Mathematical Model of the Electronic Coefficients for Different Concentrations of Argon and Mercury Mixture

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Abstract:
In this work, theoretical calculations and simulated data are presented that enable us to calculate the effect of Ar: Hg on the plasma electronic coefficients depending on the variance in the plasma field resistance, which presents in a varied electrical field and under thermodynamic equilibrium. The electric field was chosen in the limited range (1-1000) Td, and the concentrations in the limited range (0.01-0.09) mol. Results show a good agreement between the original data (using BOLSIG +) and that estimated data. There are a large number of applications, for example, material technology that uses flare discharge, thin-film deposition, invasive laser beams, and plasma screen TV. Other technological applications such as gas circuit breakers and L. of particle detectors have also been developed. The work includes calculating the effect of c variation on plasma electronic coefficients and different mercury concentrations of the argon and mercury mixture, and secondly, calculating the effect of the electric field (E / N) on electronic coefficients (mobility, the mean energy of electron, momentum frequency) by solving the Boltzmann equation using BOLSIG + where It was noticed that there is a clear effect of reducing the electric field (E / N) on the electronic transactions where the low electric field increases.

Key words: Plasma, Mean energy, Mobility, Momentum frequency, Electric field

Introduction:
Plasma is an electrically neutral medium of unbound positive and negative particles (i.e. the overall charge of a plasma is roughly zero). Although these particles are unbound, they are not "free" in the sense of not experiencing forces (1). Moving charged particles generate an electric current within a magnetic field, and any movement of a charged plasma particle affects and is affected by the fields created by the other charges. In turn this control collective behavior with many degrees of variation (2).

The properties of plasma are remarkably dependent upon the particle interactions. One of the basic features that distinguish the behavior of plasma from that of ordinary liquids and fluids is the existence of collective effects. Due to the long rage of electromagnetic forces, each charged particle in the plasma interacts simultaneously with a considerable number of other charged particles (3).

Plasma science and applications have been seeing great progress over the last few decades. This progress is the consequence of development of modern plasma sources based on plasma generation in electrical discharges in vacuum in low- and high-pressure gases (4). Yet it is also the product of innovative plasma uses in plasma dispensation of materials, in galactic propulsion and, most notably, in both plasma-based nano and biomedical technology.
In this paper, electron drift in argon with an additive of mercury vapor is considered with the aim to study the effect of the mercury concentration on the electron transport coefficients. The primary objective of the work is creating a mathematical model that accurately describes the behavior of electronic coefficients by changing discharge conditions and studying the impact of minimal concentrations of mercury vapor in argon on electronic coefficients.

Materials and Methods:

Boltzmann Equation

The Boltzmann equation is one of the most powerful tools for investigating the plasma state, from the electron kinetics in weakly ionized gases to fusion and astrophysical plasmas. Boltzmann equation introduced into physics the idea of probability, which was then used some years later in quantum physics (5).

The Boltzmann equation is a nonlinear integro-differential equation, and it is a probability density function in six-dimensional space of a particle position and momentum (6). Boltzmann equation gives the ratio of number per unit volume (the number density) of molecules, atoms, or ions, which is denoted by $N_2$, in a certain energy level to the number density in another lower energy level which is denoted by $N_1$, and it is given by:

$$\frac{N_2}{N_1} = \left(\frac{g_2}{g_1}\right) e^{-\frac{E}{kT}} \quad (1)$$

Where, $g_1$ and $g_2$ represent the multiplicity of the two energy levels; $E$ is the required energy to excite particles; $K$ represents Boltzmann constant and $T$ represents thermodynamic temperature (6).

In the present work, theoretical calculations for several electronic coefficients in a mixture of Ar-Hg gas (using several gas mixture concentrations) are presented by creating mathematical models utilizing Boltzmann distribution function and appropriated simulation process (7).

The simulation process using BOLSIG+ program was utilized under 300 k as an excitation temperature, $0.1 \times 10^{-3}$ as an ionization degree, $10^{19}/m^3$ as a density and impacted by electron-electron collision, electron-ion collision and influence of electron-electron momentum (8).

Results and Discussion

Mean Energy Modeling

The concentration affects obviously on discharge process, see Fig.2. Where the mean energy increases with the increasing of Hg concentration in Ar-Hg mixture. It can be also noticed the mean energy $\langle \varepsilon \rangle$ values dependence on reduced of the electric field ($E/N$). Where the increasing of mean energy according to the increasing of ($E/N$) is observed by eq.2:

$$\langle \varepsilon \rangle = B_0 + B_1 \left(\frac{E}{N}\right) + B_2 \left(\frac{E}{N}\right)^2 + B_3 \left(\frac{E}{N}\right)^3 \quad (2)$$

Where, $E/N= (1-1000)$ Td

This because the cross-section area is influenced by the reduced electric field (9), where the mean energy is of high sensitivity to gas mixture concentration, as a consequence this will result in a reduced electric field; attained by increasing the rate of elastic-inelastic collisions (10).
In the Fig. 1, the relationship between constants ($B_0$, $B_1$, $B_2$, and $B_3$) and Ar-Hg concentration are represented by equations (3, 4, 5, and 6):
Figure 2: Estimated values of constants $B_0, B_1, B_2$ and $B_3$ vs. concentrations Ar-Hg mixture

\[ B_0 = 0.767 + (0.689 - 0.767) / (1 + (c/0.05228)^{4.631}) \]  \hspace{1cm} (3)

\[ B_1 = 0.00269 + (0.01537 - 0.00269) / (1 + (c/0.02684)^{1.630}) \]  \hspace{1cm} (4)

\[ B_2 = 7.645 \times 10^{-7} + (-1.905 \times 10^{-5} - 7.6489 \times 10^{-7}) / (1 + (c/0.02089)^{2.2369}) \]  \hspace{1cm} (5)

\[ B_3 = -2.443 \times 10^{-10} + (8.9691 \times 10^{-9} - (-2.44 \times 10^{-10})) / (1 + (c/0.0194 \times 10^{-10})^{2.904}) \]  \hspace{1cm} (6)

where, c is the concentration, c=0.05

Fig. (3) could be obtained through figure (2), which shows a high fitting/matching ratio between original data (using Bolsig) and our simulated data equations (3, 4, 5 and 6) represent special equations that determine concentrations related to equation (2).

Figure 3: Estimated/Simulated data of Mean Energy
Mobility Modeling

Fig. 4 demonstrates decreasing in the electrons mobility starting from \( E/N = (0 - 200) \) Td for all utilized concentrations. Then the curve of the electron’s mobility begins to be almost constant. A simple/slight change starting from \( E/N = (200-1000) \) Td.(11). It can be also observed that the effect of the electric field in high concentration levels is much obvious than in low concentration levels (A decreasing of electron mobility initially starts from the range between \( 10^{23.5} \times 10^{24} \) \( \text{1/m/s} \). This effect is due to the ionization process which produces free electrons and consequently increasing the number of elastic and inelastic collisions that will limit electrons mobility (12). This influence is very evident in the limited region \( E/N = (0-200) \) Td.

![Electrons mobility as a function of reduced electric field (E/N).](image)

Through the Fig., a fitting relationship (for all concentrations) could be obtained. This relationship represents the general behavior and it can be represented by:

\[
\mu N = A_1 + (A_1 - A_2) / (1 + \left( \frac{E/N}{x_0} \right)^P)
\]  

(7)

Where, \( E/N = (1-1000)\)Td

Fig. 5 show the relationship between constants \( (A_1, A_2, X_0, \text{and } P) \) and Ar-Hg concentration. Where represented by equation (8, 9, 10 and 11)
Figure 5 Estimated values of constants $A_1, A_2, X_0$ and $P$ vs. concentrations of Ar-Hg mixture

$$A_1 = 1.4414 \times 10^{25} + (1.6637 \times 10^{25} - 1.4414 \times 10^{25})/(1 + \left(\frac{c}{0.0727}\right)^{4.061}) \quad (8)$$

$$A_2 = -4.959 \times 10^{26} + (2.349 \times 10^{24} - (-4.959 \times 10^{26})/(1 + \left(\frac{c}{9.549}\right)^{1.005}) \quad (9)$$

$$X_0 = 1.5334 \times 10^6 + (56.125 - 1.5334 \times 10^6)/(1 + \left(\frac{c}{54.291}\right)^{1.398}) \quad (10)$$

$$P = 0.104 + (1.404 - 970.104)/(1 + \left(\frac{c}{0.0697}\right)^{0.85678}) \quad (11)$$

where, $c$ is the concentration, $c=0.06$

Fig.(6) could be obtained through fig. (5), which shows high fitting/matching ratio between original data mobility (using Bolsig+) and our simulated data of mobility.
Equations (8, 9, 10 and 11) represent special equations that determine concentrations related to equation (7).

**Momentum frequency Modeling**

From fig. 7, the concentration affects obviously on discharge process, where the momentum frequency increases with the increasing of Hg concentration in Ar-Hg mixture. It can be also noticed the dependence of momentum frequency on reduced electric field (E/N), where the increasing of momentum frequency according to the increasing of (E/N) is observed. This happens because the cross-section area is influenced by the reduced electric field (13). As the momentum frequency increases with increasing the concentration of the gas mixture, as a result the elastic collision rate will increase, leading to an increase in the low electric field (14).

![Figure 6: Estimated/Simulated data (using mathematical model) of mobility](image)

![Figure 7: Electrons momentum frequency as a function of reduced electric field (E/N)](image)
The fitting relationship (for al concentrations) was obtained through the fig. 7.

\[ \langle \frac{v_m}{N} \rangle = (B_0 + B_1 \left( \frac{E}{N} \right) + B_2 \left( \frac{E}{N} \right)^2 + B_3 \left( \frac{E}{N} \right)^3 \]  

(12)

Where, \( E/N = (1-1000) \text{Td} \)

Fig.(8) shows the relationship between the constants \( (B_0,B_1,B_2\text{and } B_3) \) and Ar-Hg concentration. Where represented by equation (13, 14, 15 and 16):

Figure 8 Estimated values of constant \( B_0,B_1,B_2 \text{and } B_3 \) concentrations of Ar-Hg mixture
\[ B_0 = 8.534 \times 10^{-15} + (-6.3927 \times 10^{-4}C) + (2.137 \times 10^{-12}C^2) + (-1.3158 \times 10^{-11}C^3) \]  
(13) \[ B_1 = 2.389 \times 10^{-16} + (-6.409 \times 10^{-15}C) + (8.665 \times 10^{-14}C^2) + (-4.055 \times 10^{-13}C^3) \]  
(14) \[ B_2 = -3.469 \times 10^{-19} + (1.394 \times 10^{-17}C) + (-2.096 \times 10^{-16}C^2) + (1.031 \times 10^{-15}C^3) \]  
(15) \[ B_3 = 1.867 \times 10^{-22} + (-7.977 \times 10^{-21}C) + (1.255 \times 10^{-19}C^2) + (-6.322 \times 10^{-19}C^3) \]  
(16)

Where, \( C \) is the concentration, \( C=0.05 \)

Fig. (6) could be obtained Through fig.(5), which shows high fitting/matching ratio between original data mobility (using Bolsig+) and our simulated data.

**Equations (13,14,15and16) represent special equations that determine concentrations related to equation (12).**

**Conclusion:**

It has been closely observed in this study that the value of electronic coefficients will shift due to the change in the cross-sectional area in the case of an increase in the electric field. This in turn leads to a change in elastic and inelastic collisions. Also, it has been observed that a change in the concentration of mercury also affects the change in the value of electronic coefficients. It also enables us, through work, to obtain simple mathematical equations to extract the value of electronic coefficients easily without the need to use a simulation program BOLSIG +

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References:

1. V S Kurbanismailov S, Omar A. A. Maiorov, Gadzhimirza R. Electron drift characteristics in argon with iron vapor: coefficient of mobility, ionization and runway. J. Phys.: Conf. Ser. 2018;1115(2):1-6

2. Lipeng Liu. Physics of Electrical Discharge Transitions in Air. Sweden: electrical engineering Stockholm KTH; 2017 April

3. G. I. Sukhinin, M. V. Salnikov1 and A. V. Fedoseev1. The Effect of the Type of Ion–Neutral Collisionson Ion Cloud Formation. AIP Conf. Pro. 2018 January; 1925(1) 020029

4. Annemie B., Erik N., Renaat G., Joost v. Gas discharge plasmas and their applications. Spectrochimica Acta Part. 2002; 57(4): 609–658

5. Philip T. Gressman & Robert M. Global classical solutions of the Boltzmann equation with long-range interactions. Proceedings of the National Academy of Sciences. 2010; 07 (13): 5744–5749

6. M. Drewes, C. Weniger, S. Mendizabal. The Boltzmann equation from quantum field theory. Phys. 2013; 8 January: 718 (3): 1119–1124

7. G.J.M. Hagelaar and L.C. Pitchford. Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models. Plasma Sources Sci. Technol. 2005; 14 (0963-0252): (722-733)

8. Debbasch, Fabrice, Willem v. General relativistic Boltzmann equation I: Covariant treatment. Physica A. 2009; 388 (7): 1079–1104

9. A I Ahmed and N A Hamdon. A comparative study of electron transport coefficients in the pristine and dusty argon plasma. Indian J Phys. 2014 December; 88(12):1299–1303

10. Guangsup C., Lee J., Kim, S., Song H., Koo J., Kim B. Kang J., Choi E., Lee U., and Verboncoeur, J. Glow discharge in the external electrode fluorescent lamp. IEEE Transactions on Plasma Science. 2005; 33 (4) (1410-1415

11. V S Kurbanismailov1, S A Maiorov2, O A Omarov1, G B Ragimkhanov1 and Z R Khalikova "Electron drift characteristics in argon with iron vapor: coefficient of mobility, ionization and runway" IOP Conf. Series: Journal of Physics: Conf. Series. 2018; 10(2) 022040

12. Mathes w., Kiruthika, Gurumam, Shanmugavel. Characteristics of anodic glow pulsed plasma. Physics Lett.. 2020January; 384(1)

13. Jovanović J V, Vrhovac S B and Petrović Z L. Momentum transfer theory of ion transport under the influence of resonant charge transfer collisions: the case of argon and neon ions in parent gases. Eur. Phys J. 2002; 21: (335–342)

14. A. K. Shuaibov and A. A. Emission characteristics and plasma parameters of short glow discharge in argon-egas mixture. Teplofizika Vysokikh Temperatur. 2011; 49( 4): (505–508)