Study electron transport coefficients for Ar, O_2 and their mixtures by using EEDF program

Study electron transport coefficients for Ar, O_2 and their mixtures by using EEDF program

D S Abdul Majeed[1],B J Hussein[1], M K Jassim[1]

[1]Physics Department College of Education for Pure Science Ibn AL Haitham University of Baghdad

drbushrahussam@yahoocom

Abstract. We calculated the electron transport coefficient in Ar, O_2 and their mixtures for ratio of E/N where E denotes the electric field and N the density of gas atoms from $5 - 600$ Td $1\text{Td} = 10^{-17}\ \text{V.cm}^2$ The result and parameters mean energy mobility drift velocity and others are calculated by solving Boltzmann equation We study these gases because of its importance in thermal plasma such as shielding gas for arc welding of metals and alloys These results are useful to find best gas mixtures to reach appropriate transport parameter and to derive the same relevant cross section data

Keywords transport parameter coefficients Argon and oxygen uses and application Boltzmann equation

1. Introduction

The electron energy distribution functions EEDF play a fundamental role in plasma modeling The need of this function comes through the calculations of the reaction rates for electron collision reactions [1 – 3] The distribution functions such as Maxwellian Druyvesteyn and the solution of Boltzmann equation assume that elastic collisions are dominated and the effect of inelastic collisions on the distribution function is not important [4 – 5] However inelastic collisions of electrons with heavy particles play an essential role in the dropping of EEDF at higher electron energies On the other hand the electron transport properties can be derived from EEDF There are many resources help to figure out these properties The EEDF software package is one of those resources [6] This program gives results of the kinetic and transport coefficients of plasma in the pure and mixture of gases by numerically solving Boltzmann equation of EEDF in low – ionized plasma in an electric field In practical applications the inert gases can be mixed to specific gas in order to get special characteristic of the application In turn this needs to have accurate data about electron transport properties of gas mixtures The calculations data of a mixture of molecular Oxygen and Argon under a steady state electric field are presented in this paper There are several computational resources and numerical techniques used to find the transport properties One of them is presented in the EEDF software package This program gives results of the kinetic and transport coefficients of plasma in the mixture of gases by numerically solving Boltzmann equation of EEDF in low – ionized plasma in an electric field This program gives results of the kinetic and transport coefficients of plasma in the mixture of gases by numerically solving Boltzmann equation

of EEDF in low – ionized plasma in an electric field The gas mixtures of molecular Oxygen and Argon are very customary used for a lot of important plasma processes and plasma applications [6] The calculations of EEDF and transport coefficient of pure Argon and pure molecular oxygen and their mixtures are carried out under standard conditions $273\ ^0\text{K},\ 760\ \text{torr}$ by solving Boltzmann equation with two – term approximation using EEDF The range of reduced electric field is between 5 and 600 Td and the electron concentration is $1 \times 10^3\ \text{cm}^{-3}$ One of the goal of this paper is to compute electron drift velocity which is an important swarm parameter and may be useful to control electron energy [7]

2. Theory.

We use the program for numerical solution of Boltzmann equation for the electron energy distribution function EEDF in lowionized plasma in an electric field it is used for calculations of electron transport and kinetic coefficients in gas mixtures [8] In general the EEDF and the electron coefficients for the given discharge conditions can be calculated from the fundamental collision cross section data by solving Boltzmann equation The general form of Boltzmann equation [9]

$$(1)\left(\frac{\partial}{\partial t} + \upsilon.\nabla_r + \frac{eE}{m}.\nabla_\upsilon\right) f(r,\upsilon,t) = \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}}$$

Where $f(r,\upsilon,t)$ is the distribution function for at time t and spatial location r with velocity υ The acceleration of charged particle is given by eE/m and $\partial f/\partial t$ states that $f(r,\upsilon,t)$ changes with time at fixed values of υ and r The term $\upsilon.\nabla_r$ describes that part of change due to an external force altering υ We calculate the time evolution of in mixture of atomic or molecular gases accelerated by electric field The program also computes the diffusion coefficient as [10]

$$D = \left(\frac{1}{3N}\right)\left(\frac{2e}{m}\right)\int_0^\infty f(\epsilon)\frac{\epsilon d\epsilon}{\sum \delta_s \sigma_s(\epsilon)} \qquad (2)$$

Where q_s is the concentration of the species N_s The term $\sigma_s(\epsilon_k)$ is the cross section for elastic scattering of species$s$ and f_k is the normalized distribution function
The drift velocity is given by [10]

$$(3)\quad \upsilon_d = -\frac{1}{3}\left(\frac{2e}{m}\right)^{\frac{1}{2}}\left(\frac{E}{N}\right)\int_0^\infty \frac{1}{\sum_s \delta_s \sigma_s(\epsilon)}\frac{df_0}{d\epsilon}\epsilon d\epsilon$$

Where ϵ is electron energy in eV N is the gas density in $\text{cm}^{-3}$and E/N is in Vcm^2 The electron density n_e is in cm^{-3} and $\delta_s = N_s/N$ The term σ_s is the momentum transfer cross section for species s
The electron mobility stated as the ability of charged particles such as electron to move through a medium in response to an electric field that is pulling them we can write as [11]

$$\mu = \frac{\upsilon_d}{E} \qquad (4)$$

And also can compute the electron mean energy by [12 13]

$$(5)\langle\epsilon\rangle = \int_0^\infty f_0\,(\epsilon)\epsilon^{\frac{3}{2}}d\epsilon$$

The Boltzmann equation describes an evolution of rarefied substance whose particles during a flow undergo binary interaction It describes the physical phenomena which are often of great importance for engineering and technological applications

3 Results and discussion

'Figure 1a', 'Figure 1b' exhibit the EEDF with Mean Electron Energy MEE for pure molecular Oxygen and pure Argon for different values of reduced electric field respectively

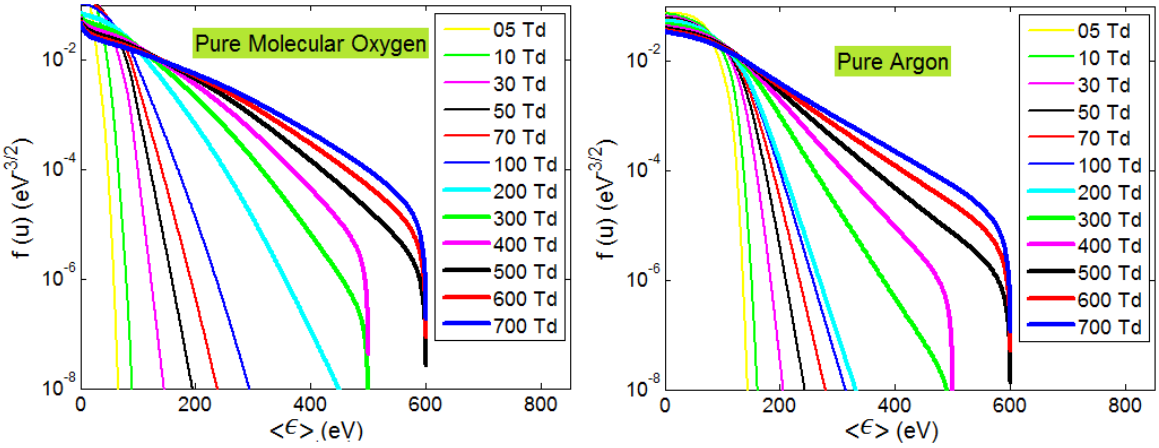


Figure1 a EEDF as a function of mean electron energy for various reduced electric fields E/N in pure molecular Oxygen and b pure Argon In both a and b the electron concentration is 1×10^3 cm^{-3} the gas temperature is 273 ^{0}K and the pressure is 760 torr

'Figure 2a',' Figure 2c' show the EEDF as a function of MEE for various reduced electric fields E/N in a described mixture It is manifesting that EEDF is strongly affected by the increasing of reduced electric field and thus the electron transport coefficients would remain affected The EEDFs for both pure molecular Oxygen and pure Argon hold different discrete curves for all electron energies due to the fact that electrons lose energy in inelastic collisions with atom In both figures applying a high E/N leads to a specific EEDF to evolve to a larger high energy tail Thus each curve is a specific depending on the value of E/N At the proximity of the origin ie at lower MEE the EEDF is low for higher E/N Near to the threshold of inelastic processes the EEDF which is strongly affected by E/N heats the electrons and thus increases the energy of cold electrons For constant value of MEE the EEDF increases as the E/N increased However as MEE increased the EEDF grows with increasing E/N

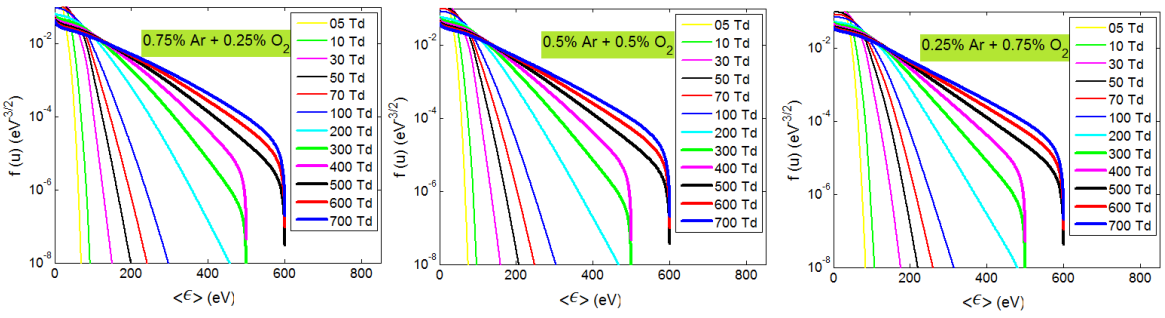


Figure 2 a The EEDF as a function of mean electron energy for various reduced electric fields E/N in a mixture of $0.75\%\ \mathrm{Ar} + 0.25\%\ \mathrm{O_2}$ 05e 2 The EEDF vslar Oxgy eld is between 3 b Mixture of $0.5\%\ \mathrm{Ar} + 0.5\%\ \mathrm{O_2}$ c Mixture of $0.25\%\ \mathrm{Ar} + 0.75\%\ \mathrm{O_2}$ In the entire calculations the electron concentration is 1×10^3 cm^{-3} the gas temperature is 273 ^{0}K and the pressure is 760 torr

'Figure 3a' shows that the MEE increases significantly as the E/N increased At $E/N \leq 350$ Td the pure Ar has upper curve and O_2 has lower curve while the curves of the mixtures are located between them Upper this value the curves are reflected the obverse The MEE of the mixtures are located between Ar and O_2 curves
The characteristic energy in pure Ar pure O_2 and their mixtures gases as a function of reduced electric field is shown in figures 3b It is clear that the characteristic energy for the pure Ar gas is higher than the pure O_2 gas and their used mixture gases For the three used mixtures of both gases the curves of the characteristic energy are located between that of pure Ar and O_2 gases The characteristic energy increases monotonously in exponentially manner with *E*/*N* until 500 Td then the increase becomes linear up from this value for all mixtures and its components

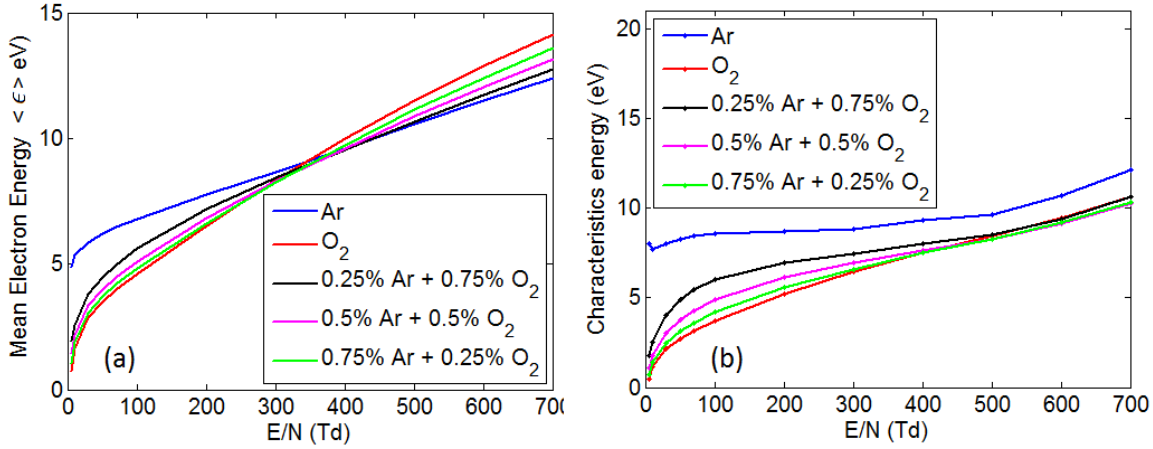
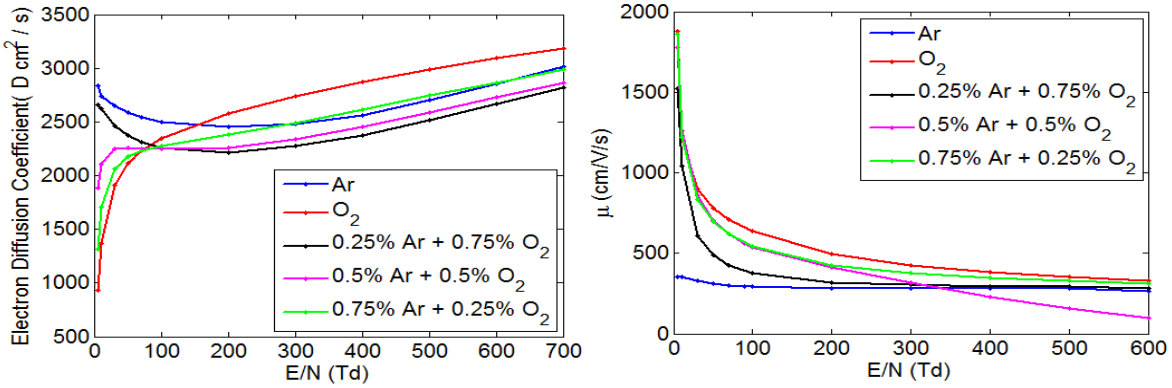


Figure 3 a Mean electron energy b Characteristic energy versus reduced field of a pure Ar O_2 and their mixtures the electron concentration is 1×10^3 cm^{-3} the gas temperature is 273 ^{0}K and the pressure is 760 torr

'Figure 4a' expresses the relation between Electron Diffusion Coefficient EDC and E/N for pure Ar O_2 and their mixtures At low E/N both pure Ar and O2 behave in a different way whilst the EDC decreases for Ar it is increasing for molecular oxygen Since EDC for O_2 is growing quickly from the start it is increasing in exponentially manner with E/N For Ar the curve of EDC against E/N looks like U shape However the curves are intersected at E/N =165 Td At lower of this value the entire values of EDC for O2 are less than for Ar Larger values of EDC than the intersection point the EDC for Ar are less than that for O2 Lower concentration used of Ar in the mixture gives similar behavior of pure Ar whilst lower concentration of O2 in the mixture yields similar behavior as pure O2 The 0.5% Ar $+$ 0.5% O_2 concentration of gas mixture gives a dual behavior of the both each pure gases This mixture obeys to the behavior of O2 at low E/N and to the behavior of Ar at large E/N Obviously at larger than E/N =165 Td the EDC of O2 is larger than all the mixtures and pure Ar
'Figure 4b' shows the electron mobility as a function E/N for a pure Ar and a pure O2 and their used mixtures The electron mobility of O2 is inversely exponential proportional with E/N This is due to the electron energy loss that results in through the collisions between the electrons and neutral molecules Clearly all the used gases mixtures have the same behavior The mobility of pure Ar is decreasing as the E/N increased at the $E/N \leq 100$ Td After this value the mobility of O2 has a plateau as E/N increased It is noted that both concentrations 50% Ar $+ 50\%$ O_2 and 75% Ar $+ 25\%$ O_2 give values of mobility are identical at low E/N but they separate at $E/N = 200$ Td The mixture 75% Ar $+$ 25% O_2 has higher values of mobility than the mixture 50% Ar $+ 50\%$ O_2 Also it is clear that the



mobility of mixture $50\%\ \mathrm{Ar} + 50\%\ \mathrm{O_2}$ continues to decrease in a way such that it is lower than that for a pure Ar

Figure 4 a Electron diffusion coefficient b Mobility versus reduced field of a pure Ar O_2 and their mixtures the electron concentration is 1×10^3 cm^{-3} the gas temperature is 273 ^{0}K and the pressure is 760 torr

'Figure 5a' shows the electron drift velocity versus reduced electric field for pure molecular O_2 and pure Ar and their mentioned mixtures The conductivity of the gases/mixture is characterized by the electron drift velocity in electric field and is the rather important electron transport parameters [14] The drift velocities of Ar O_2 and their mixtures behave in similar manner They increase as the E/N increased The increase is linear but tends to be nonlinear at higher E/N Obviously the pure Ar has lower drift velocity whereas the O_2 has higher values for constant E/N Their mixtures drift velocities stand between them It increases as the concentration of O_2 increased Figure 5b shows the electron drift velocity versus reduced electric field for pure Ar and experimental data Although the experimental data are fairly in a good agreement with the value computed by the program at *E/N* lower than 300 Td but at higher value than 300 Td the experimental data are slightly lower than the resulted from the program The differences could be attributed to experimental results due to impurities in Ar However the two set of data show the same general shape and indicate that the program realistically describes the experimental data is 273 ^{0}K and the pressure is 760 torr

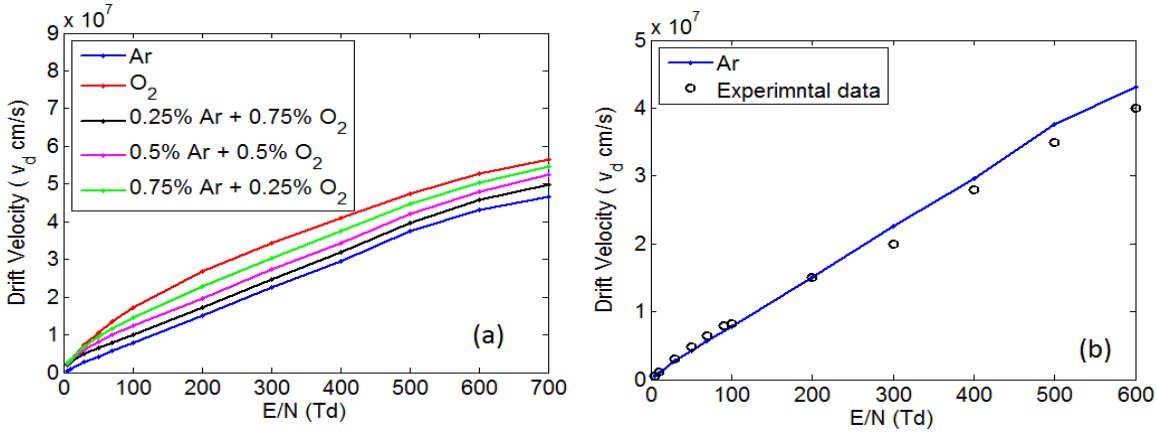


Figure 5 aThe drift velocity as a function of reduced field of a pure Ar O_2 and their mixtures b pure Ar with experimental data the electron concentration is 1×10^3 cm^{-3} the gas temperature

'Figure 6a' ,'Figure 6b' expresses the effect of electron temperature on electron diffusion coefficient and mobility for pure Ar gas at fixed pressure and plasma density The effect is to raise the curves of both parameters with *E*/*N* to a higher magnitude

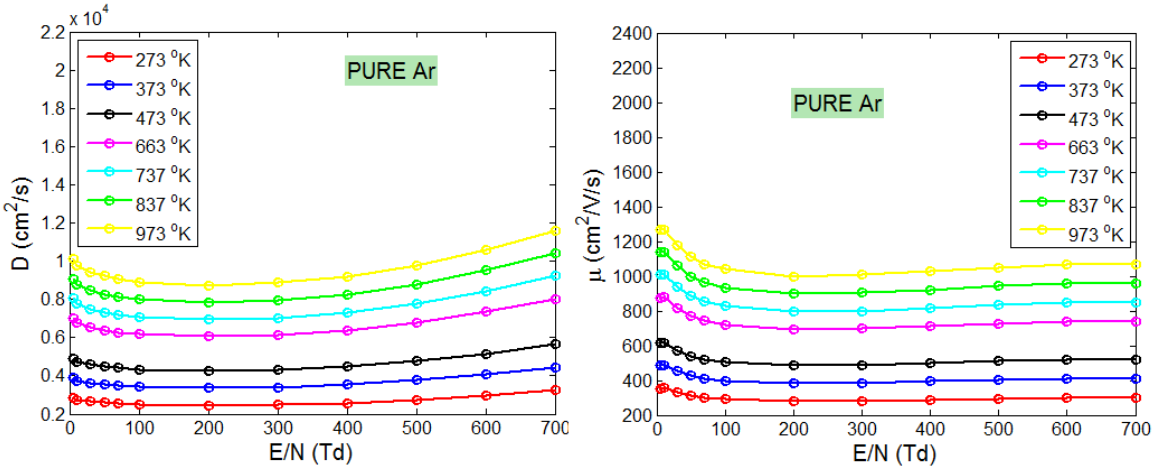


Figure 6 a Electron Diffusion Coefficient vs *E*/*N* of pure Ar for different electron temperatures b Electron Mobility vs *E*/*N* of pure Ar for different electron temperatures the electron concentration is 1×10^3 cm^{-3} and the pressure is 760 torr

'Figure 7a', 'Figure 7b' shows the effect of pressure on electron diffusion coefficient and mobility for pure for pure Ar gas at fixed electron temperature and plasma density As the pressures increased the curves of both parameters with *E*/*N* are going to be at lower magnitude

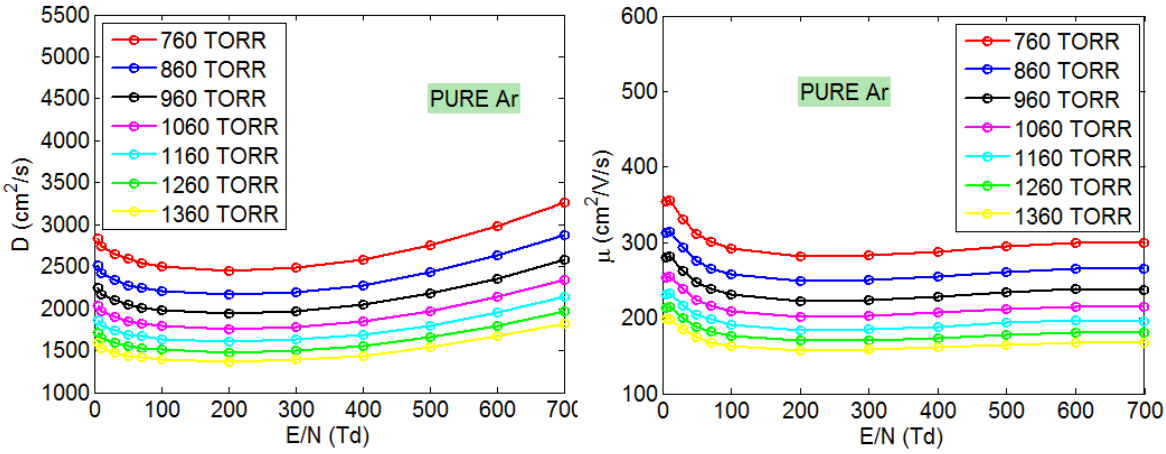


Figure 7 a Electron Diffusion Coefficient vs *E*/*N* of pure Ar for different pressures b Electron Mobility vs *E*/*N* of pure Ar for different pressures the electron concentration is 1×10^3 cm^{-3} and the temperature is 273 ^{0}K

4. Conclusion

We have introduced the transport coefficients of the electron in pure Ar and O_2 and their mixtures The coefficients result in can be adopted as model of plasma containing molecular Oxygen and Argon gases and their mixtures. We observed the effect of this mixture It was found that adding a small amount of Argon gas to molecular Oxygen gives better results in the values of transport coefficients The results of this mixture are satisfactory by comparing the drift velocity with the experimental results

Acknowledgments

The authors would like to thank physics Department College of Education for Pure Science Ibn AL Haitham University of Baghdad for their support in the present work

References

[1] Demidov V DeJoseph C Jr and Kudryavtsev A 2006 IEEE Transactions on plasma science **34** 3
[2] Meeks E and Ho P 2000 Handbook of Advanced Plasma Processing Techniques Springer Berlin Heidelberg
[3] Dahl D A Teich T H and Franck C M 2012 *Journal of Physics D Applied Physics* **45** 48 485201
[4] Boogaard A 2011 PhD thesis University of Twente Netherlands
[5] Behlman N 2009 MSc thesis Worcester Polytechnic Institute USA
[6] Dyatko N Kochetov I Napartovich A and Sukharev A 2005 EEDF the software package for calculations of the electron energy distribution function in gas mixtures
[7] Rabie M Haefliger P Chachereau A and Franck C M Journal of Physics D Applied Physics **48** 7 075201
[8] Jeon B 2003 *Journal of the Korean Physical Society* **43** 4 513 525
[9] Kuzmin D 2010 A Guide to Numerical Methods for Transport Equations Friedrich – Alexander university Germany
[10] Chen F F 1984 Introduction to plasma physics and controlled fusion Plenum Press New York and London
[11] Morgan W L and Penetrante B M 1990 Computer physics communication North Holland **58** 127 152
[12] Rockwood S D Greene A E 1980 Computer physics communication North Holland **19** 377 393
[13] Paul K Chu and XinPei Lu 2014 Low Temperature Plasma Technology Methods and Applications CRC Press USA
[14] Lisovskiy V Booth JP Landry K Douai D Cassagne V and Yegorenkov V 2006 *Journal of Physics D Applied Physics* **39** 660 665