

EEDF

The software package for calculations of the Electron Energy Distribution Function in gas mixtures

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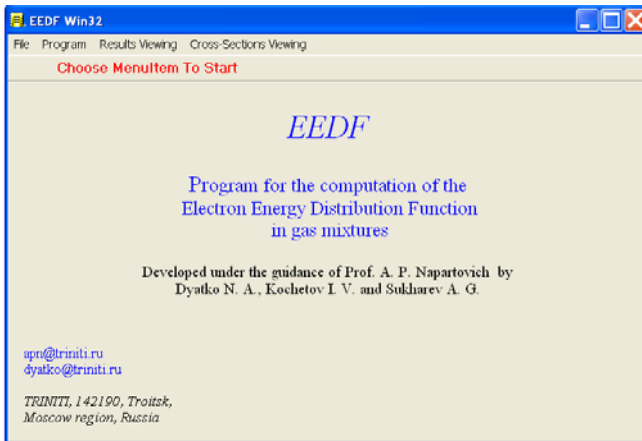
EEDF is a user-friendly program for the numerical solution of Boltzmann equation for the Electron Energy Distribution Function in low-ionized plasma in an electric field. It is used for calculations of electron transport and kinetic coefficients in gas mixtures.

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1. General comments



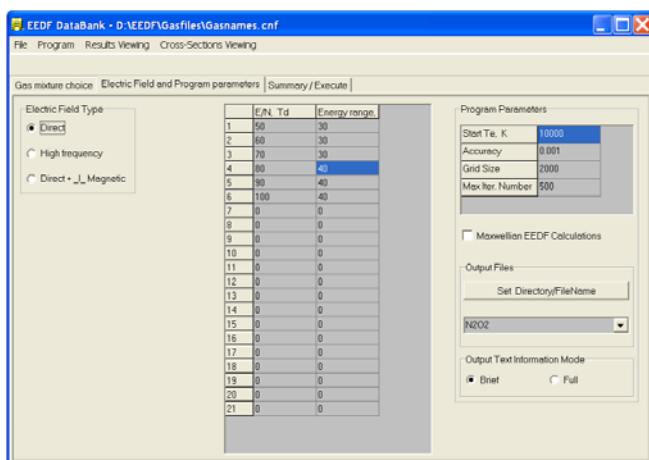
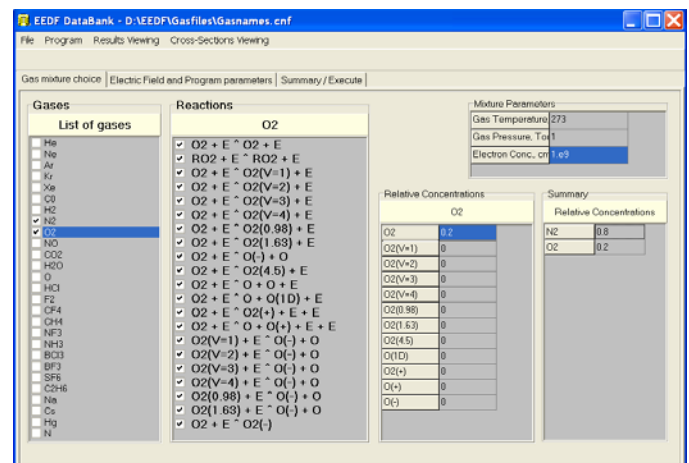
EEDF program includes:

- **Data Bank** of cross sections
- **Boltzmann Equation Solver**
- **Results Viewing** program
- **Cross-Section Viewing** program

Data Bank consists of a number of files containing data on cross-sections for the electron scattering from atoms and molecules.

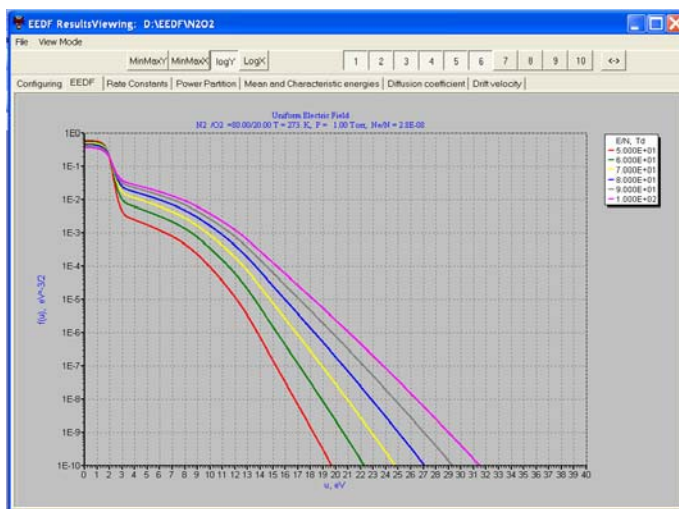
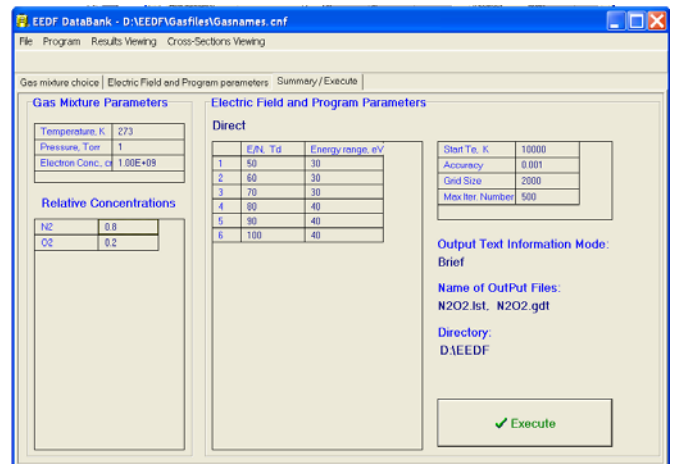
The **EEDF Access System** provides an easy, **MENU-driven** way to access the **Data Bank** and programs. Using the **MENU-system** one can do the following operations:

- ✚ Look through the list of species included in Data bank
- ✚ Choose the components of gas mixture.
- ✚ Set up the concentrations of components and the populations of excited states
- ✚ Look through the list of processes for chosen species
- ✚ Set up the parameters of gas mixture: temperature, pressure, electron concentration



- ✚ Choose the electric field type
 - Steady state
 - RF ($\omega \gg \nu_u$)
 - Crossed electric and magnetic fields
- ✚ Set up the values of field parameters
- ✚ Set up some mathematical parameters of program
- ✚ Set up the names and location of output files
- ✚ Choose the format of output text file

- Look through the summary of chosen parameters and
- Start **Boltzmann Equation Solver**



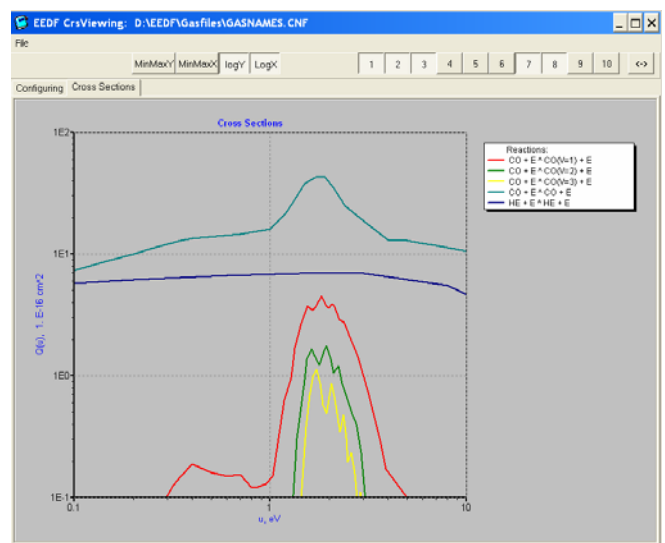
file

Start **Results Viewing** program

- Look through the results of calculation in text and graph modes
 - Electron energy distribution function
 - Mean and characteristic electron energy
 - Drift velocity
 - Diffusion coefficient
 - Rate constants
 - Power Partition
- Save images in bmp format
- Export of plotted data to text format

Start **Cross-Section Viewing** program

- Look through the list of species in Data Bank
- Choose desired species
- Choose necessary processes for each species
- Plot cross sections for all chosen processes
- Save images in bmp format
- Export of plotted data to text format file



2. EEDF package content

The EEDF package includes

- READ ME - directory, information resources
- GASFILES - directory, Data Bank of cross sections.
- EEDF.exe - executable file
- EEdfCh1.dll - dynamic library, used subprogrammes
- CrsCh1.dll - dynamic library, used subprogrammes
- Bolzproc.prg - Boltzmann equation solver

3. Data Bank structure

A Data Bank is a set of files, which are arranged in the **GASFILES** directory (the directory name can be arbitrary, a few directories with different sets can be arranged). For each species two text files are provided with the same name and different extensions. The file with **.CRS** extension contains information about electron-molecule (atom) scattering cross sections. The file with **.RC** extension contains reactions, which are written in symbolic form and some additional information used by Boltzmann equation solver. Also, Data Bank includes file **GASNAMES.CNF**, in which the correspondence between the filenames and the species names is indicated.

The structure of ***.CRS**, ***.RC** and **GASNAMES.CNF** files is illustrated by an example of **Xe1.CRS**, **Xe1.RC** and **GASNAMES.CNF** files.

The structure of **XE1.CRS** file

```
XE + E ^ XE + E 1.0 00726/07/82 1 (1)
PREPRINT IAE-3080, Moscow,1979 Momentum transfer XE +1 (2)
0.000E+00 1.000E-02 2.000E-02 4.000E-02 5.000E-02 7.000E-02 9.000E-02 1 (3)u
1.780E+02 1.160E+02 8.000E+01 4.800E+01 3.950E+01 2.900E+01 2.290E+01 1 (4)Q(u)
1.500E-01 2.000E-01 2.500E-01 3.000E-01 3.500E-01 4.000E-01 5.000E-01 1 u
1.300E+01 8.400E+00 5.350E+00 3.150E+00 2.100E+00 1.750E+00 1.380E+00 1 Q(u)
6.000E-01 7.000E-01 8.200E-01 1.000E+00 1.300E+00 2.000E+00 3.000E+00 1 u
1.280E+00 1.350E+00 1.670E+00 2.480E+00 3.900E+00 8.250E+00 1.700E+01 1 Q(u)
4.000E+00 5.000E+00 6.500E+00 8.000E+00 1.000E+01 1.600E+01 2.000E+01 1 u
2.480E+01 3.080E+01 3.200E+01 3.370E+01 3.200E+01 2.520E+01 2.050E+01 1 Q(u)
5.000E+01 1 u
1.000E+01 1 Q(u)
1 (*)

XE + E ^ XE* + E 1.0 00726/07/82 1
PREPRINT IAE-3080, Moscow, 1979 TOTAL ELECTRONIC 8.3 eV 1
8.300E+00 1.000E+01 1.250E+01 1.500E+01 2.000E+01 2.500E+01 3.000E+01 1
0.000E+00 6.000E-02 4.000E-01 4.600E-01 4.200E-01 3.300E-01 2.800E-01 1
4.000E+01 1.000E+02 1
2.100E-01 1.000E-01 1
1

XE + E ^ XE(+) + E + E 1.0 00726/07/82 1
PREPRINT IAE-3080, Moscow, 1979 IONIZATION 12.1 eV 1
1.210E+01 1.250E+01 1.500E+01 2.000E+01 3.000E+01 4.000E+01 1.000E+02 1
0.000E+00 1.100E-01 9.060E-01 2.280E+00 3.850E+00 4.480E+00 5.380E+00 1
2.000E+02 1
4.580E+00 1
1

XE2(+) + E ^ XE* + XE 1.0 00701/02/83 1
ALFA RECOMBINATION ~ (Te)**(-0.5) Q(u) ~ 1/U 1
1.000E-04 1.000E-03 2.000E-03 5.000E-03 1.000E-02 2.000E-02 5.000E-02 1
3.070E+05 3.070E+04 1.535E+04 6.140E+03 3.070E+03 1.535E+03 6.140E+02 1
1.000E-01 2.000E-01 5.000E-01 1.000E+00 2.000E+00 5.000E+00 1.000E+01 1
```

```

3.070E+02 1.535E+02 6.140E+01 3.070E+01 1.535E+01 6.140E-00 3.070E-00 1
2.000E+01 1.000E+02
1.535E-00 3.070E-01
1
1
1
1
XE* + E ^ XE(+) + E + E 1.0 00730/03/83 1
3.8EV THEORY D.TON-THAT...PHYS.REV,v.A15, p.517,1977 1
3.800E+00 5.000E-00 6.000E-00 8.000E-00 1.000E+01 1.500E+01 2.000E+01 1
0.000E+00 6.200E+00 1.000E+01 1.180E+01 1.200E+01 1.050E+01 9.000E+00 1
3.000E+01 6.000E+01 8.000E+01 1.000E+02 3.000E+02 1
7.000E+00 4.000E+00 2.500E+00 2.000E+00 1.000E+00 1
1
-1 (**)

```

The line (1) contains a reaction written in symbolic form; the number “1.0” is a scaling factor which should be put at a definite position (56-58); the data (or any other information), and, finally, " 1" or "+1" at 71 - 72 positions.

Any additional information can be written in the line (2). Usually, it contains the reference to the work where from the cross section was taken.

Line (3) contains "u" value (energy, eV) which is written in a definite format; and the line (4) contains the value of the cross section $Q(u)$ (10^{-16}cm^2) at the energy u . The lines with "u" and $Q(u)$ values are alternating in the same order. The number of specified u and $Q(u)$ pairs can be arbitrary. The values of energy should be in order of growth.

Data for different processes are separated by line (*) which has "+1" (or " 1") at 71 - 72 positions. *.CRS file is ended by the line (**), which has "-1" at 71 - 72 positions.

The structure of XE1.RC file

```

XE + E ^ XE + E -1 (**)
XE + E ^ XE* + E 1
XE + E ^ XE(+) + E + E 1
XE2(+) + E ^ XE* + XE 1
XE* + E ^ XE(+) + E + E 1
-1 (**)
XE 1.000E+00 0.000E+00 1.370E+02 +1
XE* 0.000E-00 8.300E+00 0.000E+00 +1
XE(+) 0.000E-00 1.210E+01 0.000E+00 +1
XE2(+) 0.000E-00 0.000E+00 0.000E+00 +1
-1 (**)

```

The first part of the file (between two upper (**) lines) is the list of reactions corresponding to reactions in XE1.CRS file.

The second part of the file (between two lower (**) lines) is arranged in the form of four columns.

The first column contains the list of the substance names (not longer than 8 symbols), which are figured in the reaction list.

The relative concentrations are specified in the second column.

The third column contains energies of transitions (eV) for excited particles and ionization energies for ions produced by an electron impact. It's necessary to write down 0 for XE2(+) ion.

The atomic weight is specified in the fourth column. This value is defined only for those components for which the momentum transfer cross sections are given. For other components zero should be written.

Let us note that third and fourth columns are also used to define some parameters when one describes the rotational excitation of molecules (see below).

How to handle with rotational excitation processes.

If the process of excitation of the rotational levels is described by the effective cross section and one effective excitation energy, then this process can be specified in the Data Bank like any other excitation process.

To take into account the excitation of rotational levels in the diffusion (Fokker-Plank) approximation (see comments in **Boltzmann equation** chapter) this process should be described in Data Bank in a special manner. For example, the reaction of excitation of the rotational states for nitrogen is written like **RN2 + E \wedge RN2 + E**, i.e. similarly to the reaction of the elastic scattering **N2 + E \wedge N2 + E**. The only difference is **R** letter before the component name.

		B	a	
RN2	1.000E-00	2.480E-04	6.000E+00	+1

At that the excitation energy for **RN2** in the third column (in **N2.RC** file) is defined as equal to **B**, where **B** is the rotational constant. The number **a** defined in the fourth column depends on the sort of molecule and for N2 it is equal to **6**.

Corresponding cross section for the process **RN2 + E \wedge RN2 + E** is actually not a traditional cross section. It was defined as an appropriate term in collision integral in Fokker-Plank approximation and at condition $E(j) \ll k_B T_{\text{gas}}$ ($E(j)$ is the energy of j-th rotational level and $k_B T_{\text{gas}}$ is thermal energy). Then the equilibrium rotational levels populations were approximated by linear functions of $(E(j)/k_B T_{\text{gas}})$, and summation over allowed transitions $j \rightarrow j \pm 2$, $j \rightarrow j \pm 4$ was made analytically using theoretical dependence of cross sections on j. Resulting cross section is equal to

$$Q_{\text{rot}}(u) = 6 Q_{j=0 \rightarrow j=2}(u) + 20 Q_{j=0 \rightarrow j=4}(u) = 6(Q_{j=0 \rightarrow j=2}(u) + 10/3 Q_{j=0 \rightarrow j=4}(u)) = 6Q_{\text{eff}}(u).$$

Exactly $Q_{\text{rot}}(u) = 6Q_{\text{eff}}(u)$ is used in collision integral in Fokker-Plank approximation. $Q_{\text{eff}}(u)$ is ascribed to **RN2 + E \wedge RN2 + E** process in **N2.CRS** file and multiplier **a = 6** is introduced in **N2.RC** file (see above).

Similar approach is also used for the description of the rotational excitation of O₂, H₂ and CO molecules.

Specific feature of EEDF calculations in rare gases

The specific feature of calculations in rare gases is that at low E/N values (when energy interval under consideration $[0, u_{\text{max}}]$ is such that u_{max} is less than the energy of lower electronic state) there are problems with convergence of iteration procedure. The possible way to avoid these problems is to include fictitious inelastic process (with low threshold energy and small cross section value) in set of processes for a given rare gas. In our Data Bank such a process is written as (for Ar, for example) **AR + E \wedge ARv + E**. The threshold energy is 0.1 eV and cross section is 10^{-22} cm^2 . Since the value of cross section is very small, the process has no influence on plasma characteristics, but provide convergence of iteration procedure.

The structure of **GASNAMES.CNF** file.

```
XE1 Xe
N2 N2_test
```

In each line the first term is the name of files (*.CRS and *.RC) in Data Bank. The second term in each line is a description. Exactly this term is figured in list of gases in EEDF program.

4. Modification of Data Bank

The data available in the **Data Bank** can be modified and complemented by novel data.

Modification of available cross section values

The cross section values can be modified either by replacement for a new value at a given energy or by variation of a scaling factor. In the latter case the cross section is multiplied by this factor. The value of scaling factor can be altered from **9.9** to **0.1**.

Adding of new processes to the existing files

To introduce new process into the existing files it's necessary to add this process and the correspondent cross section in ***.CRS** file. The correspondent reaction and new name of the component (if it has appeared) should be added in the reaction and name of component lists of ***.RC** file correspondingly. It's necessary to note that one may use not more than **8** symbols to designate the name of component.

Creation of files for new substances

To introduce the new components in the data bank it's necessary to create two files with the same name and ***.CRS** and ***.RC** extensions. The structure of these files is described above. Plus one should make the correspondent additions in **GASNAMES.CNF** file.

Important:

Designation of species (neutral, excited or ions) should no be longer than 8 symbols.

For the electrons designation “E” should be used.

For the positive ions designation “(+)” should be used, for example, N2(+).

For the negative ions designation “(-)” should be used, for example, O(-).

The symbol “^” should be used as separator in reactions, for example, M + E ^ M* + E

For non-commercial use, it is also possible to download cross section data collection in the native format for EEDF package (code) from open-access website LXCAT, www.lxcat.laplace.univ-tlse.fr; "MULTIPLE TEXT FILES IN ZIP ARCHIVE" option has to be selected on CROSS SECTION - DOWNLOAD page. Note, use of the data retrieved from this site should be accompanied by proper references.

5. Boltzmann equation under consideration

The EEDF code solves steady state Boltzmann equation for the isotropic part of the electron velocity distribution function in homogeneous plasma; the so-called two-term approximation for the distribution function is utilized.

Boltzmann equation under consideration can be written as follows:

$$u^{1/2} f_0(u) (dn_e/dt) = I_E(u) + I_{el}(u) + I_{in}(u) + I_{ee}(u) , \quad (1)$$

where $f_0(u)$ is isotropic part of the distribution function, u is electron energy, term $I_E(u)$ describes heating of electrons in the electric field. Terms $I_{el}(u)$, $I_{in}(u)$ and $I_{ee}(u)$ describe elastic, inelastic and electron-electron collisions.

The normalization condition for $f_0(u)$ taken to be

$$\int_0^{\infty} f_0(u) u^{1/2} du = 1 . \quad (2)$$

The first term in equation (1) takes into account variation of the electron density in the processes of ionization, recombination and attachment. The first integral of equation (1) gives an expression for the conservation of the electron density

$$dn_e/dt = n_e (v_i - v_{at} - v_{rec}) , \quad (3)$$

where v_i , v_{at} , v_{rec} are the frequencies of ionization, attachment and recombination, which can be expressed in terms of appropriate integrals of $f_0(u)$.

So the code EEDF solves the integro-differential equation (1) (with condition (3)). The physically realizable situation corresponds to PT experiment (Pulse Townsend discharge, see Thomas W.R.L., J. Phys. B., 1969, v2, p.551).

Three types of the applied electric field are considered

a) Steady state electric field. In this case

$$I_E(u) = \frac{2}{m} \frac{e^2 E^2}{3} \frac{\partial}{\partial u} \left(\frac{u^{3/2}}{\nu_m(u)} \frac{\partial f_0}{\partial u} \right), \quad \nu_m(u) = \sqrt{\frac{2u}{m}} \sum_i Q_m^i(u) N_i, \quad (4)$$

where e is the electron charge, m is the electron mass, E is the electric field strength, $\nu_m(u)$ is the momentum transfer frequency, Q_m^i is momentum transfer cross section for i -th species, number density of which is N_i .

b) Steady state electric field with crossed magnetic field. In this case

$$I_E(u) = \frac{2}{m} \frac{e^2 E^2}{3} \frac{\partial}{\partial u} \left(u^{3/2} \frac{\nu_m(u)}{\nu_m^2(u) + \omega_L^2} \frac{\partial f_0}{\partial u} \right), \quad (5)$$

where ω_L is the Larmor frequency of electrons.

c) High frequency electric field $E_0 \exp(i\omega t)$. In this case

$$I_E(u) = n_e \frac{2}{m} \frac{e^2 (E_0 / \sqrt{2})^2}{3} \frac{\partial}{\partial u} \left(u^{3/2} \frac{\nu_m(u)}{\nu_m^2(u) + \omega^2} \frac{\partial f_0}{\partial u} \right). \quad (6)$$

In the last case the taken form of Boltzmann equation is true for $\omega \gg \nu_u$, where ν_u is the effective frequency of inelastic collisions.

Collision integral

Elastic collisions

$$I_{el} = n_e \sqrt{\frac{2}{m}} \frac{\partial}{\partial u} \left(u^2 \sum_i \frac{2m}{M_i} Q_m^i(u) N_i \left(f_0(u) + k_B T_g \frac{\partial f_0(u)}{\partial u} \right) \right), \quad (7)$$

Where M_i is the mass of i -th species, T_g is the gas temperature, k_B is the Boltzmann constant.

Inelastic collisions.

Excitation of electronic states from the ground state

$$I_{elec} = -n_e \sqrt{\frac{2}{m}} \sum_i \sum_j \left[u Q_i^j(u) N_i f_0(u) - (u + \Delta_i^j) Q_i^j(u + \Delta_i^j) N_i f_0(u + \Delta_i^j) \right], \quad (8)$$

where $Q_i^j(u)$ is the cross section for the excitation of j -th electronic state of i -th species and Δ_i^j is the corresponding energy threshold. *Similar expressions are used to describe stepwise excitation processes.*

Second kind collisions with electronically excited atoms and molecules (de-excitation to the ground state)

$$I_{elec}^* = -n_e \sqrt{\frac{2}{m}} \sum_i \sum_j \left[u Q_i^{j*}(u) N_i^j f_0(u) - (u - \Delta_i^j) Q_i^{j*}(u - \Delta_i^j) N_i^j f_0(u - \Delta_i^j) \right], \quad (9)$$

where N_i^j is the population of j -th state of i -th species, corresponding cross section $Q_i^{j*}(u)$ is calculated from $Q_i^j(u)$ cross section using detailed balance principle. *Similar expressions are used to describe de-excitation to lower excited states.*

Excitation of vibrational levels

$$I_{vib} = -n_e \sqrt{\frac{2}{m}} \sum_i \sum_v \left[u Q_i^v(u) N_i f_0(u) - (u + \Delta_i^v) Q_i^v(u + \Delta_i^v) N_i f_0(u + \Delta_i^v) \right], \quad (10)$$

where $Q_i^v(u)$ is the cross section for the excitation of v -th vibrational level of i -th species and Δ_i^v is the corresponding energy threshold. *Similar expressions are used to describe stepwise excitation of vibrational levels.*

Second kind collisions with vibrationally excited molecules (de-excitation to $v=0$ vibrational state)

$$I_{vib}^* = -n_e \sqrt{\frac{2}{m}} \sum_i \sum_j \left[u Q_i^{v*}(u) N_i^v f_0(u) - (u - \Delta_i^j) Q_i^{v*}(u - \Delta_i^j) N_i^v f_0(u - \Delta_i^j) \right], \quad (11)$$

where N_i^v is the population of v -th vibrational level of i -th species, corresponding cross section $Q_i^{v*}(u)$ is calculated from $Q_i^v(u)$ cross section using detailed balance principle. *Similar expressions are used to describe de-excitation to lower vibrational levels.*

Ionization by electron impact from the ground state

$$I_{ion} = -n_e \sqrt{\frac{2}{m}} \sum_i \left[u Q_i^{ion}(u) N_i f_0(u) - (u + \Delta_i^{ion}) Q_i^{ion}(u + \Delta_i^{ion}) N_i f_0(u + \Delta_i^{ion}) \right] + n_e \delta(u) \sum_i N_i k_i^{ion}, \quad (12)$$

$$k_i^{ion} = \sqrt{\frac{2}{m}} \int_0^\infty u Q_i^{ion}(u) f_0(u) du,$$

where Δ_i^{ion} is ionization energy, $\delta(u)$ is Dirac delta function and k_i^{ion} is ionization rate constant. It is assumed that the energy of secondary electrons is equal to 0.

Similar expressions are used to describe stepwise ionization processes.

Dissociative recombination of electrons with molecular ions

$$I_{rec} = -n_e \sqrt{\frac{2}{m}} \sum_l u Q_{rec}^l(u) N_l f_0(u), \quad (13)$$

where N_l is number density of molecular ions of l -th sort and $Q_{rec}^l(u)$ is corresponding cross section.

Attachment of electrons to electronegative molecules

$$I_{att} = -n_e \sqrt{\frac{2}{m}} \sum_k u Q_{att}^k(u) N_k f_0(u), \quad (14)$$

where N_k is number density of molecular ions of k -th sort and $Q_{att}^k(u)$ is corresponding cross section.

Excitation of rotational levels

$$I_{rot} = n_e \sqrt{\frac{2}{m}} \frac{\partial}{\partial u} \left[u \sum_i B_i Q_{rot}^i(u) N_i \left(f_0(u) + k_B T_g \frac{\partial f_0(u)}{\partial u} \right) \right], \quad (15)$$

where Q_{rot}^i is effective cross section for the excitation of rotational levels of i -th species, B_i is the rotational constant. Cross section Q_{rot}^i in collision integral in Fokker-Plank approximation (15) is defined (calculated) in a special manner (see comments in subsections “Data Bank Structure”).

In some cases excitation of the rotational levels is described by the effective cross section and one effective excitation energy. In this case collision integral is similar to that for the excitation of electronic state (8).

Electron-electron collisions

$$I_{ee} = n_e \sqrt{\frac{2}{m}} 2v_{ee} u^{3/2} \frac{\partial}{\partial u} \left(P_1 f_0 + P_2 \frac{\partial f_0}{\partial u} \right), \quad P_1(u) = \int_0^u u^{1/2} f_0 du, \quad P_2(u) = \frac{2}{3} \left(\int_0^u u^{3/2} f_0 du + \int_u^\infty f_0 du \right). \quad (16)$$

$$v_{ee} = \frac{4\pi e^4 n_e}{m^2 (2u/m)^{3/2}} \ln(\Lambda), \quad \ln(\Lambda) = \ln\left(\frac{r_d}{r_0}\right), \quad r_d = \sqrt{\frac{2\bar{u}/3}{8\pi e^2 n_e}}, \quad r_0 = \frac{e^2}{\bar{u}}, \quad \bar{u} = \int_0^\infty u^{3/2} f_0 du.$$

6. Method of numerical solution

The integro-differential equation (1) is solved numerically by an iteration method. Energy interval $[0, u_{\max}]$ under consideration is divided into N equal-sized intervals and equation (1) approximated by finite differences with a uniform grid spacing in energy.

The initial approximation for $f_0(u)$ is taken be $\sim \exp(-u/k_B T_{e0})$, where T_{e0} is the parameter. The solution procedure includes two circles of iterations:

1. For a given f_0^n function the term $(dn_e/dt)^n$ is calculated from expression (3), n is the first (external) circle iteration number.

2. Calculated $(dn_e/dt)^n$ value is substituted in the equation (1) and equation is solved by iteration method (internal iteration circle) to obtain f_0^{n+1} function.

The iteration method described in (Dyatko N.A., Kochetov I.V., Napartovich A.P. Sov. J. Plasma Phys., 1992, v. 18, no. 7, pp. 462-468) is utilized for this purpose. The iteration procedure is stopped, when the relative change of f_0 in all grid points is less than given parameter ε :

$$|f_0^{m+1} - f_0^m| / f_0^m < \varepsilon, \quad (17)$$

m is the second (internal) circle iteration number. In the EEDF program the number of iterations is restricted by some value M_{\max} (defined by user). If there is no convergence for $m > M_{\max}$ program is stopped.

3. Using obtained f_0^{n+1} the term $(dn_e/dt)^{n+1}$ is calculated and calculation procedure is repeated.

The iteration process is terminated when criterion

$$((dn_e/dt)^{n+1} - (dn_e/dt)^n) / (dn_e/dt)^n < 0.001 \quad (18)$$

is satisfied and function f_0^{n+1} is considered as a sought solution.

After the distribution function was found various characteristics of plasma are calculated. In particular, the electron power balance is verified. Equation (1) is multiplied by u and integrated numerically (using calculated f_0), so the is the electric field power input (W_E) and contributions to the power balance from the various processes (W_α) are calculated. The power balance is the good criterion for the accuracy of the solution obtained. In the code the value

$$\Delta = \frac{\left| \sum_\alpha W_\alpha \right| - |W_E|}{|W_E|} 100\% \quad (19)$$

is estimated. If this value has is small

$$\Delta < 1\%, \quad (20)$$

the obtained solution may be considered as correct. Otherwise it is necessary either to change the energy interval $[0, u_{\max}]$ over which the equation is solved or to increase the number of nodes in the energy grid.

However, the realization of condition (20) still does not guarantee that the resulting solution is correct. There is one additional condition which must be satisfied. This condition is related to the treatment of electron-electron collisions in the Boltzmann equation. As is well known, electron-electron collisions do not change the total electron energy, so in the power balance equation the corresponding term (W_{ee}) must vanish. Naturally, in a numerical solution W_{ee} is some finite quantity, which differs from zero. In the code the value

$$\Delta_{ee} = \frac{|W_{ee}|}{|W_E|} 100\% \quad (21)$$

is estimated. If this value has is small

$$\Delta_{ee} < 1\%, \quad (22)$$

the obtained solution may be considered as correct.

7. Calculated characteristics

The set of characteristics depends on the type of the electric field under consideration.

Steady state electric field

1. Electron energy distribution function $f_0(u)$

2. Mean electron energy
$$\bar{u} = \int_0^{\infty} u^{3/2} f_0 du$$

3. Mean electron temperature
$$T_e = \frac{1}{k_B} \frac{2}{3} \bar{u}$$

4. Rate constants
$$k = \sqrt{\frac{2}{m}} \int_0^{\infty} u Q(u) f_0(u) du$$

5. Detailed power balance

6. Electron diffusion coefficient
$$D_e = \frac{1}{3} \frac{2}{m} \int_0^{\infty} \frac{u^{3/2}}{v_m(u)} f_0 du$$

7. Electron mobility
$$\mu_e = -\frac{1}{3} \frac{2e}{m} \int_0^{\infty} \frac{u^{3/2}}{v_m(u)} \frac{\partial f_0}{\partial u} du$$

8. Electron drift velocity
$$W_e = E \mu_e$$

8. Characteristics energy
$$u_{ch} = e \frac{D_e}{\mu_e}$$

Steady state electric field with crossed magnetic field ($\mathbf{E} \perp \mathbf{H}$)

1. Electron energy distribution function

2. Mean electron energy

3. Mean electron temperature

4. Rate constants

5. Detailed power balance

6. Diffusion coefficient ($\parallel \mathbf{H}$)
$$D_{\parallel H} = \frac{1}{3} \frac{2}{m} \int_0^{\infty} \frac{u^{3/2}}{v_m(u)} f_0 du$$

7. Diffusion coefficient ($\perp \mathbf{H}$)

$$D_{\perp H} = \frac{1}{3} \frac{2}{m} \int_0^{\infty} u^{3/2} \frac{v_m(u)}{\omega_L^2 + v_m^2(u)} f_0 du$$

8. Electron mobility ($\parallel \mathbf{E}$)

$$\mu_{\parallel E} = -\frac{e}{3} \frac{2}{m} \int_0^{\infty} u^{3/2} \frac{v_m(u)}{\omega_L^2 + v_m^2(u)} \frac{\partial f_0}{\partial u} du$$

9. Electron mobility ($\perp \mathbf{H} \perp \mathbf{E}$)

$$\mu_{\perp E \perp H} = -\frac{e}{3} \frac{2}{m} \int_0^{\infty} u^{3/2} \frac{\omega_L}{\omega_L^2 + v_m^2(u)} \frac{\partial f_0}{\partial u} du$$

High frequency electric field

1. Electron energy distribution function

2. Mean electron energy

3. Mean electron temperature

4. Rate constants

5. Detailed power balance

6. Diffusion coefficient

$$D_e = \frac{1}{3} \frac{2}{m} \int_0^{\infty} \frac{u^{3/2}}{v_m(u)} f_0 du$$

8. Complex electron mobility

$$\mu_e = \mu_{cond} + i\mu_{pol}$$

$$\mu_{cond} = -\frac{e}{3} \frac{2}{m} \int_0^{\infty} u^{3/2} \frac{v_m(u)}{\omega^2 + v_m^2(u)} \frac{\partial f_0}{\partial u} du$$

$$\mu_{pol} = -\frac{e}{3} \frac{2}{m} \int_0^{\infty} u^{3/2} \frac{\omega}{\omega^2 + v_m^2(u)} \frac{\partial f_0}{\partial u} du$$

8. Typical output listing (for the case of steady state electric field)

EEDF program permits one to look through the results of calculations in text and graph modes. Text information is stored in *.**lst** file and information needed for graph plotting is stored in *.**gdt** file. Below the typical output listing with some comments are present.

Comments to "Full" output listing

Listing consists of three parts. The parameters of the plasma are represented in the first part. The designation of parameters is close to the commonly used.

E - electric field strength
TMOL- temperature of gas
NMOL - atom and molecule number density
PTOT - pressure
E/N = E/NMOL
E/P = E/PTOT
<U> - average electron energy, eV
TE - effective electron temperature, $2/3\langle U \rangle$, K
D - diffusion coefficient
MU - electron mobility
EK - characteristic energy
VDRIFT, - drift velocity
CONDUCT/NE - conductivity per one electron
CONDUCT - fun conductivity
RHO*U - inverse value to CONDUCT/NE
J/NE - density of current per one electron

DISCHARGE - discharge power
 TOTAL POWER – total power
 INELASTIC- power dissipated into inelastic collisions
 ELASTIC HEAT- power dissipated into elastic collisions
 $E\langle U \rangle DNE/DT$ - power related to term dn_e/dt
 POWER DISS - total power ($\sum W_\alpha$)
 NU(MOM) momentum transfer collision frequency
 NE - electron number density
 NE/NMOL - degree of ionization
 $S(U = 0)/NE$ - is not considered in this version of the code
 NU(IONIZE) total frequency of the ionization
 NU(ATT,REC) -total frequency of the attachment and recombination
 $DNE/DT/NE$ - total frequency of the variation of the electron number density
 DNE/DT - $(DNE/DT/NE)*NE$

In the second part of output listing there is the table for the electron energy distribution function $f(u)$.

MESH - number of energy intervals.
 EMAX - electron energy range of integration
 $DE = EMAX/MESH$

In the third part of the output listing the data for each process are listed.

N(A) - number density of the particle A
 N(B) number density of the particle B
 U(J) inelastic energy threshold
 $DNE/DT/NE$ - frequency gain (loss) of the electrons in the process considered
 $VSIG(A \wedge B)$ forward process electron excitation rate coefficient
 $VSIG(B \wedge A)$ - reverse process electron excitation rate coefficient
 (NET)POWER - power dissipated in given process
 PERCENT POWER - fraction of this power from the total one.

The total energy balance of the electrons is given below.

DISCHARGE POWER - discharge power (W_E)
 POWER INTO INELASTIC E-MOLECULE COLLISIONS power dissipated in the inelastic collisions
 ELASTIC E- MOLECULE HEATING - power dissipated in elastic collisions
 $D/DT(STORED \text{ KINETIC ENERGY}) = E\langle U \rangle DNE/DT$ power related to the term dn_e/dt in the equation (1)
 TOTAL POWER - total dissipated power ($\sum W_\alpha$)
 E-E POWER TRANSFER DISCREPANCY - power discrepancy related to term $I_{ee}(u)$ in the equation (1).

Typical listing for the case "Full" (that is the content of the file TEST.LST)

The computation was done for pure Xe, the set of input physical parameters was the following:

Relative concentration	$XE^* 10^{-6}$
Relative concentration	$XE_2(+) 10^{-8}$
Pressure	1 Torr
Temperature	300 K
Electron density	$3.21 10^8 \text{ cm}^{-3}$
E/N	$10 \text{ Td} = 1 \cdot 10^{-16} \text{ Vcm}^2$
Energy range for integration	20 eV

-- GAS MIXTURE --

PURE XE

PLASMA PARAMETERS

UNIFORM ELECTRIC FIELD

```
-----  
E (FIELD)      =  3.2167E+00    VOLT/CM  
  
TMOL           =      300.      DEG K  
NMOL           =  3.2167E+16    CM-3  
PTOT           =      1.0      TORR  
  
E/N            =  1.0000E-16    VOLT CM2  
E/P            =      3.22      V/CM/TORR  
               =      2.44      KV/CM/ATM  
  
<U>            =      3.787      EV  
TE = 2<U>/3K   =    29306.      DEG K  
  
DIFFUSION D    =  8.5530E+05    CM2/SEC  
MOBILITY MU    =  1.4943E+05    CM2/VOLT/S  
EK = D/MU      =      5.724      EV  
VDRIIFT =MU*E  =  4.8068E+05    CM/SEC  
  
CONDUCT/NE     =  2.3939E-14    CM2/OHM  
CONDUCT        =  7.6846E-06    /OHM-CM  
RHO*NE         =  4.1772E+13    OHM/CM2  
J/NE = E*VD    =  7.7005E-14    AMP CM/EL  
  
DISCHARGE      =  7.9512E-05    W/CM3  
TOTAL POWER    =  7.9512E-05    W/CM3  
  
INELASTIC      =  6.2201E-05    W/CM3  
ELASTIC HEAT   =  1.7000E-05    W/CM3  
E<U>DNE/DT     =  3.1437E-07    W/CM3  
POWER DISS     =  7.9515E-05    W/CM3  
  
NU(MOM)        =  8.1423E+09    SEC-1  
  
NE             =  3.2100E+08    CM-3  
NE/NMOL        =  9.9793E-09  
S(U = 0)/NE    =  0.0000E+00    SEC-1  
S(U > 0)/NE   =  0.0000E+00    SEC-1  
NU(IONIZE)     =  1.6546E+03    SEC-1  
NU(ATT,REC)    =  4.0234E+01    SEC-1  
DNE/DT/NE      =  1.6144E+03    SEC-1  
DNE/DT         =  5.1822E+11    CM-3/SEC  
-----
```

CALCULATION PARAMETERS USED:

MESH =2000, EMAX = 20.00EV, DE =0.010 EV.

NORMALIZED ELECTRON DISTRIBUTION FUNCTION F(U), IN UNITS OF $EV^{**(-3/2)}$,
WITH OUTPUT AT 0.200EV INTERVALS. THE ELECTRON ENERGY RANGE(0, 20.00)EV
WAS SUBDIVIDED INTO 2000INTERVALS,GIVING A RESOLUTION=0.010EV.

UNIFORM ELECTRIC FIELD

E/NTOT = 1.000E-16VOLT CM2= 3.217 VOLT/CM/TORR = 2.445 KVOLT/CM/ATM
 FRACTIONAL IONIZATION = NE/NTOT = 9.979E-09, NE = 3.210E+08 CM-3
 PURE XE TMOL = 300. DEG K

U(EV)	F(U)	U(EV)	F(U)	U(EV)	F(U)	U(EV)	F(U)	U(EV)	F(U)
0.00	1.27E-01	0.20	1.22E-01	0.40	1.21E-01	0.60	1.21E-01	0.80	1.20E-01
1.00	1.20E-01	1.20	1.19E-01	1.40	1.18E-01	1.60	1.16E-01	1.80	1.15E-01
2.00	1.13E-01	2.20	1.11E-01	2.40	1.09E-01	2.60	1.06E-01	2.80	1.03E-01
3.00	1.00E-01	3.20	9.71E-02	3.40	9.38E-02	3.60	9.03E-02	3.80	8.67E-02
4.00	8.29E-02	4.20	7.89E-02	4.40	7.49E-02	4.60	7.08E-02	4.80	6.67E-02
5.00	6.24E-02	5.20	5.82E-02	5.40	5.41E-02	5.60	5.02E-02	5.80	4.63E-02
6.00	4.26E-02	6.20	3.91E-02	6.40	3.56E-02	6.60	3.22E-02	6.80	2.90E-02
7.00	2.59E-02	7.20	2.29E-02	7.40	2.01E-02	7.60	1.73E-02	7.80	1.47E-02
8.00	1.22E-02	8.20	9.79E-03	8.40	7.57E-03	8.60	5.60E-03	8.80	3.97E-03
9.00	2.72E-03	9.20	1.80E-03	9.40	1.15E-03	9.60	7.12E-04	9.80	4.26E-04
10.00	2.43E-04	10.20	1.29E-04	10.40	6.37E-05	10.60	2.95E-05	10.80	1.29E-05
11.00	5.35E-06	11.20	2.15E-06	11.40	8.60E-07	11.60	3.66E-07	11.80	1.83E-07
12.00	1.15E-07	12.20	8.62E-08	12.40	6.93E-08	12.60	5.79E-08	12.80	4.90E-08
13.00	4.19E-08	13.20	3.61E-08	13.40	3.12E-08	13.60	2.71E-08	13.80	2.36E-08
14.00	2.06E-08	14.20	1.80E-08	14.40	1.57E-08	14.60	1.37E-08	14.80	1.19E-08
15.00	1.03E-08	15.20	8.88E-09	15.40	7.58E-09	15.60	6.42E-09	15.80	5.37E-09
16.00	4.43E-09	16.20	3.59E-09	16.40	2.83E-09	16.60	2.17E-09	16.80	1.59E-09
17.00	1.12E-09	17.20	7.62E-10	17.40	4.99E-10	17.60	3.16E-10	17.80	1.94E-10
18.00	1.16E-10	18.20	6.62E-11	18.40	3.59E-11	18.60	1.81E-11	18.80	8.57E-12
19.00	3.81E-12	19.20	1.61E-12	19.40	6.47E-13	19.60	2.54E-13	19.80	9.80E-14
20.00	6.65E-15								

1

PLASMA KINETICS ANALYSIS WITH SUMMARY OF ELECTRON PARAMETERS, COLLISION RATES,
 AND POWER BALANCE FOR ALL ELASTIC AND INELASTIC COLLISION PROCESSES INCLUDED

UNIFORM ELECTRIC FIELD

E/NTOT = 1.000E-16VOLT CM2= 3.217 VOLT/CM/TORR = 2.445 KVOLT/CM/ATM
 FRACTIONAL IONIZATION = NE/NTOT = 9.979E-09, NE = 3.210E+08 CM-3
 PURE XE TMOL = 300. DEG K

J	REACTION(J)	N(A)	N(B)	U(J)	DNE/DT/NE
	A + E(-) ^ B + E(-)	(CM-3)	(CM-3)	(EV)	(SEC-1)

1	XE + E ^ XE* + E	3.217E+16	3.217E+10	8.30	
2	XE + E ^ XE(+) + E + E	3.217E+16		12.10	1.102E+02
3	XE2(+) + E ^ XE* + XE	3.217E+08			-4.023E+01
4	XE* + E ^ XE(+) + E + E	3.217E+10		3.80	1.544E+03

J	REACTION(J)	<VSIG(A^B)>	<VSIG(B^A)>	(NET)POWER	PERCENT
	A + E(-) ^ B + E(-)	(CM3/SEC)	(CM3/SEC)	(W/CM3)	POWER

MOMENTUM TRANSFER + ROTATION(FOR MOLECULES) =				1.700E-05	21.38
1	XE + E ^ XE* + E	4.513E-12	1.007E-08	6.182E-05	77.75
2	XE + E ^ XE(+) + E + E	3.426E-15		6.858E-08	0.09
3	XE2(+) + E ^ XE* + XE	1.251E-07		6.198E-09	0.01
4	XE* + E ^ XE(+) + E + E	4.801E-08		3.018E-07	0.38

DISCHARGE POWER =				7.951E-05 W/CM3	100.00 %

POWER INTO INELASTIC E-MOLECULE COLLISIONS =				6.220E-05 W/CM3	78.23 %
ELASTIC E-MOLECULE HEATING =				1.700E-05 W/CM3	21.38 %
D/DT(STORED KINETIC ENERGY) = E<U>DNE/DT =				3.144E-07 W/CM3	0.40 %

TOTAL POWER (COLLISIONS+ HEATING + STORAGE) =				7.952E-05 W/CM3	100.00 %
E-E POWER TRANSFER DISCREPANCY =				-3.301E-11 W/CM3	0.00 %

Comments to "Brief" output listing

Listing consists of three parts. The first part is the table of plasma parameters calculated for given E/N values. The notations, as a rule, are the same as in previous case. Note please, that $UBAR$ is the average energy and J/NE is the density of the current per one electron.

In the second part the detailed power balance (in %) is presented (the fractions, related to dn_e/dt and e-e collisions terms in Boltzmann equation are absent in this table).

The third part is the table of rate constants for all inelastic collision processes depending on E/N value.

Typical listing for the case "Brief" (that is the content of the file TEST1.LST)

The computation was done for the same conditions as in the previous example and three values for the E/N parameter (and three values for the $EMAX$) were taken.

UNIFORM ELECTRIC FIELD

SUMMARY OF PLASMA PARAMETERS AS A FUNCTION OF E/NTOT

PURE XE TMOL= 300.DEG K PTOT= 1.00 TORR

E/NTOT (E-16 V CM2)	UBAR (EV)	EK=D/MU (EV)	VD (CM/S)	MU (CM2/V/S)	D (CM2/S)	J/NE = E*VD (AMP CM/ELECT)
0.500	3.42	5.91	2.42E+05	1.51E+05	8.90E+05	3.88E-14
1.000	3.79	5.72	4.81E+05	1.49E+05	8.55E+05	7.70E-14
1.500	3.93	5.82	6.98E+05	1.45E+05	8.42E+05	1.12E-13

UNIFORM ELECTRIC FIELD

SUMMARY OF FRACTIONAL POWERPARTITION "%"

FOR ALL ELECTRON COLLISION PROCESSES AS A FUNCTION OF E/NTOT

PURE XE TMOL= 300.DEG K PTOT= 1.00 TORR

REACTION	E/NTOT --> (1.0E-16) V CM2)	0.50	1.00	1.50
XE + E ^ XE* + E		29.690	77.755	88.911
XE + E ^ XE(+) + E + E		0.259	0.086	0.060
XE2(+) + E ^ XE* + XE		0.030	0.008	0.004
XE* + E ^ XE(+) + E + E		1.079	0.380	0.193
MOMENTUM TRANSFER COLLISIONS		67.942	21.381	10.622
BALANCE ACCURACY		100.008	100.004	100.003
EMAX, EV		20.000	20.000	20.000

UNIFORM ELECTRIC FIELD

SUMMARY OF RATE CONSTANTS "cm3/s"

FOR ALL INELASTIC COLLISION PROCESSES AS A FUNCTION OF E/NTOT

PURE XE TMOL= 300.DEG K PTOT= 1.00 TORR

REACTION	E/NTOT --> (1.0E-16) V CM2)	0.50	1.00	1.50
XE + E ^ XE* + E		0.443E-12	0.451E-11	0.112E-10
XE + E ^ XE(+) + E + E		0.259E-14	0.343E-14	0.515E-14
XE2(+) + E ^ XE* + XE		0.130E-06	0.125E-06	0.123E-06
XE* + E ^ XE(+) + E + E		0.344E-07	0.480E-07	0.531E-07

9. Handling of EEDF program

I. To start

Execute **EEDF.exe** file

II. To do calculations

- 1) Use **File** menu item to change Data Bank directory (if necessary). To do it one should “**Open**” **Gasnames.cnf** file in chosen directory.

By default, Data Bank placed in Gasfiles directory is used.

- 2) Click on **Program** menu item

- Use **Gas mixture choice** sheet to assign gas mixture and gas mixture parameters.
 - Choose mixture component in **Gases** box by marked corresponding rectangle.
 - Look through the list of processes in **Reactions** box and delete some processes (if it is needed) by unmarking corresponding rectangle.
 - Assign relative concentration of chosen mixture component and relative populations of excited states in **Relative Concentrations** box.
To obtain in calculations rate constants for the processes with participation of excited particles (or ions) nonzero concentrations of corresponding states (or ions) should be assigned.
 - Repeat procedure to add one more gas mixture component.
 - Assign gas mixture parameters (pressure, temperature, electron concentration) in **Mixture parameters** box.

To assign some parameter type a number and press ENTER

If electron concentration $n_e = 0$, then electron-electron collisions are not taken into account and power balance characteristics are calculated per one electron. By default, $n_e = 0$.

- The box **Summary** is used only for the information about chosen gas mixture.
- Use **Electric field and program parameters** sheet to assign electric field type and parameters of calculations.
 - Choose electric field type in **Electric Field Type** box, and assign electric field frequency (in the case of **High Frequency** field) and magnetic field strength (in the case of **Direct + \perp Magnetic**).
 - Assign a set of E/N (or E_0 values in the case of high frequency field). For each E/N (or E_0) value **Energy rage** value should be assign (energy interval u_{max} , which will be used in calculations).
 - Assign some program parameters in **Program Parameters** box. **Start T_e** is T_{e0} , **Accurasy** is ε , is N , **Max. Iter. Number** is M_{max} (see chapter **Method of numerical solution** for details). **By default, $\varepsilon=0.001$, $M_{max}=500$, $N=2000$. Maximum possible Grid Size value is $N=20000$.**
 - Mark **Maxwellian EEDF Calculations** box to calculate plasma parameters using Maxwellian EEDF with T_{e0} temperature.
 - Press **Set Directory/FileName** button to specify directory, in which two files (with **.lst** and **.gdt** extensions) with results of calculations will be placed.

- Specify format of data in output .txt file by marking of corresponding circle in **Output Text Information Mode** box.
- Use **Summary/Execute** sheet to see the summary of chosen parameters and start Boltzmann equation solver.
 - Press **Execute** button to start Boltzmann equation solver.

III. To look through the results of calculations (current or previous)

- Click on **Results Viewing** menu item to start the results viewing program. Using **File/Open** menu item specify output file (with **.gdt** or **.lst** extension).
- If file with **.lst** extension is chosen then results of calculations in text form is presented. To switch from text to graphic presentation mode choose **View Mode/Graphics** menu item.
- If file with **.gdt** extension is chosen then graphics presentation mode is opened. To switch from graphics to text presentation choose **View Mode/Listing** menu item.
- We believe that user interface in graphic presentation mode is rather understandable, so we do not describe it in detail.
- Use **File/Save** menu item to save plotted graph in bmp or jpg format, **File/Print** menu item to print graph and **File/Export** menu item to save plotted data in text format (in the form of (x,y) columns).

IV. To examine cross sections collected in Data Bank

- Click on **Cross-Sections Viewing** menu item to start cross sections viewing program. Using **File/Open** menu item open file with **cnf** extension in chosen Data Bank directory (in presented EEDF package, **gasnames.cnf** file in **Gasfiles** directory).
- Use **Configuring** sheet to specify processes, cross sections of which will be plotted.
 - By mouse clicking select the species in **Gases** box.
 - For chosen species specify required processes by marking rectangular in **Reactions** box
- Use **Cross Sections** sheet to examine graphs of chosen processes. We believe that user interface is rather understandable, so we do not describe it in detail.
- Use **File/Save** menu item to save plotted graph in bmp or jpg format, **File/Print** menu item to print graph and **File/Export** menu item to save plotted data in text format (in the form of (x,y) columns).

10. Reference to EEDF program

The reference to EEDF program should be given as follows:

Dyatko N.A., Kochetov I.V., Napartovich A.P. Sukharev A.G.

EEDF: the software package for calculations of the electron energy distribution function in gas mixtures. <http://www.lxcat.laplace.univ-tlse.fr/software/EEDF/>