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Simulation Analyses and Investigation of the Induced Electric Field and Ar-Hg Mixture on the Gas Discharge Processes

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ABSTRACT

In this work, theoretical calculations and simulated data were presented to investigate the effect of the Ar-Hg mixture on electronic plasma coefficients, in addition to study the influence of the electric field and focus on electronic coefficients. The low electric field was chosen in the range (1-1000) Td, and concentrations in a limited range (0.01-0.09) mol. The results showed a clear effect of the electric field on electronic transactions, especially at low levels. These parameters values are higher for high concentrations due to the effect of the electric field on the excitation and ionization energy. In compare to elastic and inelastic collision, and cross-section collision of gas discharges. The results showed good agreement between the original data (using BOLSIG +) and the estimated data in the current work.

KEYWORDS: Boltzmann Equation; Electronic Coefficients; Gas Discharge; Elastic and Inelastic Collision; Mean Energy.

INTRODUCTION

The term "gas discharge" comes from the discharging designation process of a charged capacitor circuit that includes a gas gap between the electrodes at a sufficiently high voltage. The ionizing state occurs under the influence of the electric field, where The electric gas breakdown happened and the gas becomes an electrical conductor When the circuit is closed between the plates, and the capacitor is discharged [1, 2]. Discharge is a type of plasma formed by applying an electrical potential between the cathode and the anode in a tube containing gas [3]. External charge density $\rho_{ext}(r,t)$, is contained in the dielectric function to calculate the electronic. The discharge is called for any electric current process that flows through an ionizing gas, any process of ionization occurrence, and the property of electrical conductivity under the influence of an applied electric field [4, 5]. Since the ionized gas mostly glows and the discharge is flame due to combustion [4].

Transfer coefficients were first studied theoretically or empirically for equilibrium plasma, such as pure hydrogen, nitrogen, oxygen, air and noble gases. The theory of transport properties of gas mixtures was developed by Chapman and Cowling, by Hirsch elder, Curtis, and Bird[5]. Many researchers have theoretically calculated electron transport coefficients using the Boltzmann Equation method. There are many researchers have been studied changing electronic coefficients and their effect on discharge operations such as Wei Yang *et al.* [4]. They are calculated electron transport coefficients in copper vapor plasma by two-term expansion of Boltzmann equation (BOLSIG+: A series of runs to increase E / N linearly, for initial and final E / N values and a certain number of runs. The typical E / N range for standard conditions ranges from 1Td to a few 1000 Td). R.I. Golyatinaa *et al.* [7], are calculated the properties of the electron drift in the argon mixture with mercury in a low electrical field (E / N = 1-100 Td). A. I. Ahmed *et al.* [8], are studied the Boltzmann transfer equation for the electron energy distribution function and the values of the various electron transfer coefficients using the reduced electric field in the range (30-200) Td. There are a large number of applications, for example, material technology that uses glare discharge, gas lasers, thin-film deposition, and plasma screen television [6-8].

THEORETICAL PART

Boltzmann Equation (BE)

Equation (1) describes the behavior of charged particles in gases by the phase space distribution function f (r, c, t). The physical assumptions and numerical techniques used by solving the Boltzmann equation [9]:

$$\frac{\partial f}{\partial t}+ c.\frac{\partial f}{\partial r}+\frac{\partial E}{m}.\frac{\partial f}{\partial c}=-J(f,f_0) \qquad (1)$$

Where *e* and m are the charge and mass of the electrons and *t* is the time. The electric field is assumed to be spatially homogeneous force *E**r*, c: velocity coordinates and $J(f,f_0)$ indicates to the rate of change of *f* due to the two collide with neutral particles only [10].

Total frequency collision can be calculated from the following equation [12]:

$$(\upsilon_{tot}/N)=\gamma\int_0^{\infty}\sum_{k=all}x_k\,\sigma_k\varepsilon f_0 d\varepsilon \qquad (2)$$

Where, x_k: fractional particle number density of target gas species of collision process k.

σ_k: cross section of electron-neutral collision process k. for inelastic processes and f_0: electron energy probability function (EEPF) $eV^{3/2}$ [11].

$$(P_{ei}/N)=\sum_{K=elastic}\gamma x_k\frac{2m_e}{M_K}\int_0^{\infty}\left[\sigma_k\left(\varepsilon^2 f_0+\frac{k_BT}{e}\frac{\partial f_0}{\partial\varepsilon}\right)\right]d\varepsilon \qquad (3)$$

Where, γ: constant coefficient $(2e/m_e)^{1/2}$ $C^{1/2}$ $Kg^{-1/2}$, m_e: electron mass kg, M_K:particle mass of target particles of collision process k, σ_k:cross section of electron-neutral collision process k. for inelastic processes, k_B: Boltzmann's constant= 1.380×10^{-23} J K^{-1} and e: electron charge=1.6×10^{-19} C.

Inelastic power loss can be calculated from the following equation [14]:

$$(P_{inel}/N)=\sum_{K=inel}U_k\,x_k\left(y_k^{low}K_k-\,y_k^{up}K_k^{inv}\right) \qquad (4)$$

Where, U_k: threshold energy of inelastic collision process k, K_k: Rate coefficients (m^3/s) y_k^{low}: fractional population of lower quantum state of excitation process k, y_k^{up}: fractional population of upper quantum state of excitation process k. and K_k^{inv}: Inverse rate coefficients (m^3/s).

RESULTS AND DISCUSSION

Influence of the Reduced Electric Field (E/N) On Total Collision Frequency

Figure 1 shows increasing the total collision frequency with the increasing of (E / N). From (E/N=1-345.5) Td the total collision frequency increases sharp, while from (345.5.9-1000) Td the increase will represent a slight, this is due to the energy of the electron depends on the ionization energy, and the increase of the electric field will increase the processes of the ionization and the kinetic energy which leads to an increase the total collision frequency. Also note the non-linear increase in the total collision frequency, especially for concentrations (0.01, 0.02 and 0.03) mole, where the effectiveness of inelastic collisions in the electric field ranges from (0-260) Td, after which the behavior stabilizes in the linear increase, which is the common increase for the rest concentrations (0.04 - 0.09) mole, the reason is that the impact of collision varies from region to region due to the electric field [12].

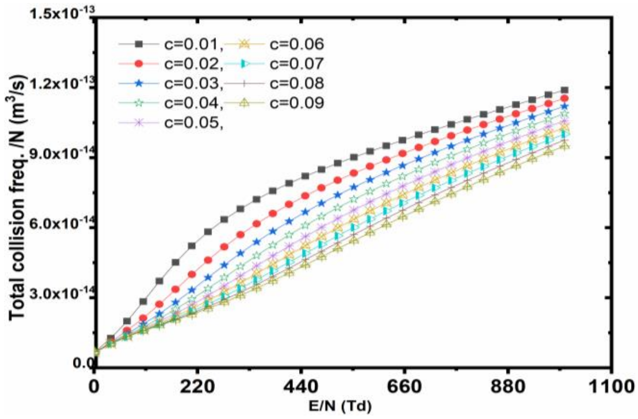

Figure 1. Total collision frequency as a function of reduced electric field (E/N).

Influence of Concentration of mixture Ar-Hg on Total Collision Frequency

Table 1 demonstrated the relationship between collision frequency and concentration of Hg that are observed a decrease in the collision frequency value when the concentration increases from (0.1 to 0.9) mole, this attributed to the collision's ratio decrease when the increase of concentration[13].

Table 1. The relationship between total collision frequency & concentration of Hg.

E/N=517.7 Td	
Concentration (mole)	**Total coll. Freq. $*10^{-14}$ (m^3 /s)**
0.01	8.765
0.02	8.033
0.03	7.402
0.04	6.861
0.05	6.396
0.06	5.996
0.07	5.653

Total Collision Frequency Modeling

Equation 5 represents the fitting relationship (for all concentrations) obtained from Figure 2 which represents a matching between the BOLSIG+ program values and proposed model that based of using logistic function and third degree polynomial in Origen program which gives optimal matching equation.

$$(\boldsymbol{v_{tot}/N}) = B_0 + B_1(\tfrac{E}{N}) + B_2(\tfrac{E}{N})^2 + B_3(\tfrac{E}{N})^3 \qquad (5)$$

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

Also, the parameters B_0, B_1, B2, and B_3 can be calculated by third degree of logistic and polynomial functions using equations (6), (7), (8), (9) respectively, then utilized to determine the concentration aforementioned in equation (5).

$$B_0 = 4.26056 \times 10^{-15} + (-1.00994 \times 10^{-13})C + (3.95323 \times 10^{-12})C^2 + (-2.6001 \times 10^{-11}C^3) \qquad (6)$$

$$B_1 = 3.79061 \times 10^{-16} + (-1.07769 \times 10^{-14})C + (1.30011 \times 10^{-13})C^2 + (-5.59552 \times 10^{-13})C^3 \qquad (7)$$

$$B_2 = (-5.14059 + (2.45711 \times 10^{-17}) + (-3.41544 \times 10^{-16})C^2 + (1.57345 \times 10^{-15})C^3 \qquad (8)$$

$$B_3 = (2.56292 \times 10^{-22}) + (-1.43251 \times 10^{-20})C + (2.1313 \times 10^{-19})C^2 + (-1.01365 \times 10^{-18})C^3 \qquad (9)$$

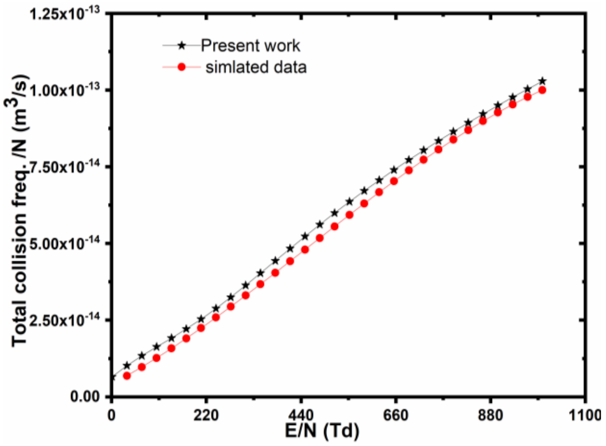

Figure 2. Estimated/simulated data (using mathematical model) of total collision frequency.

Influence of Reduced Electric Field on Elastic Power Loss

Figure 3 shows the relationship between the elastic power loss and reduced electric field (E/N), where the elastic power loss increased with in (E/N) increasing) for different concentrations of Hg in Ar-Hg mixture (0.01-0.09) mole. The increasing in elastic power loss is very small for the lower values of the reduced electric field, while this increasing is the sharpness for the high values of the electric field. The increase in the electric field leads to an increase in the velocity of electrons and thus an increase in power loss due to collisions [17].

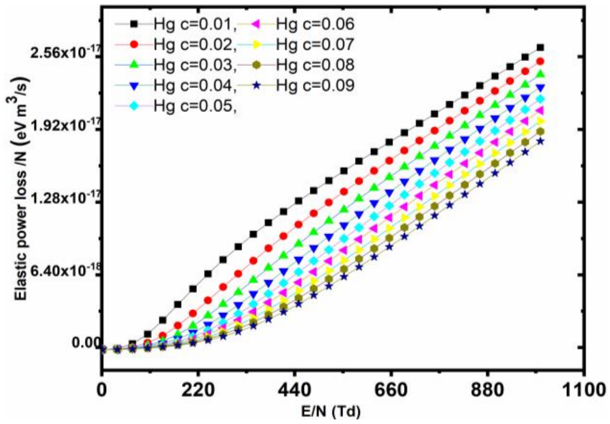

Figure 3. Elastic power loss as a function of reduced electric field (E/N).

Influence of Concentration of mixture Ar-Hg on Elastic Power Loss:

Table 2 shows the effect of the mercury concentration on the elastic power loss. One can observed that the elastic power loss decreases with increasing of mercury concentration in the Ar-Hg mixture due to increase in the strength of the external reduced electric field as well as this will increase the rate of elastic collisions[14] especially when moving from a high concentration to a low concentration.

Table 2. The relationship of elastic power loss with concentration of Hg.

E/N=517.7 Td	
Concentration (mole)	**Total coll. Freq. $*10^{-14}$ (m^3 /s)**
0.01	8.765
0.02	8.033
0.03	7.402
0.04	6.861
0.05	6.396
0.06	5.996
0.07	5.653
0.08	5.357
0.09	5.102

Elastic Power Loss Modeling

Equation (10) represented the fitting relationship (for al concentrations) and was obtained according to figure (4) using the second order of logistic and polynomial functions because it gave the best matching equation:

$$(P_{ei}/N) = B_0 + B_1\left(\frac{E}{N}\right) + B_2\left(\frac{E}{N}\right)^2 \quad (10)$$

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

Also, the parameters B_0, B_1, B_2, and B_3 are calculated using second and third degree of logistic and polynomial functions, then these values utilized to determine the required concentration in equation (10).

$$B_0 = (-1.03285 \times 10^{-18}) + (-6.8339 \times 10^{-17})\,C + (1.64511 \times 10^{-15})C^2 + (-9.4468 \times 10^{-15})C^3 \quad (11)$$

$$B_1 = (4.15106 \times 10^{-20}) + (-7.44993 \times 10^{-19})\,C + (3.59195 \times 10^{-18})C^2 \quad (12)$$

$$B_2 = (-1.27749 \times 10^{-23}) + (6.7325 \times 10^{-22})C + (-3.9445 \times 10^{-21})C^2 \quad (13)$$

Figure 4 shows high fitting/matching ratio between original elastic power loss (using BOLSIG+) and our simulated data.

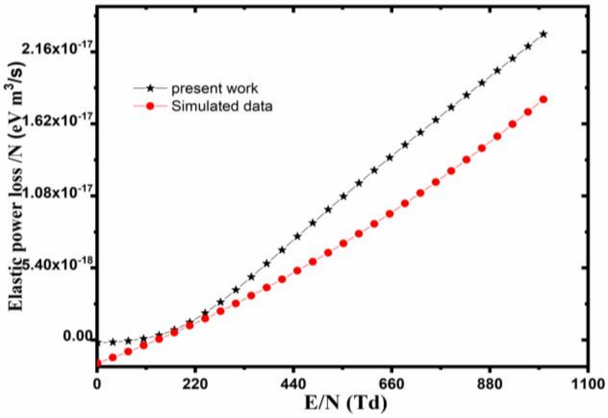

Figure 4. Estimated/simulated data (using mathematical model) of elastic power loss.

Influence of the Reduced Electric Field (E/N) On Inelastic Power Loss

Figure 5 shows the relationship between inelastic power loss and the reduced electrical field (E / N) for different concentrations of the Ar-Hg mixture (0.01-0.09) Mole. While the inelastic power loss increases with increasing reduce electric field (E / N), where its effect is at (1 - 207.7) Td more compared to other values (276.6-1000) Td for all concentrations.

Influence of Concentration of Mixture Ar-Hg on Inelastic Power Loss

Table 3 cleared the effect of Hg concentration on the inelastic power loss which is decreased by increased Hg concentration in Ar -Hg mixture. Furthermore, it is noticed from Figure 5 and Table 3, increasing in the rate of inelastic collision with diminishing the concentration, which is attributed to irritate the neutral atoms and increased their energies by colliding with electrons[15].

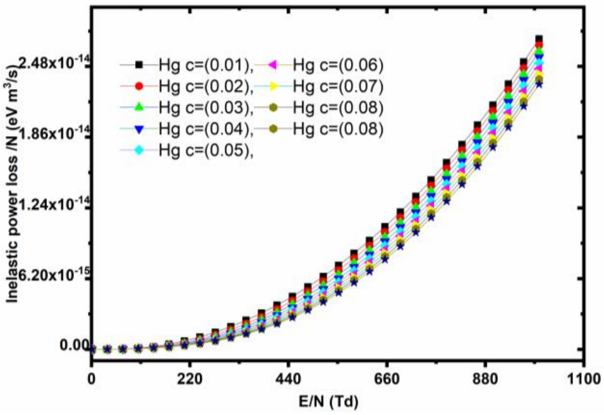

Figure 5. Inelastic power Loss as a function of the Electric Field (E/N).

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Table 3. The relationship between inelastic power loss & concentration of Hg.

E/N=552.2Td	
Concentration (mole)	Inelastic power loss $*10^{-15}$ (eV m3/s)
0.01	7.371
0.02	6.942
0.03	6.554
0.04	6.21
0.05	5.902
0.06	5.625
0.07	5.381
0.08	5.164
0.09	4.97

Inelastic Power Loss Modeling:

Equation (14) represented the fitting relationship (for all concentrations) that was obtained according to figure (5) by using function of logistic and polynomial of second degree in program origin.

$$(P_{inel}/N) = B_0 + B_1\left(\frac{E}{N}\right) + B_2\left(\frac{E}{N}\right)^2 \quad (14)$$

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

The parameters B0,B1, B2,and B3 are calculated in equations (15),(16) and (17) by using logistic and polynomial functions of both second and third degree, and utilized to determine the concentration in equation (14).

$$B_0 = (8.6146 \times 10^{-17}) + (8.19677 \times 10^{-15})\, c + (-2.57877 \times 10^{-14})c^2 \quad (15)$$

$$B_1 = (-2.75162 \times 10^{-18}) + (-1.34018 \times 10^{-16})\, c + (6.90434 \times 10^{-16})c^2 \quad (16)$$

$$B_2 = (3.03062 \times 10^{-20}) + (6.84063 \times 10^{-20})\, c + (-6.12229 \times 10^{-19})c^2 \quad (17)$$

Figure 6 shows high matching ratio between data of inelastic power loss (using BOLSIG+) and present work.

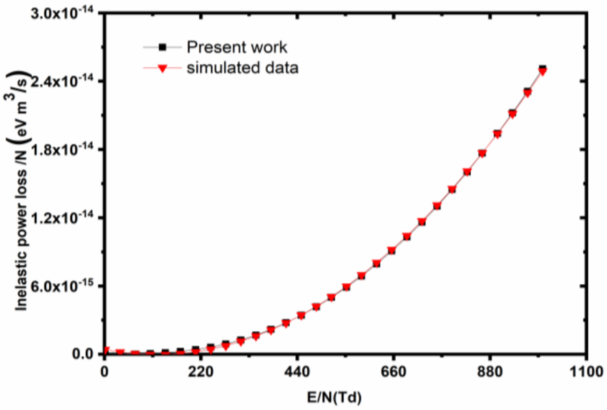

Figure 6. Estimated/simulated data (using mathematical model) of Inelastic Power Loss

CONCLUSIONS

In this work, we have noticed that the electric field has a major role in the gas discharge process with a different effect from one place to another. For the total collision frequency, the influence of the electric field is high in the region (0-260) Td. It is noted that the reduced electric field for both the inelastic power loss and the elastic power loss have the same effect, especially in the region (1 -207.7) Td where, the reason for this is due to the role of elastic and inelastic collisions and cross-section for collisions. As for concentrations, electronic coefficients have high values at low concentrations due to the effectiveness of elastic and inelastic collisions and cross-section collisions at these concentrations. In addition, the mathematical model was obtained appeared a great match between percent work and the values of the electronic transactions obtained using the BOLSIG+ program. The study also showed the importance of relying on logistic and polynomial functions, because, these functions showed a higher matching than other functions.

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