Study of Argon and Xenon gas properties on DC-glow discharge plasma

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Abstract. With the advances in the plasma technology in several fields as waste management, space technology and medical applications, non-thermal plasmas have become popular. They replace the combustion fuels for stationary hall thrusters and require minimal voltage to sustain longer duration. Generally, non-reactive gases such as Xenon, Argon, Krypton in a pure or mixture form is used to generate plasma, in order to have overall better performance of the system. Hence, the study of these gases and its properties becomes very crucial for further improvement in any kind of application. Xenon has proven to be most efficient in Hall thruster as compared to the other gases, but its limited availability and high cost has led to the idea of replacing it with other gases that are in abundant. As the DC glow discharge is considered to be canonical problem of interest, the paper focuses on modelling and simulation of 1-D and 2-D. DC glow discharge tubes using Argon and Xenon as gases to generate plasma and study its properties. The trend in distribution of electron density, electron temperature and electric potential has shown little variation. However, the magnitude on electron density is slightly higher for Argon relative to Xenon for given operating conditions in 1-D simulation and in the case of 2-D simulation the diffusive nature in lateral direction has shown higher peak value for Xenon.

1. Introduction:

The rise in application of non-thermal plasma in several fields imparts research attention. The ionized state of plasma makes it different from a normal gas. The laboratory plasmas are formed when an electric current is passed through the discharge tube ionizing the gas [1]. The study of glow discharge plasmas in pure or mixed gases are very crucial for the industrial and medical applications [2-4]. Few applications include the utilization of chemical energy through the active species in surface treatment of thin film deposition [5], microelectronics, sterilization, volume treatment of waste decomposition, pollution control and bio-medical applications. Several authors have published their studies about plasma technology in gas mixtures like, Ne-Ar by klomich et al [6] found the solution to the problem of metal surface modification. Similarly, space technology like stationary plasma Hall thrusters use plasma technology for a thrust generation up to 5 N for an operating power going up to 100 kW. Xenon is the most efficient noble gas used from a long time in the Hall thrusters. Studies have mentioned due to its less abundance in nature (87 ppb), the production worldwide is limited to an approximate of 6000 m³ per year [7]. The increase in demand due to its highly efficient nature in these applications has led to the price swings in the past decade as much to a factor of ten. Therefore, this paper focusses on the usefulness of the other economic gases like Argon, Krypton and other mixtures. A simple canonical 1-D and 2-D glow discharge...
problem is considered with the help of commercial software COMSOL Multiphysics Plasma solver. Simulations are made for Xenon and Argon gases to identify its influence on properties like electron density, electric potential and electron temperature.

2. The Glow Discharge Model:

A DC- Glow discharge is built and operated by applying an electric potential difference with low gas pressure of 10-100 Pa between the electrodes that are, anode (high potential) and a cathode (low potential). Applied potential accelerates the free electrons within the neutral gas to the higher potential, that ionizes the neutral gas particles along their path resulting in release of more electrons. The ions produced are accelerated towards the lower potential cathode, where they collide with the electrode acquiring an electron and colliding with the other electrons off the electrode into the plasma.

![Figure 1. A 3-D sketch of the different regions present within a glow discharge with labelled regions. Figure as represented in Livoskiy et al [8].](image)

A qualitative phenomenon is displayed across the discharge tube that helps in the study of the properties of the gas. Regions within a glow discharge are differentiated with the expanse of light they produce and have been the primary feature to distinguish each section during the 19th century, when the discharge glow tubes were first being studied [9]. This difference in the luminosity explains the physical phenomena of each region. Figure 1 shows a DC glow discharge tube with different glow regions visible.

To start with anode the region that comes first is the positive column. It is a region with high electron current and a low ion current. Due to a relatively low electric field, the electrons possess energy to excite the neutral atoms, but some ionization occurs in this region. This region of the column is responsible for the glow in the gas. As we move towards from anode to cathode the region next to positive column is the Faraday dark space. The electrons do not possess sufficient energy in order to ionize neutral particles, and therefore the region appears to be dark.

Negative glow coming after the Faraday dark space possess high electric field which accelerates the electrons, causing avalanche of electrons and ions. The region observes high concentrations of electrons and ions where a large amount of recombination of ions and electrons takes place that in turn is responsible for the light in the region.

A large amount of electrons drift towards the anode region and into the Faraday dark space, that have reduced energy due to the ionizing collisions. The ions created newly now drift towards the cathode and enter the cathode dark space. This region is the area where ions gain reasonable kinetic energy to ionize the neutral particles. Kinetic energy of the ions is quite higher than the excitation energy and hence higher number of ion collisions due to which the region remains dark. [9,10]

Next comes the cathode glow region where cathode is bombarded with ions that recombine with an electron from the surface of the cathode and collapse the neutral atoms to the ground state, emitting light. In each of these different regions, the electric potential and currents of the various species are distinct. The experimental results are analyzed based on the variation in the emitted light whereas simulations are compared based on the variation in parameters like electric potential, electron density and so on.
3. The Mathematical Formulation

The mathematical modelling of plasma is broadly categorized in kinetic model, fluid model and hybrid model [11]. In the case of kinetic model, particles are solved with Boltzmann equation [10], which is computationally time consuming. On the other hand, the fluid model is arrived by taking moment to Boltzmann equation which gives the form identical to Euler equations in fluid flow. There are some limitations of fluid models at low pressures [12]. The fluid approach is considered in this study. The equations for 1-D and 2-D are well reported in the literature. This involves, computation of the electron density and mean electron energy by solving a pair of drift diffusion equations.

3.1 Drift Diffusion Equations

The simplest mathematical model of a DC glow discharge comprises of a balance equation for particle densities (for electrons $n_e$ and positive ions, $n_p$), Poisson’s Equation. The set of drift diffusion equations are solved and are used to compute the electron density and mean electron energy as shown below [13,14],

$$\frac{\partial}{\partial t} (n_e) + \nabla \cdot [-n_e (\mu_e \cdot E) - D_e \cdot \nabla n_e] = R_e$$  (1)

$$\frac{\partial}{\partial t} (n_p) + \nabla \cdot [-n_p (\mu_p \cdot E) - D_p \cdot \nabla n_p] + E \cdot \nabla E = -\nabla \cdot \Gamma_E$$  (2)

$$\Gamma_E = -n_e (\mu_e \cdot E) - D_e \cdot \nabla n_e$$  (3)

The electron source $R_e$ and the energy loss due to inelastic collisions $\Gamma_e$ are defined later. The electron mobility is used to compute electron diffusivity, energy mobility and energy using the below equations,

$$D_e = \mu_e T_e, \quad \mu_e = \left(\frac{5}{3}\right) \mu_e, \quad D_e = \mu_e T_e$$  (4)

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Assuming that $M$ number of reactions contribute to the $P$ number of inelastic electron-neutral collisions and the growth or decay of electron density. Generally, $P \gg M$. The electron source term in terms of rate coefficients, is given by,

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$  (5)

where $x_j$ is the mole fraction of the target species for reaction $j$, $k_j$ is the rate coefficient for reaction $j$ ($\text{m}^3/\text{s}$), and $N_n$ is the total neutral number density ($1/\text{m}^3$). It is a better practice to use the Townsend coefficients instead of rate coefficients to define the reaction rates. A better description of the phenomena in the cathode fall region is better explained with the help of Townsend coefficients. When the Townsend coefficients are used, the electron source term is given by,

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n |\Gamma_e|$$  (6)

where $\alpha_j$ is the Townsend coefficient for reaction $j$ ($\text{m}^2$) and $\Gamma_e$ is the electron flux ($1/(\text{m}^2 \cdot \text{s})$). The stability of the numerical computation is improved with the use of the Townsend coefficients [12,13] when the electron flux is field driven. The electron energy loss is obtained by summing the collisional energy loss over the reaction,

$$R_e = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta \varepsilon_j$$  (7)
where $\Delta \epsilon_j$ is the energy loss from reaction j. The rate coefficients are computed using the cross-section data applying the following integral,

$$
\rho = q \int_0^\infty \epsilon \sigma_k(\epsilon) f(\epsilon) d\epsilon
$$

where $\gamma = (2q/m_e)^{1/2} (C_{1/2}/kg^{1/2})$, $\sigma_k$ is the collision cross section ($m^2$), $m_e$ is the electron mass (kg), $\epsilon$ is energy (V), and $f$ is the electron energy distribution function. In this case a Maxwellian EEDF is assumed. The electron energy loss is,

$$
R_\epsilon = \sum x_j p_j = \alpha_j n_j |\gamma_e| \Delta \epsilon_j
$$

For the non-electron species, mass fraction of each species is computed using the following equation,

$$
\rho = \frac{\partial}{\partial t} w_k - \rho (u \cdot \nabla) w_k = \nabla \cdot j_k + R_k
$$

The following equation is used to compute electrostatic field,

$$
-\nabla \cdot \epsilon_0 \nabla V = \rho
$$

The space charge density $\rho$ is computed using the plasma chemistry specified in the model with the below equation,

$$
\rho = q \sum_{k=1}^N Z_j n_k - n_e
$$

### 3.2 Boundary Conditions

The sustenance of the discharge is due to the emission of secondary electrons from the cathode. When an ion bombards the cathode with a specified probability an electron is emitted from the cathode surface. The emitted electrons are then accelerated by a strong electric field close to the cathode where they acquire enough energy that can initiate ionization. This results in a rapid increase of electron density close to the cathode in a region often known as the cathode fall or Crookes dark space.

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and are gained due to secondary emission effects, resulting in the following boundary condition for the electron flux,

$$
\n \Gamma_e = \left( \frac{1}{2} v_e n_e \right) - \sum_p \gamma_p (\Gamma_p \cdot n) \epsilon_0
$$

and the electron energy flux is given by

$$
\n \Gamma_\epsilon = \left( \frac{1}{2} \epsilon \epsilon_0 \right) - \sum_p \epsilon_p \gamma_p (\Gamma_p \cdot n) \epsilon_0
$$

The second term on the right-hand side of Equation 13 is the gain of electrons due to secondary emission effects, $\gamma_p$ being the secondary emission coefficient. The second term in Equation 14 is the secondary emission energy flux, $\epsilon_p$ being the mean energy of the secondary electrons.
3.3 Plasma Chemistry

The plasma chemistry of Argon and Xenon such as different cross section energies for Elastic, Excitation and Ionization type of reactions are given in table 1 and table 3 respectively. They are also termed as volumetric reactions and apart from them the surface reactions to Argon and Xenon are provided in the table 2 and table 4 respectively. The sticking coefficient specified in the tables describe the probability of a metastable atom reverting to a ground state atom when it comes in contact with the wall.

Table 1. Tables of Collisions and Reaction Modeled for Ar [13,14].

| Reaction | Formula     | Type       | Δε (eV) |
|----------|-------------|------------|---------|
| 1        | e + Ar => e + Ar | Elastic    | 0       |
| 2        | e + Ar = > e + Ar s | Excitation | 11.5    |
| 3        | e + Ar s => e + Ar | Superelastic | -11.5  |
| 4        | e + Ar = > 2e + Ar+ | Ionization | 15.8    |
| 5        | e + Ar s => 2e + Ar+ | Ionization | 4.24    |
| 6        | Ar s + Ar s => e + Ar + Ar s | Penning Ionization | -     |
| 7        | Ar s + Ar => Ar + Ar | Metastable quenching | -     |

Table 2. Tables of Collisions and Reaction Modeled for Ar [13,14]

| Reaction | Formula | Sticking Coefficient |
|----------|---------|----------------------|
| 1        | Ar s => Ar | 1                    |
| 2        | Ar s+ => Ar | 1                    |

Table 3. Tables of Collisions and Reaction Modeled for Xe [15]

| Reaction | Formula     | Type       | Δε(eV) |
|----------|-------------|------------|--------|
| 1        | e + Xe => e + Xe | Elastic    | 4.2    |
| 2        | e + Xe = > e + Xes | Excitation | 8.31   |
| 3        | e + Xes => e + Xe | Superelastic | -8.31  |
| 4        | e + Xe = > 2e + Xe+ | Ionization | 12.13  |
| 5        | e + Xes => 2e + Xe+ | Ionization | 3.8    |
| 6        | Xes+ Xes => e + Xe +Xe+ | Penning Ionization | -     |
| 7        | Xes + Xe => Xe + Xe | Metastable quenching | -     |

Table 4. Tables of Collisions and Reaction Modeled for Xe

| Reaction | Formula | Sticking Coefficient |
|----------|---------|----------------------|
| 1        | Xes => Xe | 1                    |
| 2        | Xe+ => Xe | 1                    |
The 1-D and 2-D simulation for Argon is very well reported in COMSOL plasma simulation module.

4. Simulation, Results and Discussion

Simulations were performed on 1-D and 2-D DC glow discharge tubes using COMSOL Multiphysics Plasma module with necessary data extracted from LXCAT [15]. The analysis is based on the comparison of parameters like electron density, electric potential and electron temperature of the two gases Argon and Xenon.

4.1 1-D DC glow discharge of Argon and Xenon

The variation of electron density, electric potential and electron temperature for Argon and Xenon are considered in this study on a 1-D DC discharge column of 0.36 m with a low gas pressure of 13 Pa. The cross-section energies for different gas reactions of the Argon and Xenon are imported from LXCAT [15].

Figure 2 (a) and 2(b) show the plot of electron density of Argon and Xenon respectively against the length of the column 0 m (Cathode) to 0.36 m (Anode) and it is observed that the electron density peaks in the region between the cathode fall and positive column which is the region of negative glow region. The maximum electron density is 1.47 E+15 (1/m$^3$) for xenon which is quite less compared to the electron density of argon which comes to 8.82 E+15 (1/m$^3$) at the same axial length of the column. There is a rapid increase in the electron density close to the cathode due to the acceleration of the secondary electrons released from the cathode are accelerated by a strong electric field.

![Graph of electron density against length of column](image)

(a) Argon  
(b) Xenon

**Figure 2.** Distribution of electron density against the length of the column

The variation of electron temperature against the axial length of the column is plotted for Argon and Xenon in figure 3 (a) and (b) respectively. It shows that the strong electric field in the cathode region can lead to high energy ion bombardment of the cathode. Heating of the cathode surface occurs which may in turn lead to thermal electron emission where additional electrons are emitted from the cathode surface with high drift velocity. The electron temperature for Argon peaks at 12.39 V whereas for Xenon it is 15.44 V at a column length of cathode dark space region where the ions gain energy to bombard with the cathode to release the secondary electrons with high kinetic energy leading to peak in temperature at the region. The peak electron temperature of Xenon is about 3V higher than Argon.
Figure 3. Distribution of electron temperature of against the length of the column

Figure 4 (a) and (b) shows the plot of electric potential of Argon and Xenon against the axial length of the column and it is observed that the electron potential drops from the potential close to 120 V as it comes closer to the Cathode fall region due to high ion density of the ions that are ready to bombard the cathode for the release of secondary electrons.

Figure 4. Distribution of electric Potential against the length of the column

4.2 2-D DC glow discharge of Argon and Xenon

2-D DC discharge tube of 0.05 m width x 0.4 m height as shown in figure 5 under 66 Pa of low pressure is considered with cross section data of Argon and Xenon obtained from LXCAT [15] and the following results were obtained in terms of analysing the electron density, electric potential and electron temperature and the line graphs of the respective quantities are also plotted. The variation of electron density, electric potential and electric temperature are observed along the axial length of the column.
Figure 5. Geometry of 2-D glow discharge tube

Figure 6 (a) and 6 (b) shows the plot of electron density of Argon and Xenon against the length of the column 0 (cathode) to 0.4 (anode) respectively. It is observed that the electron density peaks to 1.18 E+16 (1/m$^3$) for Argon and 3.84 E+16 (1/m$^3$) for Xenon which falls in the region between faraday dark space and the cathode glow region that is called the negative glow space where most of the electrons are accelerated toward the anode region. The electrons accelerate with high mean electron energies from the cathode region due to the strong electric field at this region. Further, there is decrease in the electron density at the Faraday dark space to the positive column where most of the electrons ionize the incoming gas particles. Due to the low ionization potential of Xenon, the plot shows a small difference in the densities of Xenon and Argon.

Figure 6. Plot of electron density at the centre of the tube, against the axial length of the discharge channel

Figure 7 (a) and 7 (b) are the electron temperature plots of Argon and Xenon respectively. The electron temperature at the cathode glow region is much higher due to the reason that a lot of electrons released from the cathode gain enough mean electron energy and possess high kinetic energy and get accelerated towards the positive column. The peak in electron temperature of Xenon (18 V) is higher to the peak in electron temperature of Argon (10 V) due to the fact that the electron temperature is dependent on the number of inelastic collisions taking place which is high for Xenon due to its low ionization potential that tends to ionize and excite the gas at an earlier stage in the column. Further decrease in the electron temperature occurs due to the gradual start of recombination of the electrons with the gas particles away from the cathode glow region into cathode fall to the Faraday dark space. The peak electron temperature of Xenon is about 8V higher than Argon.
Figure 7. Distribution of electron temperature at the centre of the tube, against the axial length of the discharge

Figure 8 (a) and 8 (b) shows the Distribution of electric potential of Argon and Xenon against the length of the column and it is observed that the electron potential drops at the cathode fall region majorly because the high electric field in the region where the ion concentration near the cathode is much higher than the electrons. The peak in the potential shows the accumulation of charged particles that are mostly ions. There is a slight difference in the maximum potential of the gases due to the difference in ion densities of Xenon and Argon in the region.

Figure 8. Distribution of electric potential at the centre of the tube, against the axial length of the discharge

4.2.1 2-D Axial symmetrical Surface Distributions of DC glow discharge

Figure 9 (a) and (b), Figure 10 (a) and (b) and Figure 11 (a) and (b) show the electron density, electron temperature and electric potential distributions of Argon and Xenon axial symmetrical surface model of DC glow discharge tube in 2-D respectively.

The electron density as per the figure shows different values axially and is observed to be more at the region between cathode glow region and the positive column. The electron density also decreases rapidly
in the radial direction. This is caused by diffusive loss of electrons to the outer walls of the column where they accumulate a surface charge. The build-up of negative charge leads to a positive potential in the centre of the column with respect to the walls.

**Figure 9.** Distribution of electric density at the centre of the tube, against the axial length of the discharge

**Figure 10.** Distribution of electron temperature at the centre of the tube, against the axial length of the discharge

The Electron temperature is seen to be more at either sides of the cathode glow region in terms of Xenon. Whereas for Argon, it is observed to be radially spreading across in the cathode glow region.
Figure 11. Distribution of electric potential at the centre of the tube, against the axial length of the discharge.

Electric Potential is almost similar in case of both the gases with a gradual drop in potential near the cathode fall region.

5. Conclusions:

Numerical simulations are performed with the help of COMSOL software to study the influence of Argon and Xenon gases in DC glow discharge problem. It solves a pair of drift diffusion equations for electron density and mean electron energy, along with species equation and equation for electrostatic field. The model parameters and reaction terms are used from the literature. The 1-D and 2-D simulation for Argon is very well reported in COMSOL plasma simulation module. By considering Argon and Xenon, it has shown similar trend in electron density, electron temperature and electric potential with less variation. However, the magnitude of electron density is slightly higher for Argon compared to Xenon at a lower pressure of 13 Pa in 1-D Glow discharge. The 2-D simulation with 66 Pa pressure has also shown a similar trend with slight difference in electron density of Argon and Xenon due to the diffusive nature in the lateral direction. The electron density of Xenon is slightly larger compared to Argon in 2-D glow discharge. The electric potential shows no much difference for both the gases in 1-D and 2-D. The electron temperature of Xenon is about 3 V and 8 V higher than Argon in 1-D and 2-D glow discharge respectively. Future analysis will be taken to identify the sensitivity of model parameters and its influence. Mixture of Argon and Xenon will be considered.

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