the index j denoting the state; σ_s = momentum transfer cross section for species s; σ_{sj}, ϵ_{sj} = excitation cross section and energy loss, respectively, for the jth state of species s; $\delta_s = N_s/N$. The first term in eq. (3) represents the energy gain by electrons from the electric field. The second term represents the energy loss in elastic collisions with the heavy species, with a correction term to account for the thermal energy of the heavy species. The quantity $R_{sj}(\epsilon)$ is the rate at which electrons with energy ϵ produce excitation from the ground state of species s to excited state j losing energy ϵ_{sj} in the process. The quantity $R^*_{sj}(\epsilon)$ is the rate at which electrons with energy ϵ gain an energy ϵ_{sj} due to superelastic collisions with molecules in state N_s^j. As it stands, eq. (3) is actually independent of electron density, and in the steady state,

$$\frac{\partial n(\epsilon)}{\partial t} = n_e\epsilon^{1/2}\frac{\partial f_0(\epsilon)}{\partial t} = 0,$$

independent of N in the sense that the key parameters become E/N and the fractional composition of the heavy species.

When processes such as attachment and ionization, which do not conserve the number density of free electrons, are included in the calculation the distribution function can reach steady state and the LHS of eq. (3) can still be non-zero. That is,

$$\frac{\partial n(\epsilon)}{\partial t} = \epsilon^{1/2}f_0(\epsilon)\frac{\partial n_e}{\partial t} + n_e\epsilon^{1/2}\frac{\partial f_0(\epsilon)}{\partial t}, \tag{9}$$

$$\frac{\partial f_0(\epsilon)}{\partial t} = 0 \quad \text{does not imply} \quad \frac{\partial n(\epsilon)}{\partial t} = 0 \quad \text{unless} \quad \frac{\partial n_e}{\partial t} = 0.$$

Although the electron density in the Boltzmann calculations is variable, the neutral atom and molecule densities are not. Modeling of the time evolution of these species generally involves solving a set of chemical kinetics rate equations. This provision is not included in ELENDIF, although ELENDIF has been used as a subroutine in a chemical kinetics code to provide electron collision rate coefficients appropriate to the non-equilibrium chemistry that occurs in discharges [11] and laser-produced plasmas [18].

3. Inclusion of additional processes in the boltzmann equation

3.1. Rotational processes

Collisional excitation of molecular rotational modes can be included in the Boltzmann equation explicitly or by use of the "continuous approximation to rotation" (CAR) [4] In this approximation $f_0(\epsilon+\epsilon_j)$ is expanded in a Taylor series to first order, the $\Delta j = \pm 2$ selection rule is invoked, and the Gerjuoy and Stein [25] Born approximation formulae are used for $\sigma_{j,j+2}(\epsilon)$ to obtain the following simplification,

$$\sum_j \frac{N_j}{N}\left[(\epsilon+\epsilon_j)\sigma_{j,j+2}(\epsilon+\epsilon_j)f_0(\epsilon+\epsilon_j) - \epsilon\sigma_{j,j+2}(\epsilon)f_0(\epsilon) + (\epsilon-\epsilon_j)\sigma_{j,j-2}(\epsilon-\epsilon_j)f_0(\epsilon-\epsilon_j)\right.$$
$$\left. -\epsilon\sigma_{j,j-2}(\epsilon)f_0(\epsilon)\right] = 4B_0\sigma_0\frac{d}{d\epsilon}\left[\epsilon f_0(\epsilon)\right],$$

Table 1
Parameters, for various molecules, for calculations using the continuous approximation to rotational states

Molecule	B_0 (eV)	q_2 (ea_0)	q_4 (ea_0^2)	CAR
CO	2.43E-4	0.046		1.45E-12
CO_2	4.85E-5		3.000	4.10E-4
H_2	7.35E-3		0.586	2.37E-3
H_2O	1.78E-3	0.730		2.11E-9
N_2	2.43E-4		1.040	2.47E-4
O_2	1.78E-4		1.800	5.40E-4

where B_0 = the rotational constant and

$$\sigma_0 = \frac{8\pi}{15} a_0^2 q^2,$$

with q = electric quadruple moment.

This same approach can be used for the case of rotational excitation via a permanent dipole moment as shown by Hake and Phelps [6]. Following Luft [26], we defined the CAR parameters for dipole and quadrupole excitation respectively by

$$C_2 = q_2^2 B_0^{7/8} 10^{-6} \tag{10a}$$

and

$$C_4 = q_4^2 B_0 a_0^2 \frac{16\pi}{15} 10^{16}, \tag{10b}$$

where the units of the dipole and quadrupole moments and rotational constants are ea_0 for q_2, ea_0^2 for q_4, and eV for B_0. a_0 is the Bohr radius in cm. One can use the dipole or quadrupole moments and the rotational constant or the CAR parameter as input to ELENDIF. A list of these parameters, compiled by Luft [26], for several common molecules is shown in table 1.

The rotational cross section is obtained from the CAR parameter using

$$Q^{\mathrm{CAR}} = \begin{cases} \dfrac{C_4 M}{kTm\epsilon}, & \text{if the species has a quadrupole moment,} \\ 3.7613 \times 10^6 \dfrac{C_2 R_y M}{(kT)^{1.875} m\epsilon^{1.75}}, & \text{if the species has a dipole moment.} \end{cases} \tag{11}$$

A difficulty encountered in finite differencing the Boltzmann equation is that $\Delta\epsilon$ should be much smaller than the smallest energy loss in any inelastic process. This makes it difficult to include processes in which there is great disparity in the size of the energy quantum; one must use very small $\Delta\epsilon$. This strains the capabilities of all but the largest supercomputers. The CAR approach allows us to circumvent this limitation when rotational processes are included.

3.2. Attachment and recombination

Electron attachment can be properly included in eq. (3) as an inelastic process by retaining the loss term $-R_{sj}(\epsilon)n(\epsilon)$, and deleting the gain term $R_{sj}(\epsilon+\epsilon_{sj})n(\epsilon+\epsilon_{sj})$.

Electron molecule dissociative recombination is treated similarly when a cross section is available. In general, recombination data are available only in the form of an electron temperature dependent rate coefficient. If the recombination rate coefficient, $\alpha(\mathrm{cm}^3/\mathrm{s})$, is of the form

$$\alpha = \alpha_0 (kT_e)^{-q},$$

with kT_e in eV and the cross section is assumed to be of form

$$\sigma = \sigma_0 (kT_e)^{-q},$$

then one can show that

$$\sigma(\epsilon) = \frac{1.5^{-8}}{\Gamma\left[\left(\frac{3}{2}\right) - q\right]} \frac{\alpha_0}{\epsilon^{q+1/2}} (\mathrm{cm}^2), \tag{12}$$

with the electron energy ϵ in eV. The special case of $q = \frac{1}{2}$ corresponds to the $\alpha = \alpha_0 (kT_e)^{-1/2}$ rate coefficient derived by O'Malley [27]. Note that $\Gamma(z)$ possesses simple poles at $z = 0, -1, -2, \ldots$, implying that q cannot take on the values $\frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \ldots$.

The subroutine RECOMB that treats recombination in ELENDIF must be modified by the user for the specific problem being modeled.

3.3. Ionization

Secondary electrons due to ionization can be included in the formalism in two ways:

(i) Delta function

All of the secondaries are assumed to enter the distribution with zero energy, thus adding the term [8]

$$\left[\frac{\partial n(\epsilon)}{\partial t}\right]_{\text{ionization of species } s} = \delta(\epsilon)\left(\frac{2}{m}\right)^{1/2} N_s^0 \int_{\epsilon_{si}}^{\infty} \sigma_{si} \epsilon^{1/2} n(\epsilon)\, \mathrm{d}\epsilon + N_s^0 \left[R_s^i(\epsilon + \epsilon_{si}) n(\epsilon + \epsilon_{si}) - R_s^i(\epsilon) n(\epsilon)\right] \tag{13a}$$

to the RHS of eq. (3). The primaries are treated as are any other electrons, undergoing inelastic collisions with the energy loss equal to the ionization potential, ϵ_{si}.

(ii) Secondary electrons distributed in energy

If the differential cross section, $\mathrm{d}\sigma_{si}(\epsilon_2, \epsilon)/\mathrm{d}\epsilon_2$, for the production of secondary electrons of energy ϵ_2 by a primary of energy ϵ is available, ionization processes and secondary electrons would be properly represented on the RHS of eq. (3) by the terms

$$\begin{aligned}\left[\frac{\partial n(\epsilon)}{\partial t}\right]_{\text{ionization of species } s} &= \left(\frac{2}{m}\right)^{1/2} N_s^0 \int_{\epsilon_{si}}^{\infty} (\epsilon + \epsilon_2 + \epsilon_{si})^{1/2} \frac{\mathrm{d}\sigma_{si}(\epsilon_2 + \epsilon_{si},\, \epsilon + \epsilon_2 + \epsilon_{si})}{\mathrm{d}\epsilon_2} n(\epsilon + \epsilon_2 + \epsilon_{si})\, \mathrm{d}\epsilon_2 \\ &\quad - \left(\frac{2}{m}\right)^{1/2} N_s^0 \int_{\epsilon_{si}}^{(\epsilon+\epsilon_{si})/2} \epsilon^{1/2} \frac{\mathrm{d}\sigma_{si}(\epsilon_2 + \epsilon_{si},\, \epsilon)}{\mathrm{d}\epsilon_2} n(\epsilon)\, \mathrm{d}\epsilon \\ &\quad + \left(\frac{2}{m}\right)^{1/2} N_s^0 \int_{2\epsilon+\epsilon_{si}}^{\infty} \epsilon_1^{1/2} \frac{\mathrm{d}\sigma_{si}(\epsilon + \epsilon_{si},\, \epsilon_1)}{\mathrm{d}\epsilon} n(\epsilon_1)\, \mathrm{d}\epsilon_1.\end{aligned} \tag{13b}$$

Note that the second term in this expression reduces to

$$-\left(\frac{2\epsilon}{m}\right)^{1/2} N_s^0 n(\epsilon)\sigma_{si}(\epsilon) = -N_s^0 R_s^i(\epsilon) n(\epsilon),$$

where $\sigma_{si}(\epsilon)$ is the total ionization cross section.

The differential cross section $d\sigma_{si}(\epsilon_2, \epsilon)/d\epsilon_2$ must be written into the function DSIGMA by the user. Due to the work of Peterson and Green and their collaborators [28–31], such differential cross sections are available in the form of semi-empirical analytic formulae for a number of atoms and molecules.

3.4. Electron–electron collisions

The terms describing the effect of electron–electron collisions on the distribution function are given by Rockwood [8] as

$$\left(\frac{\partial n}{\partial t}\right)_{e-e} = \alpha\left[\frac{3}{\epsilon^{1/2}} n^2 + 2\epsilon^{3/2}\frac{\partial \psi}{\partial \epsilon}\frac{\partial}{\partial \epsilon}\left(\frac{\partial n}{\partial \epsilon} - \frac{n}{2\epsilon}\right) + \frac{\psi}{\epsilon^{1/2}}\left(\frac{\partial n}{\partial \epsilon} - \frac{n}{2\epsilon}\right)\right], \tag{14}$$

where

$$\psi(\epsilon, t) = 3\int_0^{\epsilon} n(\epsilon')\, d\epsilon' - \frac{1}{\epsilon}\int_0^{\epsilon} \epsilon' n(\epsilon')\, d\epsilon' + 2\epsilon^{1/2}\int_{\epsilon}^{\infty} \frac{n(\epsilon')}{\epsilon'^{1/2}}\, d\epsilon',$$

$$\alpha = \tfrac{2}{3}\pi e^4\left(\frac{2}{m}\right)^{1/2} \ln \Lambda, \quad \Lambda = \frac{\langle mv^2\rangle}{2e^2}\left(\frac{kT_e}{4\pi n_e e^2}\right)^{1/2}.$$

The theory, which involves obtaining $\partial f_0/\partial t$ due to electron–electron collisions by solving the Fokker–Planck equation using the Rosenbluth potentials, is described in detail by Shkarofsky et al [32], Rosenbluth et al [33], Dreicer [34] and by Megill and Cahn [35].

3.5. Electron–ion collisions

Collisions between electrons and ions can be treated by modifying the momentum transfer cross section in the following manner [36]:

$$\sigma_s(\epsilon) \to (\delta_{s,n} - \delta_{s,i})\sigma_s(\epsilon) + \delta_{s,i}\sigma_{ei}(\epsilon), \tag{15a}$$

where

$\delta_{s,n}$ = fraction of species s that are neutral,

$\delta_{s,i}$ = fraction of species s that are ions,

such that

$$\delta_{s,n} + \delta_{s,i} = 1$$

and

$$\sigma_{ei}(\epsilon) = 4\pi\frac{e^4}{\epsilon^2} \ln \Lambda. \tag{15b}$$

$\sigma_{ei}(\epsilon)$ is the Coulomb cross section with the maximum impact parameter set equal to the Debye shielding length [32,37].

3.6. Photon–electron processes

The free–free interaction between photons and electrons (inverse bremmstrahlung) in the field of neutral species is included in eq. (3) by use of the relation [38,39]

$$K_a(\epsilon) = \frac{8\pi e^2}{3mc\omega^2}\left[\frac{2(\epsilon + h\nu)}{m}\right]^{1/2}\frac{(\epsilon + h\nu/2)}{h\nu}\sum_s \delta_s\sigma_s\left(\epsilon + \frac{h\nu}{2}\right) \tag{16a}$$

for the free–free absorption coefficient (cm^5) for photons of energy $h\nu$. The terms in eq. (3) are then

$$FN\left[-K_a(\epsilon)n(\epsilon) + K_a(\epsilon - h\nu)n(\epsilon - h\nu) - K_e(\epsilon)n(\epsilon) + K_e(\epsilon + k\nu)n(\epsilon + h\nu)\right], \tag{16b}$$

where F is the photon flux ($cm^{-2}\ s^{-1}$) and the coefficient for stimulated emission, K_e, is related to the absorption coefficient by the detailed balance formula

$$\epsilon K_e(\epsilon) = (\epsilon - h\nu)K_a(\epsilon - h\nu). \tag{16c}$$

These processes are of interest, for example, in laser breakdown problems where the photon flux is large enough to heat electrons directly via inverse bremsstrahlung.

4. Transport coefficients, rate coefficients and energy balance

Using the distribution function one can compute the electron mean energy,

$$\bar{\epsilon} = \int_0^\infty f_0(\epsilon)\epsilon^{3/2}\,d\epsilon(eV), \tag{17}$$

drift velocity,

$$v_d = -\frac{1}{3}\left(\frac{2e}{m}\right)^{1/2}\left(\frac{E}{N}\right)\int_0^\infty \frac{1}{\sum_s \delta_s\sigma_s(\epsilon)}\frac{df_0}{d\epsilon}\epsilon\,d\epsilon(cm/s) \tag{18}$$

and rate coefficients,

$$k_{sj} = \left(\frac{2e}{m}\right)^{1/2}\int_0^\infty \sigma_{sj}(\epsilon)f(\epsilon)\epsilon\,d\epsilon(cm^3/s), \tag{19}$$

for electron impact processes. Additionally, one can compute the characteristic energy, D_T/μ, where $\mu = v_d/E$ is the electron mobility and D_T is the transverse diffusion coefficient

$$D_T = \frac{1}{3N}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty f(\epsilon)\frac{\epsilon\,d\epsilon}{\sum_s \delta_s\sigma_s(\epsilon)}(cm^2/s). \tag{20}$$

For a Maxwellian energy distribution $D_T/\mu = \frac{2}{3}\bar{\epsilon}$.

One can obtain an energy balance relation by integrating eq. (3) over all energy [8,12]. This gives an equation with rate of energy gain (from the field, free–free absorption, and superelastic collisions) on one

side and the rate of energy loss (due to elastic and inelastic collisions) on the other. This equation is, for $f_0(\epsilon,t)$,

$$v_d\frac{E}{N}n_eN + n_eN\sum_{s,j}\delta_s\frac{N_s^j}{N_s^0}\epsilon_{sj}k_{s,-j} + \bar{\epsilon}\frac{\partial n_e}{\partial t} + n_e\frac{\partial\bar{\epsilon}}{\partial t}$$
$$= \left(\frac{2e}{m}\right)^{1/2} n_eN\int_0^\infty \epsilon^2\left[\sum_s \delta_s\frac{2m}{M_s}\sigma_s(\epsilon)\right]\left[f_0(\epsilon) + \frac{kT_e}{e}\frac{df_0}{d\epsilon}\right]d\epsilon + n_eN\sum_{s,j}\delta_s\epsilon_{sj}k_{sj}$$
$$+\left(\frac{2e}{m}\right)^{1/2} n_eNF\int_0^\infty K_a(\epsilon)f_0(\epsilon)\epsilon^2\,d\epsilon\,(\mathrm{eV/cm^3/s}). \tag{21}$$

The $\partial n_e/\partial t$ term arises because $\partial n(\epsilon)/\partial t$ can be non-zero even though the distribution function is in steady state. Thus the integral over energy becomes

$$\int_0^\infty \frac{\partial n(\epsilon)}{\partial t}\epsilon\,d\epsilon = \frac{\partial n_e}{\partial t}\int_0^\infty f_0(\epsilon)\epsilon^{3/2}\,d\epsilon + n_e\frac{\partial}{\partial t}\int_0^\infty f_0(\epsilon)\epsilon^{3/2}\,d\epsilon$$
$$= \bar{\epsilon}\frac{\partial n_e}{\partial t} + n_e\frac{\partial\bar{\epsilon}}{\partial t}. \tag{22}$$

The program also computes the energy loss and momentum transfer collisions frequencies, ν_u and ν_m, respectively, which have been devised by A.V. Phelps [4] for evaluating the cross section data. These collision frequencies are defined by:

$$\frac{\nu_u}{N} = \frac{v_d e(E/N)}{D/\mu - kT} \tag{23}$$

and

$$\frac{\nu_m}{N} = \frac{e}{m\mu N}. \tag{24}$$

In practice ν_m is sensitive primarily to the momentum transfer cross section and ν_u to the vibrational and electronic cross sections.

5. Numerical method

If the function $n(\epsilon, t)$ is put in finite difference form as a vector $n(\epsilon_i, t) = n_i(t)$ $(i = 1, \mathrm{NPTS})$ on an NPTS point energy grid, eq. (3) has the general form [8,9]

$$\frac{\partial \boldsymbol{n}}{\partial t} = \mathbf{A}\cdot\boldsymbol{n} + \mathbf{B}(t)\cdot\boldsymbol{n} + \mathbf{C}[\boldsymbol{n}(t)]\cdot\boldsymbol{n} + \boldsymbol{Q}(t), \tag{25}$$

where **A** represents the constant matrix of coefficients for the field, elastic, inelastic and superelastic processes, **B** represents the matrix of coefficients for a time dependent process (such as recombination), **C** represents the matrix of coefficients for processes dependent upon $\boldsymbol{n}$ (such as electron–electron collision), and $\boldsymbol{Q}$ represents an external source of electrons (such as an electron beam). As pointed out by Rockwood [8], and Elliot and Greene [9], this equation can be solved using a combination of implicit and explicit

methods. The algorithm for this solution is developed as follows:

$$\frac{\partial \boldsymbol{n}(t)}{\partial t} = \frac{\boldsymbol{n}(t+\delta t) - \boldsymbol{n}(t)}{\delta t}$$

$$= \mathbf{A}\cdot\boldsymbol{n}(t+\delta t) + \mathbf{B}(t)\cdot\boldsymbol{n}(t) + \mathbf{C}[\boldsymbol{n}(t)]\cdot\boldsymbol{n}(t+\delta t) + \boldsymbol{Q}(t),$$

$$\boldsymbol{n}(t+\delta t) = \delta t\mathbf{A}\cdot\boldsymbol{n}(t+\delta t) + \delta t\mathbf{B}(t)\cdot\boldsymbol{n}(t) + \delta t\mathbf{C}[\boldsymbol{n}(t)]\cdot\boldsymbol{n}(t+\delta t) + \delta t\boldsymbol{Q}(t) + \boldsymbol{n}(t)$$

$$= (1-\delta t\mathbf{A})^{-1}\cdot\delta t\mathbf{C}[\boldsymbol{n}(t)]\cdot\boldsymbol{n}(t+\delta t) + (1-\delta t\mathbf{A})^{-1}\cdot\{[1+\delta t\mathbf{B}(t)]\cdot\boldsymbol{n}(t) + \delta t\boldsymbol{Q}(t)\},$$

$$\boldsymbol{n}(+\delta t) = \left\{1-(1-\delta t\mathbf{A})^{-1}\cdot\delta t\mathbf{C}[\boldsymbol{n}(t)]\right\}^{-1}\cdot(1-\delta t\mathbf{A})^{-1}\cdot\{[1+\delta t\mathbf{B}(t)]\cdot\boldsymbol{n}(t) + \delta t\boldsymbol{Q}(t)\}.$$

If δt is small, the factor on the RHS involving $\mathbf{C}$ is approximately $[1-\delta t\mathbf{C}]^{-1}$ so that

$$\boldsymbol{n}(t+\delta t) = \{1-\delta t\mathbf{C}[\boldsymbol{n}(t)]\}^{-1}\cdot(1-\delta t\mathbf{A})^{-1}\cdot\{[1+\delta t\mathbf{B}(t)]\cdot\boldsymbol{n}(t) + \delta t\boldsymbol{Q}(t)\}. \tag{26}$$

In ELENDIF, secondary electrons from ionization, electron depletion due to recombination or attachment, and electron–ion collisions are include in the **B** array, which is treated explicitly, and electron–electron collisions are included in the **C** array. The order of computation goes from right to left. Since **C** is tridiagonal, the final operation in the calculation of $\boldsymbol{n}(t+\delta t)$ is the solution of a tridiagonal system. Each diagonal of the tridiagonal **C** array is the product of an n_e and T_e dependent factor, a constant matrix, and the vector representing $n(\epsilon)$. Hence the electron–electron collision term is effectively quadratic in electron density. Details are given by Rockwood [8].

Regarding the choice of δt that allows us to use this approximation, if δt is chosen such that

$$\max(\delta t A_{ij}) < 1 \quad \text{for all } i,\ j,$$

then the matrix $(\delta t A_{ij})$ is nilpotent in a limiting sense in that

$$(\delta t A_{ij})^r \to 0 \quad \text{as } r \to \infty.$$

In this case the matrix $(1-\delta t\mathbf{A})$ possesses an inverse such that [40,41]

$$(1-\delta t\mathbf{A})^{-1} = 1 + (\delta t\mathbf{A}) + (\delta t\mathbf{A})^2 + \cdots.$$

Hence,

$$1-(1-\tau t\mathbf{A})^{-1}\cdot\delta t\mathbf{C} = 1-\delta t\mathbf{C},$$

dropping the terms having quadratic and higher powers of δt.

The matrix **A**, having dimensions of s^{-1}, represents the collision frequencies for the flow of electrons up an down the energy axis due to the electric field and elastic, inelastic and superelastic collisions. As one of the key assumptions in the use of the first order spherical harmonic expansion of the distribution function is $\nu_{\text{elastic}} \gg \nu_{\text{inelastic}}$, the **A**-matrix should be diagonally dominant. Because the electric field acceleration and momentum transfer energy loss are treated as continuous processes in the Boltzmann equation, the flow of electrons along the energy axis due to these processes is written in terms of a current in eq. (3). These terms, in finite difference form, are given by Rockwood [8] as

$$A_{km}n_m \propto a_{k-1}n_{k-1} + b_{k+1}n_{k+1} - (a_k + b_k)n_k, \tag{27}$$

where

$$\left.\begin{matrix} a_k \\ b_{k+1} \end{matrix}\right\} = \frac{2N_e^2}{3m}\left(\frac{E}{N}\right)^2\frac{1}{\nu_k^+/N}\left(\frac{1}{\Delta\epsilon}\right)^2\left(\epsilon_k^+ \pm \frac{\Delta\epsilon}{4}\right) + \frac{\bar{\nu}_k^+}{2\Delta\epsilon}\left(\pm\frac{kT_{\text{gas}}}{2} \mp \epsilon_k^+ + \frac{2kT_{\text{gas}}}{\Delta\epsilon}\epsilon_k^+\right)(s^{-1}) \tag{28}$$

and

$$\epsilon_k^+ = k\Delta\epsilon, \quad \nu_k^+/N = \left(\frac{2\epsilon_k^+}{m}\right)^{1/2} \sum_s q_s\sigma_s(\epsilon_k^+), \quad \bar{\nu}_k^+ = 2mN\left(\frac{2\epsilon_k^+}{m}\right)^{1/2} \sum_s \frac{q_s\sigma_s(\epsilon_k^+)}{M_s}.$$

For use in choosing a value for δt, these terms are approximately

$$\left.\begin{matrix} a \\ b \end{matrix}\right\} \approx 1.2^{15}\frac{N^2}{\nu_{el}}\left(\frac{E}{N}\right)^2 \frac{1}{\Delta\epsilon}\left(\frac{\epsilon}{\Delta\epsilon}\right) \mp \frac{2m}{M}\nu_{el}\left(\frac{\epsilon}{\Delta\epsilon}\right)(s^{-1}),$$

where ϵ and $\Delta\epsilon$ are in eV, N is the gas density in cm^{-3}, E/N is in V cm^2 and ν_{el} is the elastic collision frequency in s^{-1}.

Having chosen the time step δt for integration of the Boltzmann equation, one needs to estimate the time needed for the distribution function to relax to a steady state under the influence of electron–electron collisions. This time is of the order of the electron–electron energy exchange time discussed by Spitzer [37]. He gives this time as

$$t_E = \frac{v^2}{4A_D G(L_v)},$$

where

v = electron speed (cm/sec),

$L \equiv \dfrac{m}{2kT_e}$ such that for a Maxwellian distribution $L^2v^2 = \epsilon/kT_e$,

$A_D = \dfrac{8\pi e^4 n_e \ln\Lambda}{m^2}$,

n_e = electron density (cm^{-3}),

$\ln\Lambda$ = Coulomb logarithm,

$G(x) \equiv \dfrac{\Phi(x) - x\Phi'(x)}{2x^2}$ with $\Phi(x) = \mathrm{erf}(x)$.

Evaluating the constants,

$$t_E = \frac{3.24^4\epsilon^{3/2}}{n_e \ln\Lambda G\left[(\epsilon/kT_e)^{1/2}\right]}(s), \tag{29}$$

where ϵ = electron energy (eV). Values of $\ln\Lambda$ and $G(x)$ are tabulated by Spitzer [37].

These implicit computational techniques have been used because of their inherent stability. For the electron–electron problem restrictions have been imposed upon δt by the approximation used, not by stability considerations. When electron–electron processes are not being included in the calculation, the stability characteristics of the implicit scheme allow an arbitrary choice of δt. It should be noted, however, that although all choices of δt converge to the same solution, the temporal development of the distribution function will be represented accurately only for "small" δt. The integration is not unconditionally stable when the source term $Q(t)$, or the term $B(t)$ (which is how recombination, for instance, is included in the calculations) are large. These terms are treated explicitly and, consequently, have a stability criterion associated with their presence in the finite difference equations.

As a final note, the electron–electron calculation can also be performed explicitly, the algorithm being

$$\boldsymbol{n}(t+\delta t) = (1-\delta t\mathbf{A})^{-1} \cdot \{1 + \delta t\mathbf{B}(t) + \delta t\mathbf{C}[\boldsymbol{n}(t)]\} \cdot \boldsymbol{n}(t) + \delta t\boldsymbol{Q}(t). \tag{30}$$

With this approach there are stability considerations that place a restriction on δt of the form $\delta t = F[\boldsymbol{n}, (\mathrm{d}\boldsymbol{n}/\mathrm{d}t), (\mathrm{d}\boldsymbol{n}, \mathrm{d}\epsilon), \Delta\epsilon]$ where F is some complicated function of electron density and energy bin size. However, this stability criterion has not been worked out.

6. Choice of parameters

The choice of time step was discussed in the previous section. The choice of energy bin size and maximum energy are dictated by several considerations. Normalization and conservation of electrons requires that $f_0(\epsilon_{\max}) \ll \max f_0(\epsilon)$, i.e. the calculation must be performed into the "tail" of the distribution. Also, for accuracy in the calculation and in the normalization of the distribution function, $\Delta\epsilon \ll \bar{\epsilon}$, where $\bar{\epsilon}$ is the mean energy. To minimize discretization error, $f_0(\epsilon_i)/f_0(\epsilon_{i+1})$ should be of order unity. To minimize discretization error with regard to the physical processes being included in the calculation, we desire $\Delta\epsilon \ll \epsilon_{ij}$ represents the excitation energies of the important electron impact processes in the calculation. $\Delta\epsilon$ should also be small with respect to the energy dependence of the cross sections for these processes. An example of this latter consideration is the inclusion of vibrational processes in the calculation. The $\Delta\epsilon \ll \epsilon_{ij}$ constraint is particularly important in a time-dependent calculation in order to conserve electrons.

7. Program structure and subroutines

PARAMETER statements in the main routine and in the subprograms are used to control the dimensions of the arrays used in ELENDIF. The user may want to modify these dimensions depending on the amount of computer memory available. These parameters are:

NPTSF the maximum number of points in the finite differenced electron energy distribution function;
NPTSEE the dimension of the arrays used in the electron–electron calculation; must equal NPTSF if e–e collisions are being treated, but can be set equal to 1 to make the code smaller if e–e collisions are being neglected;
NSP the maximum number of chemical species that the code can handle;
NLEV the maximum number of states or levels which are allowed for each species.

The entire flow of calculation is controlled from the main program ELENDIF, but the routine responsible for the matrix calculation of the distribution function is subroutine FDIFF. The flow charts are shown in figs. 1 and 2.

The input parameters and cross sections are read into program ELENDIF. Details of the input data are described in a later section. Subroutine QCAR computes the cross section parameter for rotational states in the continuous approximation described in section 3, if this process is being included. In some cases an effective rotational cross section with a computationally tractable effective energy loss is used to represent the effect of the rotational states. ELENDIF then calls FDIFF, which is the main routine for calculating the distribution function. Once the distribution function is known, subroutine INTGRL normalizes the distribution function and calculates the mean energy (eq. (17)). The rate coefficients (eq. (19)) for all the inelastic and superelastic processes are then computed in subroutine RATE. Calculation of the transport coefficients (eq. (18) and (20) and check of the energy balance (eq. (21)) is done in subroutine ENBAL. In

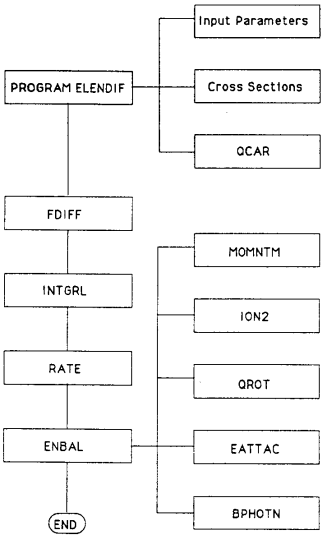

Fig. 1. Flow chart for program ELENDIF.

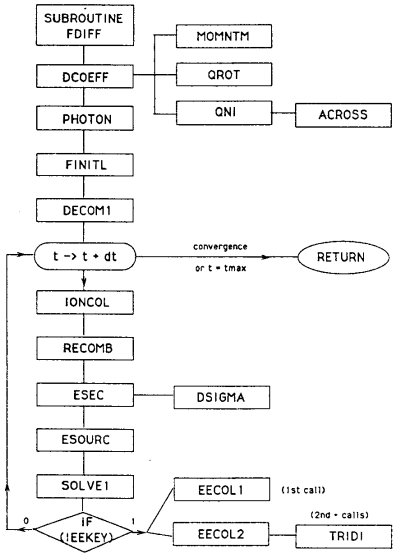

Fig. 2. Flow chart for subroutine FDIFF.

setting up the energy rate balance, ENBAL calls subroutines MOMNTM, ION2, QROT, EATTAC and BPHOTN. Subroutine MOMNTM interpolates the momentem transfer cross section for use in calculating the energy gain rate from the external electric field. Subroutine ION2 computes the electron–ion collision cross section, which is then added to the total momentum transfer cross section, as described in section 3.5. Subroutine QROT computes the cross section for rotational excitation in the continuous approximation (eq.(11)). Subroutine EATTAC computes the energy loss due to attachment. Subroutine BPHOTN calculates the absorption and emission rates for the free–free processes (eqs. (16a) and (16c)).

The matrix calculation of the distribution function is managed by subroutine FDIFF. The matrix of coefficients is calculated by subroutine DCOEFF, which calls subprograms MOMNTM, QROT, QNI and ACROSS for the collisional cross sections. Function QNI interpolates the inelastic (vibrational and electronic) cross sections. Function ACROSS is user-provided and is used for cross section evaluation using analytic formulae. Subroutine PHOTON is called to calculate the terms in the coefficient matrix relating to free–free processes. Subroutine FINITL provides the initial distribution function, if a non-Maxwellian is desired. Subroutine DECOM1 does the matrix decomposition. Other processes depend on the distribution function and will to be updated at each time step. Subroutine IONCOL computes the electron–ion collision terms. Subroutine RECOMB provides the rate of energy loss versus energy due to recombination. Subroutine ESEC adds the secondary electrons due to ionization to the distribution. There are two choices provided: (1) the secondaries are all put into the lowest energy bin, or (2) the secondaries are distributed along the energy grid using the secondary electron energy spectrum computed in the user-provided function DSIGMA. Subroutine ESOURC provides the external source of electron, e.g. an electron beam, if the problem involves such. Subroutine SOLVE1 solves the resulting set of matrix equations. If electron–electron collisions are included, subroutine EECOL1 computes the matrix used in the electron–electron calculations, while EECOL2 computes the right hand side for the implicit calculation. Subroutine TRIDI is used for solving the tridiagonal system of equations resulting from the inclusion of electron–electron interaction.

Subroutine FDIFF first sets up the matrix calculation by partitioning the electron energy axis into NPTS cells of width DELTAZ $= \Delta\epsilon$. The number density of electrons with energy between $(k-1)\Delta\epsilon$ and $k\Delta\epsilon$ is defined as n_k. Equation (25) is then represented as a set of NPTS coupled differential equations. The matrix of coefficients in eq. (25) is calculated in the subroutines described in the following. The time evolution of the electron distribution proceeds as given in eq. (26) or (27).

Subroutine DCOEFF calculates the contributions to the A-matrix of eq. (25) due to the field, and the elastic, inelastic and superelastic processes. The elements of the A-matrix are identified from refs. [8,9],

$$A_{km}n_m = a_{k-1}n_{k-1} + b_{k+1}n_{k+1} - (a_k + b_k)n_k + \sum_{s,j} N_s^0\left(R_{sj,k+m_{sj}}n_{k+m_{sj}} - R_{sj,k}n_k\right) - \sum_{s,j} N_s^j\left(R^*_{sj,k}n_k - R^*_{sj,k-m_{sj}}n_{k-m_{sj}}\right), \tag{31}$$

where a_k and b_k are given by eq. (28), and $R_{sj,k} = R_{sj}(k\Delta\epsilon)$. The functions $R_{sj}(\epsilon)$ and $R^*_{sj}(\epsilon)$ are defined in eqs. (6) and (7). a_k is the rate at which electrons in the kth energy cell are promoted to the $(k+1)$th cell, and b_k is the rate at which they are demoted to the $(k-1)$th cell. $R_{sj,k+m_{sj}}$ is the rate at which electrons in the $(k+m_{sj})$th cell are demoted to the kth cell because of inelastic collisions. $R^*_{sj,k-m_sj}$ is the rate at which electrons in the $(k-m_{sj})$th cell are promoted to the kth cell because of superelastic collisions. In the calculation of a_k and b_k, calls are made to subroutine MOMNTM, which interpolates the momentum transfer cross section data to the defined energy grid points. Calls are also made to subroutine QROT, which calculates the rotational cross section using eq. (11). The effective momentum transfer cross section automatically includes the rotational contribution if the CAR parameter is non-zero. In calculating the inelastic and superelastic terms of A_{km}, calls are made to function QNI, which interpolates the vibrational and electronic cross sections.

Subroutine EECOL1 calculates the C-matrix of eq. (25) when electron–electron collisions are taken into account. The elements of the C-matrix are identified from refs. [8,9],

$$C_{km}n_m = a'_{k-1}n_{k-1} + b'_{k+1}n_{k+1} - (a'_k + b'_k)n_k, \tag{32}$$

where

$$a'_k = \sum_j A'_{kj}n_j, \quad b'_k = \sum_k A'_{kj}n_k,$$

$$A'_{kj} = \left[A_{kj}A_{j-1,k+1}(\epsilon_{j-1}\epsilon_{k+1})^{1/2}(\epsilon_j\epsilon_k)^{-1/2}\right]^{1/2},$$

$$A_{kj} = \begin{cases} \alpha\left[\epsilon_{k+1}^{-1/2} + \epsilon_k^{-1/2}\right]\left(\epsilon_j\epsilon_k - \frac{3}{4}\right), & k > j, \\ \alpha[\epsilon_{k+1} + \epsilon_k]u_k\epsilon_j^{-1/2}, & k < j-1, \\ \alpha\left[\left(\epsilon_{k+1}^{-1/2} + \epsilon_k^{-1/2}\right)\left(\epsilon_j u_k - \frac{3}{4}\right) + \epsilon_k u_k \epsilon_j^{-1/2}\right], & k = j, \\ \alpha\left[\left(\epsilon_j u_k - \frac{3}{4}\right)\epsilon_{k+1}^{-1/2} + (\epsilon_{k+1} + \epsilon_k)u_k\epsilon_j^{-1/2}\right], & k = j-1, \\ 0, & k = 1 \quad \text{or } k = \text{NPTS}, \end{cases}$$

$$u_k = \frac{1}{\Delta\epsilon} + \frac{0.25}{\epsilon_k + 0.5\,\Delta\epsilon}.$$

and α is given in eq. (14).

Subroutine PHOTON computes the contribution to the A-matrix of eq. (25) when photon–electron processes are taken into account. The terms used in calculating this contribution are easily identified from eq. (16).

Subroutine ESOURC provides an external source of electrons through the array Q. Subroutine ESEC provides for secondary electrons from ionization, while subroutine RECOMB provides for electron depletion due to recombination. These contributions are included in the B-array. Subroutine IONCOL uses the cross section in eq. (15b) to calculate the contribution to the B-array from electron–ion collisions.

Subprograms ACROSS, DSIGMA, ESOURC, ESEC, FINITL and RECOMB are user provided, and are described in the next section. We have provided the shells of these subprograms and have included the appropriate calls so that users can easily adapt the code to their specific application.

8. User provided subroutines for special problems

Calls on the following routines and dummy routines are included in the program:

(a) Subroutine for providing initial distribution function (if non-Maxwellian is desired):

```
SUBROUTINE FINITL(B,DE,EMAX,EDENS,N)
DIMENSION B(N)
```

Definitions:

B(i) = $n(\epsilon_i, t=0) = n_i(t=0)$ = number of electrons/cm^3/eV,
DE = energy grid size,
EMAX = maximum energy = N × DE,
EDENS = electron number density n_e (cm^{-3}),
N = number of grid points.

(b) Subroutine for providing external source of electrons, such as might come from an electron beam or fission fragment ionization of a gas:

```
SUBROUTINE ESOURC(Q,DE,EMAX,T,N)
DIMENSION Q(N)
```

Definitions:

Q(i) = $Q(\epsilon_i)$ = number of electrons/cm^3/eV/s,
DE,EMAX,N = same as before,
T = time (s).

The quantity to be furnished by the user is the spectrum Q(i), the number of electrons/cm^3/eV/s at energy ϵ_i.

(c) Function for providing secondary electron spectrum (called by subroutine ESEC):

```
FUNCTION DSIGMA(W,EP,NC,L)
```

Definitions:

W = energy loss = secondary energy + ionization potential,
EP = primary electron energy,
NC = species index (consistent with data being used in the code),
L = state index.

The unit of the differential cross section DSIGMA, i.e. $d\sigma_{si}(\epsilon_2,\epsilon)/d\epsilon_2$, is Å^2/eV.

(d) Function for analytic cross section evaluation (called by function QNI):

```
FUNCTION ACROSS(E,NC,NL,P1,P2)
```

Definitions:

E = electron energy (eV),
NC = species index,
NL = state index,
P1,P2 = arbitrary parameters,
ACROSS = cross section (Å^2).

This function is called for a given species NC and state NL when the number of cross section data points is equal to one. In this event the data value E(NC,1,NL) and Q(NC,1,NL) may serve as arbitrary parameters to be used in the formulae being evaluated in ACROSS. The function also passes the electron energy E for use in the user written formula.

(e) Subroutine for providing rate of electron loss versus energy due to recombination:

```
SUBROUTINE RECOMB(N,NP1,B,U,USQRT,DT,EDENS,TEL,GDENS)
DIMENSION B(N), U(NP1), USQRT(NP1)
```

Definitions:

N = number of grid points,
NP1 = N + 1,
B = $n_e(\epsilon)$(electrons/cm^3/eV),

U = energy (eV); $U_{i+1} = i\delta\epsilon$ = energy of ith grid point,
USQRT = $U^{1/2}$,
DT = time step Δt (s),
EDENS = total electron density (cm^{-3}),
TEL = reduced mean energy, $2\langle\epsilon\rangle/3$,
GDENS = gas density (cm^{-3}),
RECRATE = loss rate of electrons from the distribution (electrons/cm^3/s/eV),
EREC = energy loss rate due to recombination/product of electron and gas densities (eV cm^3/s); this is used in the energy balance calculation.

Recombination is included in the Boltzmann calculation as a time dependent process represented by $\mathbf{B}(t)$. Recombination processes fall into three categories:

i) $e^- + X^+ \rightarrow X + h\nu$, two-body collisional-radiative recombination,
ii) $e^- + X_2^+ \rightarrow X + X$, dissociative recombination,
iii) $e^- + X^+ + Y \rightarrow X + Y$, three-body recombination.

A form of recombination cross section that can be derived from an electron temperature dependent rate coefficient was discussed in a previous section. A review of recombination cross sections and rate coefficients is given by Biondi [42]. For an accurate treatment of recombination $\sigma_{recomb}(\epsilon)$ and an assumption concerning the ion densities $[X^+(t)]$, $[X_2^+(t)]$, etc. are required. In the absence of an energy dependent cross section one could use a rate coefficient and remove electrons from the distribution in the lowest energy bin. In either case, this calculation is performed explicitly in the Boltzmann code due to the time dependent ion density.

Subroutine RECOMB must be modified appropriately for different kinds of recombination (radiative, three-body, etc.) or more than one kind of recombining ion. For example, given α_0 for dissociative recombination, the coding to be written into RECOMB would be:

```
      sigma0 = 1.5e - 8*alpha0
      erec = 0.
      do 10 i = 1,n
            v = 5.93e7*usqrt(i + 1)
            sigma = sigma0/u(i + 1)
            recrate(i) = v*sigma*edens*b(i)
            erec = erec + recrate(i)*de
10    continue.
```

9. Input data description

The sample input data serves as a template for creating other input data files. The sample input file and the code itself are commented well enough so that the user can modify the structure of the input (e.g. the cross section data format) to his/her liking. The following briefly describes what the input variables are.

COMENT	comment line containing anything.
NCOMP	number of chemical species.
NAME(i)	
i = 1,NCOMP	name of chemical species.
COMP(i)	
i = 1,NCOMP	fractional composition, i.e. mole fraction of species i in the mixture.
VTEMP(i,j)	These define the excited state populations so that superelastic effects can be

	included in the calculations. The following conventions apply: vibrational states: VTEMP(i,j) = vibrational temperature (K) for jth excited state of species i; electronic states: VTEMP < 0: abs(VTEMP) is the fractional population of the jth excited state relative to that of the ground electronic state; VTEMP > 0: VTEMP is the fractional population of the jth excited state relative to the total gas density.
EBYN	E/N in V cm^2.
TGAS	gas temperature in K.
DT	time step size.
EPS	distribution function convergence criterion.
PRESS	gas pressure in atmosphere.
TEL	initial electron temperature.
EDENS	electron density (cm^{-3}).
DNEBDT	rate of increase of electron density due to external electron beam.
FLOOR	minimum allowed value of distribution function; this prevents underflow/overflow in subroutine FDIFF.
IFKEY	= 0: maxwellian initial distribution with electron temperature TEL is used; = 1: user provided initial distribution function (in subroutine FINITL).
IONKEY	= 0: secondary electrons due to ionization not included; = 1: secondaries are included; also, subroutine RECOMB is called.
IEEKEY	= 0: no electron–electron collisions; = 1: electron–electron collisions included; = 2: electron–ion collisions also included.
ISMAX	maximum number of time steps.
IPRINT	print interval.
IFPR	= 0: do not print out distribution function; = 1: print out distribution function.
IFPL	= 0: do not plot distribution function; = 1: plot distribution function.
VTCODE	= 0: vibrational temperature defined with respect to ground state; = 1: vibrational temperature defined with respect to next lower state.
FION(i) i = 1,NCOMP	fractional ionization for species i.
DELTAZ	grid spacing for the energy axis.
ZMATRX	maximum energy used in the calculation.
ID(i) i = 1,4	degree of polynomial used in the interpolation of, i = 1, momentum transfer cross section, i = 2, vibrational cross section, i = 3, electronic cross section, i = 4, distribution function.

M(i,j)
i = 1,NCOMP
j = 1,5
	i = species index;
	j = 1: number of vibrational states;
	j = 2: number of electronic states;
	j = 3: number of other states (ionization, etc);
	j = 4: not used (= 0);
	j = 5: number of data points for momentum;
	transfer cross section.

Parameters for continuous approximation to rotation:

CROT(i,1)	= B0 (eV) [If CROT(i,2) = 0 then CROT(i,1) is the usual CAR parameter];
CROT(i,2)	= the dipole moment (ea_0) or the quadrupole moment (ea_0^2).
KEYR(i)	= 2 for electron-dipole collisions or = 4 for electron-quadrupole collisions.
OMEGA(i,j)	applies only to diatomic molecules;
j = 1,2	contains the vibrational constants.
MV(i,j)	If (M(i,1) < 0 this input gives the number of data points for the vibrational cross
j = 1,M(i,1)	section of each state.
EM(i,k)	energy points for momentum transfer cross section.
QM(i,k)	
k = 1,M(i,5)	momentum transfer cross section points (in units of 10^{-16} cm^2).
LOGO(j,i)	commentary information about the cross section.
ET(i,j)	energy loss for the jth state of species i.
MV(i,j)	number of cross section data points.
QSCALE	scale factor for the cross section.
E(i,j,k)	kth energy point for the cross section of the jth state of species i.
Q(i,j,k)	kth data point for the cross section of the jth state of species i.
STATWT(i,j)	statistical weight ratio or = −1, attachment, = +1, ionization with secondary electrons having zero energy, = +2, ionization with secondaries distributed in energy via function DSIGMA, = 0, none of the above.

There is a provision for making multiple runs of the code allowing E/N, ZMATRX and DELTAZ to be changed between runs. This is accomplished in the last line of the input data:

EBYN,DELTAZ,ZMATRX,IEND

where IEND = 0 terminates the code.

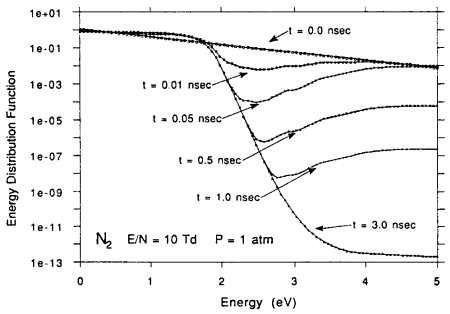

Fig. 3. Time evolution of the energy distribution function for very-weakly ionized N_2 at $E/N = 10$ Td, starting from an initial Maxwellian distribution with a mean energy of 1 eV.

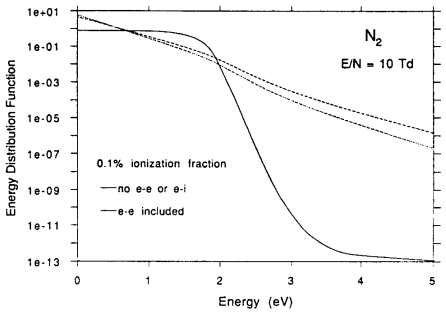

Fig. 4. Steady-state energy distribution function for partially ionized N_2 at $E/N = 10$ Td, showing the effects of electron–electron and electron–ion collisions.

10. Sample run

The test run input data for the sample run included in this paper is for N_2 at $E/N = 10$ Td $= 1 \times 10^{-16}$ V cm^2. The energy grid size is chosen to be 0.025 eV, which is much smaller than the lowest vibrational energy threshold. Instead of using a continuous approximation to rotation, this particular set of N_2 cross section data uses an effective rotational cross section with an effective energy threshold of 0.2 eV. The maximum energy used in the calculation is 5 eV, which goes well into the tail of the energy distribution, as seen in the test run output. The convergence criterion for a steady-state energy distribution function is chosen to be 10^{-5}. The calculation starts with an initial Maxwellian distribution (the default) with a temperature of 1 eV. In this sample input data the ionization fraction of the gas is chosen to be small enough so that electron–electron and electron–ion collisions are negligible. The time evolution of the energy distribution function is shown in fig. 3. Note how very highly non-Maxwellian the steady-state energy distribution is due to the large vibrational excitation cross sections. By increasing the electron density and by setting the flag IEEKEY, the effects of electron–electron and electron–ion collisions can be studied, as shown in fig. 4. Electron–electron collisions drive the energy distribution towards a Maxwellian, as expected.

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References

[1] H.A. Lorentz, Theory of Electrons (Lecture Notes, 1906), 2nd ed. (Stechert, New York, 1923), Dover Reprint (Dover, New York, 1952).
[2] W.P. Allis, Handbuch der Physik, vol. 21 (Springer, Berlin, 1956).
[3] T. Holstein, Phys. Rev. 70 (1946) 367.
[4] L.S. Frost and A.V. Phelps, Phys. Rev. 127 (1962) 1621.

[5] L.S. Frost and A.V. Phelps, Phys. Rev. A 136 (1964) 1538.
[6] R.D. Hake and A.V. Phelps, Phys. Rev. 158 (1967) 70.
[7] A.V. Phelps, Rev. Mod. Phys. 40 (1968) 399.
[8] S.D. Rockwood, Phys. Rev. A 8 (1973) 2348.
[9] C.J. Elliot and A.E. Greene, J. Appl. Phys. 47 (1976) 2946.
[10] W.L. Morgan and E.R. Fisher, RIES Report 74-56, Wayne State University (August 1974).
[11] W.L. Morgan and E.R. Fisher, Phys. Rev. A 16 (1977) 1186.
[12] W.L. Nighan, Phys. Rev. A 2 (1970) 1989.
[13] W.L. Morgan, JILA Information Center Report No. 19, University of Colorado (1979).
[14] W.L. Morgan and L. Vriens, J. Appl. Phys. 51 (1980) 5300.
[15] R.W. Lee and W.L. Morgan, Phys. Rev. A 32 (1985) 448.
[16] W.L. Morgan, R.D. Franklin and R.A. Haas, Appl. Phys. Lett. 38 (1981) 1.
[17] W.L. Morgan and A. Szöke, Phys. Rev. A 23 (1981) 1256.
[18] W.L. Morgan, Appl. Phys. Lett. 42 (1983) 790.
[19] R.M. Thomson, K. Smith and A.R. Davies, Comput. Phys. Commun. 11 (1976) 369.
[20] S.D. Rockwood and A.E. Greene, Comput. Phys. Commun. 19 (1980) 377.
[21] L.C. Pitchford, S.V. O'Neil and J.R. Rumble, Phys. Rev. A 23 (1981) 294.
[22] L.C. Pitchford and A.V. Phelps, Phys. Rev. A 25 (1982) 540.
[23] P. Segur, M. Bordage, J. Balaguer and M. Yousfi, J. Comput. Phys. 50 (1983) 116.
[24] B.M. Penetrante, J.N. Bardsley and L.C. Pitchford, J. Phys. D 18 (1985) 1087.
[25] E. Gerjuoy and S. Stein, Phys. Rev. 97 (1955) 1671.
[26] P.E. Luft, JILA Information Center Report No. 14, University of Colorado (1975).
[27] T.F. O'Malley, Phys. Rev. 185 (1969) 101.
[28] L.R. Peterson, S.S. Prasad and A.E.S. Green, Can. J. Chem. 47 (1969) 1774.
[29] L.R. Peterson and J.E. Allen, J. Chem. Phys. 12 (1972) 6068.
[30] A.E.S. Green and T. Sawada, J. Atmos. Terr. Phys. 34 (1972) 1791.
[31] T. Sawada, D.L. Sellin and A.E.S. Green, J. Geophys. Res. 77 (1972) 4819.
[32] I.P. Shkarofsky, T.W. Johnston and M.P. Bachynski, The Particle Kinetics of Plasmas (Addison-Wesley, Reading, MA, 1966).
[33] M.N. Rosenbluth, W.M. MacDonald and D.L. Judd, Phys. Rev. 107 (1957) 1.
[34] H. Dreicer, Phys. Rev. 117 (1960) 343.
[35] L.R. Megill and J.H. Cahn, J. Geophys. Rep. 69 (1964) 5041.
[36] L.A. Schlie, J. Appl. Phys. 47 (1976) 1397.
[37] L. Spitzer, Physics of Fully Ionized Gases (Interscience, New York, 1956).
[38] T. Holstein, Westinghouse Scientific Paper, 65-1E2-GASES-P2 (February 1965).
[39] A.V. Phelps, Theory of growth of ionization during laser breakdown, in: Physics of Quantum Electronics, eds. P.L. Kelley et al. (McGraw-Hill, New York, 1966).
[40] I.N. Herstein, Topics in Algebra (Xerox, Waltham, MA, 1964).
[41] B. Higman, Applied Group-Theoretic and Matrix Methods (Dover, New York, 1964).
[42] M.A. Biondi, Recombination, in: Principles of Laser Plasmas, ed. G. Bekefi (Wiley, New York ,1976).