acta physica slovaca vol. 55 No. 6, 507 – 514 **December 2005**

WEB-EEDF: OPEN SOURCE SOFTWARE FOR MODELING THE ELECTRON DYNAMICS[1]

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Received 18 April 2005, in final form 13 July 2005, accepted 13 July 2005

We present a free software for modeling the electron dynamics in the uniform electric field named Web-EEDF. It uses a Monte Carlo algorithm to calculate electron energy distribution functions (EEDFs) and other plasma parameters in various gas mixtures. Obtained results are in good agreement with literature. This software represents the first stage in a more complex modeling of plasma chemical processes leading to the decomposition of various air pollutants in electrical discharges at atmospheric pressure.

PACS: 52.65.Pp, 02.50.Ng, 51.50.+v

1 Introduction

It is well known that gas discharge plasmas are able to initiate chemical reactions in normally inert gas mixtures. Since the initiation factor are electrons, it is inevitable to know the electron energy distribution functions (EEDFs) to calculate the rate coefficients of elementary electron processes.

In this paper we present the software for modeling the electron dynamics in gas mixtures in weakly ionized plasmas in the uniform electric field named 'Web-EEDF'. The electron modeling code we use is not discharge and conditions-specific, and therefore is generally applicable for a large variety of discharges and gas mixtures.

The algorithm used in Web-EEDF is based on the algorithm developed by Tas et al. [1], with several modifications. The current version includes cross-sections for CO_2, H_2O, O_2, and N_2. We use compilation of cross sections obtained from Joint Institute for Laboratory Astrophysics, available at *'ftp://jila.colorado.edu/collision_data/'* [2]. The set of cross-sections for CO_2 was updated according to Itikawa [3].

[1] Presented at Joint 15th Symposium on Applications of Plasma Processes (SAPP) and 3rd EU-Japan Symposium on Plasma Processing, Podbanské (Slovakia), 15 – 20 January 2005.

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Direct results from the simulation are EEDF, electron drift velocity (v_d), electron mobility and collisional frequency of electrons with neutrals. From EEDF, we derive electron mean energy, electron mean free path, rate coefficients of elementary electron processes (e.g. excitations to various levels, ionization, electron attachment...), and the branching of the electron energy towards different processes.

The model presented here represents the first stage in a more complex modeling of plasma chemistry initiated by non-equilibrium atmospheric plasmas used for air pollution control. In further stages, we will adapt the model to the specific conditions of our investigated discharges, calculate the net production of reactive species, assess their steady-state concentrations, and finally evaluate the importance of different pathways of the destruction of the studied pollutants.

2 Algorithm

Initial parameters are the gas composition, pressure and temperature, the strength of reduced electric field (E/N) in $[\mathrm{Td}]$, the number of calculation cycles and the degree of ionization.

Pressure and temperature do not influence the EEDF directly. If the electric field is given in $[\mathrm{kV/cm}]$, then the value of the reduced electric field strength is calculated according to the given pressure and temperature. They are also used to calculate the average distance between gas molecules (Δs).

The degree of ionization in weakly ionized plasmas can be defined as a ratio of concentrations of electrons and neutral particles. The maximum value allowed in Web-EEDF is 10^{-3}. The E/N can be in the range from 20 to 600 Td.

At the beginning of the simulation, Web-EEDF randomly chooses the energy, and a direction of the motion of a thermalized test electron relative to the electric field. Then it follows its motion in a required number of calculation cycles.

One calculation cycle means that the electron changes its position by the distance Δs, and new values of its energy and direction of its motion are calculated. Then, the type of molecule is randomly decided (in case of the a calculation in gas mixtures). Another random number decides whether the electron during this cycle will collide with this molecule or not, and the type of the eventual collision. The probability of each type of collision at a given electron energy depends on the values of cross-sections of all included processes for a given molecule.

For non-zero degree of ionization, the electron-electron interactions are also included in the simulation, and therefore it is necessary to choose the EEDF of background electrons from previous calculations. These background electron are treated as if a new type of molecules was added to the mixture, with just one type of interactions described by so called Coulomb cross-section taken from Mitchner and Kruger [4].

The values of electron energy, the time from the last collision, and the component of the velocity vector parallel to the vector of electric field are stored after each calculation cycle. From these data we get EEDFs, electron drift velocity (v_d), electron mobility and collisional frequency of electrons with neutrals. After the last calculation cycle, obtained EEDFs are normalized so that

$$\int_0^\infty f(\varepsilon) \cdot \sqrt{\varepsilon}\, \mathrm{d}\varepsilon = 1 \tag{1}$$

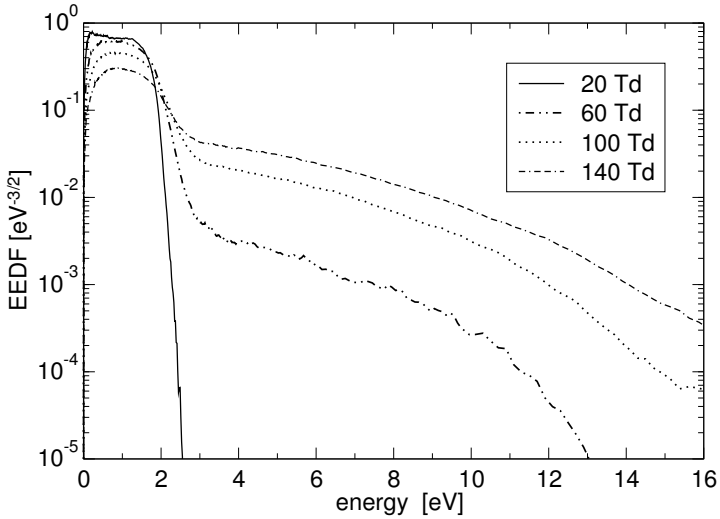

Fig. 1. EEDF in pure nitrogen for different E/N.

and used for the calculation of further parameters: electron mean energy, electron mean free path, rate coefficients of elementary electron processes (e.g. excitations to various levels, ionization, electron attachment...), and the branching of the electron energy towards different processes.

3 Results and Discussion

The direct results from our simulations are EEDFs. Fig. 1 shows the example of the calculated EEDFs for various E/N in pure N_2. They were calculated for the pressure 1 atm, the temperature 293 K, and with 20 million calculation cycles, as well as all other data presented here.

One can see that at 60 Td, the EEDF is not very smooth for electron energies over 6 eV. The reason is in the statistics, because in such a weak electric field the electron reaches energy higher than 6 eV only about 600000 times during these 20 million cycles. So, the improvement of the quality of the high energy 'tail' of obtained EEDFs in weak fields would require more calculation cycles, which might be time consuming. For illustration, one million steps take approximately 1 minute and 15 s on a computer with processor AthlonXP$^{\mathrm{TM}}$ 2000+ with frequency 1667 MHz (OS Linux SuSE 9.2).

This high energy 'tail' does not influence significantly parameters such as electron mean energy, drift velocity of electrons, or their collisional frequency with neutrals. So, it is sufficient to perform the simulation with 2 – 3 million cycles to get reasonable values of these parameters. On the contrary, this high energy 'tail' of the EEDF is crucial for the calculation of rate coefficients of various electron-impact processes, such as ionization or dissociation, because their energy threshold is usually over 10 eV.

Our calculations also show that the degree of ionization only starts to play a significant role, i. e. it changes the shape of the EEDF and values of the derived parameters, if it is higher than

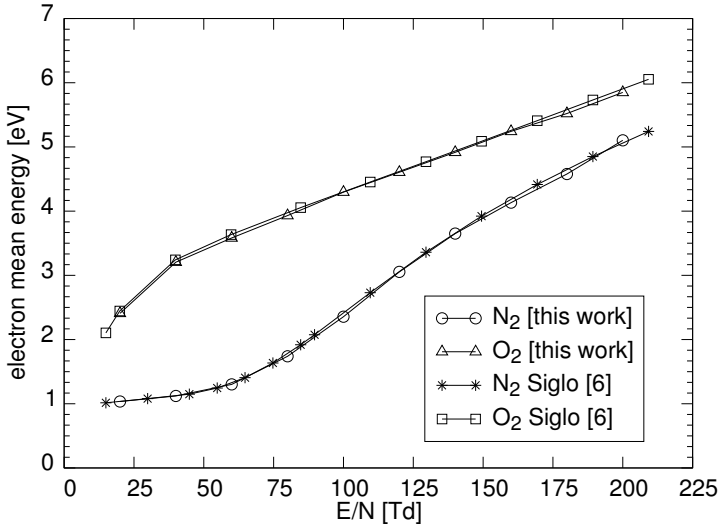

Fig. 2. Electron mean energies in nitrogen and oxygen.

10^{-5}. The concentration of electrons in atmospheric pressure glow discharges studied in our work group are in the range 10^{12} – 10^{13} cm^{-3}, with gas temperature in the discharge channel around 2000 K [5]. So, the corresponding degree of ionization is in the order of 10^{-6}. The situation is similar in case of other atmospheric pressure discharges (e. g. corona).

Besides, the inclusion of electron-electron interactions slows down the calculation by about 30 %. Therefore, all data presented here were obtained from simulations neglecting electron-electron interactions (zero degree of ionization).

To ensure the reliability of our data, we compare them with literature. We find out that electron mean energies (ε_{mean}) in pure N_2 and O_2 in the range of E/N from 20 to 200 Td are almost identical with the values found at SIGLO Series Software homepage [6] (see Fig. 2). We also find very good agreement of electron drift velocities in dry air with values measured by Verhaart et al. [7] and values calculated by program IVTAN [8] (Fig. 3). Our values of ε_{mean} and v_d in N_2, O_2, CO_2 and dry air (80% N_2, 20% O_2) can be in the range from 20 to 200 Td fitted by the polynomial functions of up to 4^{th} order

$$\varepsilon_{mean} = a_0 + a_1 \cdot E/N + a_2 \cdot (E/N)^2 + \ldots \tag{2}$$

$$v_d = b_0 + b_1 \cdot E/N + b_2 \cdot (E/N)^2 + \ldots \tag{3}$$

where the reduced electric field strength (E/N), the electron mean energy (ε_{mean}) and the drift velocity (v_d) are expressed in $[\mathrm{Td}]$, $[eV]$ and $[\mathrm{m} \cdot \mathrm{s}^{-1}]$, respectively. The regression coefficients a_i and b_i can be found in Tab. 1 and in Tab. 2, respectively.

We find a good agreement with literature also for the rate coefficients of various elementary electron processes. For illustration, we show here the rate coefficient of the ionization and dis-

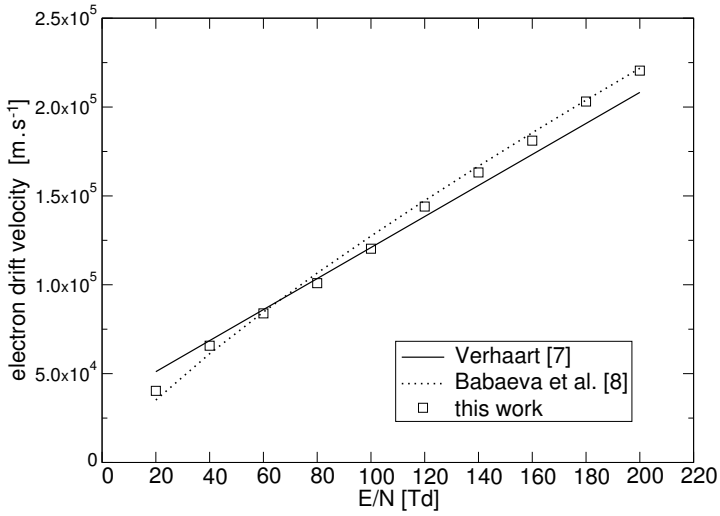

Fig. 3. Electron drift velocity in dry air.

sociation of N_2 in pure nitrogen (Fig. 4). Our results are compared with the data presented by Guerra et al. [9], their rate coefficients were calculated for N_2 vibrational temperature of 300 K.

Achieving the best agreement of the calculated rate coefficients with literature is desirable especially in the range from 80 to 140 Td, which is the most important for plasma chemistry induced by atmospheric pressure discharges.

Gas	a_0 [eV]	a_1 [eV·Td^{-1}]	a_2 [eV·Td^{-2}]	a_3 [eV·Td^{-3}]	a_4 [eV·Td^{-4}]
N_2	1.560	-3.851×10^{-2}	7.694×10^{-4}	-3.588×10^{-6}	5.714×10^{-9}
O_2	1.409	6.171×10^{-2}	-5.804×10^{-4}	3.106×10^{-6}	-5.969×10^{-9}
CO_2	-1.012	8.404×10^{-2}	-5.073×10^{-4}	1.939×10^{-6}	-3.041×10^{-9}
dry air	1.4058	-3.050×10^{-2}	7.271×10^{-4}	-3.555×10^{-6}	5.817×10^{-9}

Tab. 1. Regression coefficients of electron mean energy in different gases.

Gas	b_0 [m·s^{-1}]	b_1 [m·s^{-1}·Td^{-1}]	b_2 [m·s^{-1}·Td^{-2}]	b_3 [m·s^{-1}·Td^{-3}]	b_4 [m·s^{-1}·Td^{-4}]
N_2	19353	939	0	0	0
O_2	10063	2528	-9.2	0.016	0
CO_2	6183	3653.5	-37.167	0.2043	-4.063×10^{-4}
dry air	22960	994	0	0	0

Tab. 2. Regression coefficients of drift velocity of electrons in different gases.

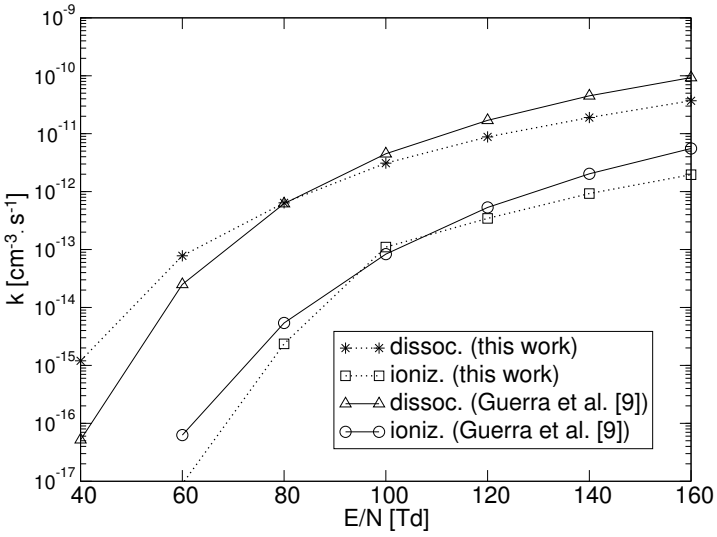

Fig. 4. Rate coefficients of ionization and dissociation of nitrogen.

A slight disagreement observed might be caused by the usage of different sets of cross sections. The sets of cross sections used by SIGLO Series Software [6] are almost identical with our sets. But we cannot check the sets of cross sections used by Guerra et al. [9].

However, the disagreement for lower E/N is most probably caused by statistical error of our simulations. Longer calculations will be necessary to eliminate this error. Explaining the slight disagreement at higher E/N requires further investigation.

Another interesting information obtained from Web-EEDF is the branching of the energy of electrons. For example, in dry air at 100 Td, with the electron mean energy of 2.7 eV, approximately only 0.16% and 0.13% of the input energy goes to the ionization of O_2 and N_2, respectively, whereas more than 50% of the energy goes to the vibrational excitation of N_2. This is in agreement with data presented by Penetrante et al. [10], thought the exact comparison is not possible, since they have calculated power dissipation in an atmospheric pressure dry air discharge as the function of the electron mean energy, and not as the function of E/N.

Figure 5 shows the branching of energy in the range from 20 to 200 Td, where 'vib' means vibrational excitation, 'exc' means electronic excitation and 'ion' means ionization of N_2 and O_2, respectively. Other processes, such as electron attachment or elastic collisions are not figured out in this graph but their contribution is also evaluated in the output from Web-EEDF.

4 Conclusions

Web-EEDF is an open source software for modeling the electron dynamics in uniform electric fields. It provides EEDF, electron drift velocity, electron mobility, and collision frequency of electrons with neutrals as functions of E/N. EEDF enables to calculate electron mean energy,

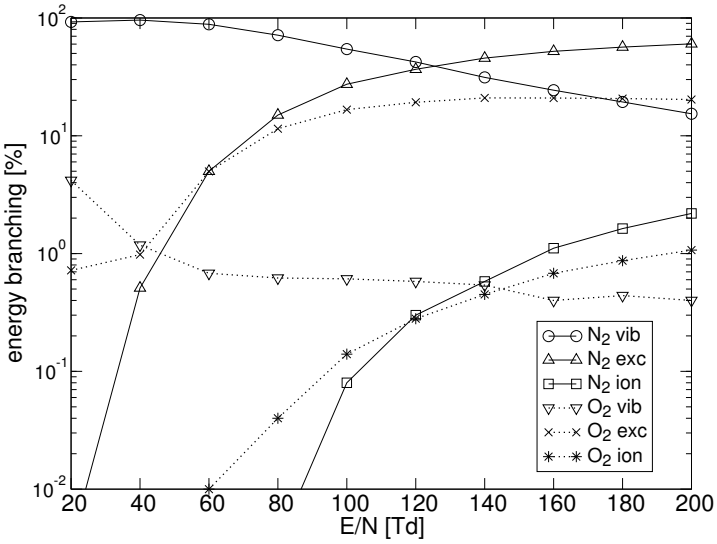

Fig. 5. The branching of electron energy in dry air.

electron mean free path, rate coefficients of electron-molecule collisional processes (e.g. excitation, attachment, ionization), and the branching of the electron energy towards these processes.

Calculated rate coefficients of electron-induced processes can facilitate better understanding of the importance of various reaction pathways leading to the decomposition of air pollutants in various gas mixtures.

The principle goal of this paper is to inform the plasma physics community about this new open source software, and to demonstrate that despite its simplicity the Web-EEDF results are in good agreement with literature. Web-EEDF is also suitable for educational purposes by providing clearer insight in understanding physical and chemical mechanisms in plasma processes.

We hope that this program will be useful for a large public and will warmly welcome any suggestions for its further development. Web-EEDF source code can be downloaded from *http://jandam.host.sk/web-eedf/*.

Acknowledgement: The authors wish to thank the Slovak Grant Agency VEGA for the financial support under projects 1/0256/03 and 1/2013/05, and the APVT agency for the project of bilateral Slovak-US cooperation No. 027/2001.

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