Monte Carlo simulation of electron drift characteristics in an inert gas with mercury vapor

V S Kurbanismailov¹, S A Maiorov²,³, G B Ragimkhanov¹ and Z R Khalikova²

¹Dagestan State University, M Gadjieva st. 43a, Makhachkala, Russia 367003
²A.M. Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova Str. 38, Moscow, Russia, 119991
³Joint Institute for High Temperatures of RAS, Izhorskaya st. 13 Bd.2, Moscow, Russia 125412

e-mail: gb-r@mail.ru

Abstract. The Monte Carlo method calculated the kinetic characteristics of electron drift in three inert gases (He, Ar, Xe) in the presence of small impurities (up to 1%) of mercury vapor at an electric field strength $E/N = 1\text{–}2000 \text{Td}$ taking into account inelastic collisions and analyzed the effect of the concentration of metal vapor on the drift velocity, average electron energy, diffusion and mobility coefficients. In addition, the Townsend ionization coefficient and electron runaway, the electron energy distribution function, and their comparison with the Maxwell and Druvestein distributions are calculated. It has been shown that even insignificant additions of mercury atoms to an inert gas, starting with a fraction of a percent, strongly affect the discharge, in particular, the characteristics of inelastic processes and the charge composition.

1. Introduction
Electron diffusion and drift in gas mixtures have significant features that can be used in numerous gas-discharge plasma applications.

It is known that the transition from the volumetric form of combustion to the spark channel is preceded either by the explosion of the micropoints of the cathode surface, or by the initiation of the emission center during breakdown of dielectric inclusions [1, 2]. Consequently, a certain number of atoms of the material from which the electrodes are made can fall into the feed gas [3, 4]. For example, a mixture of an inert gas with a large ionization potential and a small addition of a heavy easily ionized gas can radically change the characteristics of a gas discharge [5–7]. Indeed, the ionic composition in this case will be determined by an easily ionized additive, and the movement of heavy ions in an improper gas leads to the formation of a supersonic ion flow [8].

In this paper, we consider the drift of electrons in an inert gas (He, Ar, Xe) with mercury vapor in order to study the effect of mercury concentration on electron transfer coefficients.

2. Research methods and analysis of the results
2.1. Problem statement Monte Carlo simulation of electron drift in a gas.
The collision model is based on a random number generation procedure, i.e., on a Monte Carlo method. The implementation of electron – atom collisions by the Monte Carlo method allows one to
take into account the energy balance of electrons based on elementary events, including inelastic collisions.

In the future, when drawing electron - atom collisions, we will assume that:

1) gas atoms have a Maxwell velocity distribution and do not change their temperature due to collisions with electrons;

2) elastic electron–atom collisions occur as collisions of solid spheres, that is, isotropic scattering occurs in the center of mass system, but the collision cross section is assumed to depend on the energy of their relative motion;

3) the loss of electrons on the excitation of atomic levels is irreplaceable, i.e., it is believed that excited atoms lose excitation energy in the mode of volumetric emission, and metastable atoms quickly diffuse beyond the boundaries of the considered volume and do not affect the energy distribution of electrons;

4) during ionization by electron impact, an electron incident on an atom loses energy equal to the sum of the ionization energy and kinetic energy of the knocked out electron;

5) the processes of recombination of electrons and atoms, quenching of excited levels and transfer of resonant radiation do not change the energy of electrons;

6) the probability of ionization and excitation is determined by the cross section of reactions for which a linear approximation is used, starting from the reaction threshold.

2.2. Calculation results of electron drift characteristics in an inert gas with mercury vapor and their analysis.

Tables 1-3 show the calculated values of the drift velocity $V_{dr}$ km/s, average electron energy $<e>$ eV, and the reduced ionization coefficient of Townsend $\alpha/N_o$ $10^{-16}$ cm$^2$ in helium, argon and xenon with small admixtures of mercury vapor. It can be seen from the data presented that even 0.1% of iron atoms already affect the characteristics of electron drift, i.e. the drift velocity and the average electron energy decrease. The results also indicate a sharp change in the ionization characteristics when mercury vapor is added to an inert gas. It should also be noted that the studied quantities strongly depend on the mass of the inert gas atom, the smaller the mass of the gas, the greater the value of the drift characteristic. In helium, all drift characteristics have the highest values, and in xenon the smallest. When mercury vapors are added to an inert gas, the drift velocity and average electron energy decrease. The mercury vapors have the greatest influence on the drift characteristics of electrons in helium.

Table 1. Characteristics of electron drift in helium with mercury vapor at gas temperature $T_g=300$ K.

| $E/N_o$, Td | in pure He | in He with 0.1% Hg | in He with 1% Hg |
|-------------|------------|------------------|------------------|
| $V_{dr}$ km/s | $<e>$ eV | $\alpha/N_o$, $10^{-16}$ cm$^2$ | $V_{dr}$ km/s | $<e>$ eV | $\alpha/N_o$, $10^{-16}$ cm$^2$ | $V_{dr}$ km/s | $<e>$ eV | $\alpha/N_o$, $10^{-16}$ cm$^2$ |
| 1 | 5.018 | 0.5567 | 4.621 | 0.5346 | 4.359 | 0.5278 | 0 |
| 2 | 6.868 | 1.07 | 6.96 | 1.06 | 6.202 | 1.01 | 0 |
| 5 | 11.28 | 2.79 | 12.59 | 2.77 | 12 | 2.38 | 0 |
| 10 | 21.33 | 5.95 | 0.00241 | 21.79 | 5.31 | 0.00717 | 21.33 | 3.75 | 0.00669 |
| 20 | 44.34 | 7.98 | 0.00458 | 43.49 | 7.55 | 0.0115 | 42.07 | 5.56 | 0.03765 |
| 50 | 125.5 | 10.9 | 0.03068 | 121.3 | 10.3 | 0.02783 | 110.3 | 8.78 | 0.06168 |
| 100 | 293.6 | 15.73 | 0.06432 | 279.5 | 14.64 | 0.05895 | 248.5 | 13.03 | 0.08378 |
| 200 | 621.2 | 22.69 | 0.06983 | 608.8 | 22.02 | 0.07041 | 563.1 | 21.2 | 0.09822 |
| 500 | 1208 | 30.72 | 0.05998 | 1198 | 30.39 | 0.06116 | 1143 | 29.86 | 0.07833 |
| 1000 | 1698 | 35.76 | 0.05389 | 1685 | 35.18 | 0.05358 | 1632 | 34.95 | 0.06812 |
| 2000 | 2028 | 39.97 | 0.05254 | 1919 | 40.57 | 0.05765 | 1992 | 38.5 | 0.0629 |
distribution in this range is determined by a drift in the \( k_{\text{eff}} \), energy space with a diffusion coefficient determined by the cross section of elastic collisions; acts of excitation and ionization, after which the electrons are in the low energy ranges, the distribution in which is determined by the dominance or competition of various functions in helium.

In the presence of 1% mercury vapor, the distribution function in helium and argon changes markedly, vapor

| Table 2. Characteristics of electron drift in argon with mercury vapor at gas temperature \( T \equiv 300 \text{ K} \). |
| --- |
| $E/N$, Td | \( V_{dr} \), km/s | \(< \varepsilon > \), eV | \( \alpha/N_{e} \), \(10^{16}\text{cm}^{-2}\) | \( V_{dr} \), km/s | \(< \varepsilon > \), eV | \( \alpha/N_{e} \), \(10^{16}\text{cm}^{-2}\) | \( V_{dr} \), km/s | \(< \varepsilon > \), eV | \( \alpha/N_{e} \), \(10^{16}\text{cm}^{-2}\) |
| 1 | 4.73 | 2.003 | 0 | 4.01 | 1.93 | 0 | 3.41 | 1.83 | 0 |
| 2 | 5.01 | 2.934 | 0 | 4.51 | 2.771 | 0 | 5.47 | 2.553 | 0 |
| 5 | 4.69 | 4.413 | 0 | 5.38 | 4.45 | 0 | 9.13 | 3.22 | 0 |
| 10 | 9.80 | 5.383 | 0.0005 | 11 | 5.27 | 0.00221 | 15.2 | 4.08 | 0.0016 |
| 20 | 18.7 | 5.836 | 0.00421 | 17.8 | 5.69 | 0.00726 | 21.1 | 5.16 | 0.01355 |
| 50 | 39.2 | 6.633 | 0.08335 | 41.1 | 6.59 | 0.05699 | 41.5 | 6.25 | 0.06472 |
| 100 | 74.5 | 7.774 | 0.3224 | 76.4 | 7.487 | 0.1779 | 75.9 | 7.233 | 0.1831 |
| 200 | 138 | 9.648 | 0.7102 | 137 | 8.748 | 0.3937 | 140 | 8.689 | 0.4053 |
| 500 | 341 | 14.35 | 0.9424 | 331 | 13.13 | 0.7975 | 330 | 12.94 | 0.8026 |
| 1000 | 596 | 17.94 | 0.8202 | 607 | 17.4 | 0.7787 | 606 | 17.34 | 0.7889 |
| 2000 | 933 | 21 | 0.6861 | 942 | 20.61 | 0.6617 | 933 | 20.54 | 0.6787 |

| Table 3. Characteristics of mercury ion drift in xenon at gas temperature \( T \equiv 300 \text{ K} \). |
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| $E/N$, Td | \( V_{dr} \), km/s | \(< \varepsilon > \), eV | \( \alpha/N_{e} \), \(10^{16}\text{cm}^{-2}\) | \( V_{dr} \), km/s | \(< \varepsilon > \), eV | \( \alpha/N_{e} \), \(10^{16}\text{cm}^{-2}\) | \( V_{dr} \), km/s | \(< \varepsilon > \), eV | \( \alpha/N_{e} \), \(10^{16}\text{cm}^{-2}\) |
| 1 | 4.31 | 1.15 | 0 | 3.601 | 1.184 | 0 | 3.601 | 0.926 | 0 |
| 2 | 4.97 | 1.58 | 0 | 3.642 | 1.708 | 0 | 3.642 | 1.399 | 0 |
| 5 | 5.53 | 3.488 | 0 | 5.548 | 3.192 | 0 | 5.548 | 3.007 | 0 |
| 10 | 11.34 | 3.631 | 0.0015 | 11.34 | 3.631 | 0.0015 | 11.34 | 3.605 | 0.001 |
| 20 | 25.3 | 4.400 | 0.09 | 25.37 | 4.368 | 0.046 | 25.37 | 4.339 | 0.051 |
| 50 | 53.6 | 5.149 | 0.4 | 53.64 | 4.944 | 0.22 | 53.64 | 4.979 | 0.21 |
| 100 | 125.5 | 6.631 | 0.84 | 111.9 | 5.891 | 0.50 | 111.9 | 5.885 | 0.51 |
| 200 | 356.1 | 9.947 | 1.0 | 353.5 | 9.518 | 0.95 | 353.5 | 9.476 | 0.94 |
| 500 | 657.3 | 12.88 | 0.91 | 656.1 | 12.56 | 0.88 | 656.1 | 12.52 | 0.87 |
| 1000 | 1012 | 15.64 | 0.81 | 1019 | 15.39 | 0.77 | 1019 | 15.41 | 0.81 |

2.3. The results of the calculation of the electron distribution function in an inert gas with mercury vapor. In figure 1a, b. characteristic dependences are given for the electron energy distribution function in an inert gas with 0.1%, 1%, and the content of mercury atoms at $E/N = 15$ Td. As can be seen from the figure, even 0.1% changes the electron distribution function, although this effect is barely noticeable. In the presence of 1% mercury vapor, the distribution function in helium and argon changes markedly, while in xenon the actual does not change. Mercury vapors are most affected by the distribution function in helium.

A detailed analysis of the distribution functions shows that they can in no way be described by any one-parameter function with an effective temperature determined by the relation $1.5T_{\text{eff}} = <\varepsilon >$.

In the EEDF calculated in the computational experiment, one can distinguish several characteristic energy ranges, the distribution in which is determined by the dominance or competition of various processes:

1) region of subthermal energies $\varepsilon < T_{\text{eff}}$, the distribution in this range is largely determined by the acts of excitation and ionization, after which the electrons are in the low-energy region;

2) thermal energy region $\varepsilon < E_{\nu, I}$, the distribution in this range is determined by a drift in the energy space with a diffusion coefficient determined by the cross section of elastic collisions;
3) energy region $E_i < \varepsilon < I$, the distribution in this range is determined by the drift in the energy space and the slope of the straight line in a linear approximation of the excitation cross section;

4) energy region $I < \varepsilon < I + 3T_{\text{off}}$, the distribution in this range is determined by the drift in the energy space and the slope of the straight line in a linear approximation of the ionization cross section;

5) energy region $\varepsilon >> I + 3T_{\text{off}}$, the distribution in this range is determined by the effect of runaway electrons. This division of the characteristic regions of electron energy is very arbitrary.

Figure 1. Characteristic dependences of the electron energy distribution function in inert gases (He, Ar, Xe) with mercury vapor for $E / N = 15$ Td.

3. Conclusions
The characteristics of electron drift in inert gases with mercury vapor were calculated and analyzed at an electric field strength $E / N = 1–1000$ Td with allowance for inelastic collisions. It was shown that even insignificant additions of mercury atoms to an inert gas, starting with a fraction of a percent, strongly affect the discharge, in particular, on the characteristics of inelastic processes. The influence of the percentage of mercury atoms in an inert gas on the kinetic characteristics is studied: diffusion and mobility coefficients, ionization frequency, etc. The values of the drift velocity, average electron energy, characteristic Townsend energy, and Townsend ionization coefficient are calculated. The effect of mercury vapor on the distribution function in inert gases was studied, and the greatest effect of mercury vapor in helium was established.

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