زانكۆی سەلاحەددین - هەولێر
Salahaddin University-Erbil

Determination of Distribution Functions and swarm parameter in N_2-CO gas mixtures using cross section Data and Boltzmann Transport Equation

Research Project
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بسم الله الرحمن الرحيم

لما بلغ أشده آتيناه

حكماً وعلماً

وكذلك نجزي

المحسنين

76 سورة يوسف اآلية

DECLARATION

I declare that the BSc. project entitled: **Determination of distribution Function and swarm parameter in N2-CO gas mixtures using cross section data and Boltzmann transport equation**, is my own original work, and hereby certify that unless stated, all work contained within this thesis is my own independent research and has not been submitted for the award of any other degree at any institution, except where due acknowledgment is made in the text.

Student Name: Elaf Bahjat Ismael

Signature:

Date: April-2024

DEDICATION

This thesis is dedicated to:
Allah Almighty, my Creator and my Master,
My great teacher and messenger, Mohammed (May Allah bless and grant him), who taught us the purpose of life,
My homeland Kurdistan, the warmest womb,
The University of Salahaddin-Erbil; my second magnificent home; my great parents, who never stop giving of themselves in countless ways,
My beloved brothers and sisters;
To all my family, the symbol of love and giving,
My friends who encourage and support me,
All the people in my life who touch my heart.

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Summary

Plasma is described as an electrically neutral medium of unbound positive and negative particles. It is important to note that although they are unbound, these particles are not 'free'. When the charges move, they generate electric current with magnetic fields, and as a result, they are affected by each other's fields.

Theoretical calculations are performed on the electron swarm parameter (i.e. Drift Velocity) and electron energy distribution function (EEDF) in N_2/CO gas mixtures by using the two-term approximation of the distribution in Boltzmann equation within the international computer code Boltz.

A set of electron cross-section data have been used in this calculation.

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ABBREVIATIONS

Abbreviation	Details
V_d	Drift velocity
N	Total number density
Σ_m	Momentum transfer cross-section
K	Boltzmann Constant
T	Temperature
EEDF	Electron energy distribution function
CFDL	Current-free double layer
V	Electron velocity
E	Electric field
∇_v	Velocity-gradient
t	Time
ε	The electron mean energy
eV	Electron volt
σ_m	Momentum transfer-cross-section for elastic collision of electron
P	pressure
E/N	Electric Field to the gas density

Chapter One
Introduction

Plasma is one of the four fundamental states of matter, along with solid, liquid, and gas it is a state of matter in which an ionized substance becomes highly electrically conductive to the point that long-range electric and magnetic fields dominate its behavior.

Plasma is typically an electrically quasimetric medium of unbound positive and negative particles, meaning that the overall charge of plasma is roughly zero; however, these particles are not "free" in the sense of not experiencing forces.

Moving charged particles generate electric currents, and any movement of a charged plasma particle affects and is affected by the fields created by the other charges, which governs collective behavior with many degrees of variation.

Plasma can appear in nature in various forms and locations, including artificially produced, terrestrial, space, and astrophysical plasmas.

Nearly all the visible matter in the universe exists in the plasma state, occurring predominantly in this form in the Sun and stars and in interplanetary and interstellar space. (Andrey Starikovskiy.2015).

Plasma science and technology are studied by the vast academic field of plasma science or plasma physics, including several sub-disciplines such as space plasma physics. It has many applications, including electric lamps, lasers, medical devices, energy converters, water purifiers, and flat-panel video displays.

The study of energy distribution of electrons in weakly ionized gases has a long history and become increasingly important for the quantitative understanding of gas discharges plasma physics, laser physics… etc.

The electron distribution function can be computed for typical electric discharge conditions by solving numerically the Boltzmann equation for especially uniform steady state, with knowledge of the elastic and inelastic electron-molecular cross-section

A fundamental assumption is that the large number of atoms or molecules making up the gas is in a continuous state of random motion that is intimately dependent on their temperature. As they move, the gas particles collide with each other as well as with the walls of the confining vessel. Just how many molecule–molecule or molecule–wall impacts occur depends on the concentration or pressure of the gas. (Kazunori Takahashi….*etal*,2011).

In the perfect or ideal gas approximation there are no attractive or repulsive forces between molecules. Rather, they may be considered to behave like independent elastic spheres separated from each other by distances that are large compared to their size.

Boltzmann distribution is a probability function used in statistical physics to characterize state of a system of particles, with respect to temperature and energy.

The distribution function can be specialized with respect to a particular set of dimensions, such as the momentum distribution, which gives the number of particles in the momentum phase space having approximately the momentum.

A Boltzmann approximation analysis for electrons in nitrogen and Carbon monoxide mixture under an electric field were intending for determination of the electron collision cross section (Edward V. Rostomyan,2019).

In molecular kinetic theory, the distribution function can be used to solve the self-consistent problem of the mutual influence of N_2CO molecular gases.

In addition, the electron energy distribution function can be obtained for electrically excited N_2, CO, CO_2, and their mixtures by numerically solving the self-consistent Boltzmann equation.

In summary, the distribution function of N_2CO in physics is a function that gives the number of particles per unit volume in single-particle phase space. It can be used to solve the self-consistent problem of the mutual influence of N_2CO-type molecular gases in molecular kinetic theory. The distribution function can be specialized with respect to a particular set of dimensions, such as the momentum distribution. Particle distribution functions are often used in plasma physics to describe wave-particle interactions and velocity-space instabilities.

The role of electron swarm parameter (drift velocity) is an important one because it provides a link between electron-gas collision cross-section and gas breakdown and discharge phenomena. Once the validity of this parameter is assured that may be used to explain pre-breakdown and breakdown phenomena as well as providing some information for understanding of discharges. (M.Benhenni…*etal*, 2009).

Drift velocity is the average velocity attained by charged particles, such as electrons, in a material due to an electric field, or it is the net velocity at which electrons drift in one direction when subjected to an electric field

The evolution of electron swarms in gases has been studied as a fundamental approach of the engineering of weakly ionized plasma. Typically, the primary purpose of investigation of electron swarms are analysis of essential features of electron swarm behavior and the derivation of qualitative data conserving the electron transport coefficients.

N_2 and CO are important component gases of the CO laser, which is one of the most efficient gas lasers. The two are almost identical in molecular mass, equilibrium nuclear distance, dissociation energy and fundamental vibrational constants. The momentum transfer cross-section are also alike (Gulala.M.F, 2000).

The net result of the continual elastic collisions and exchange of kinetic energy is that a steady-state distribution of molecular velocities emerges given by the celebrated Maxwell–Boltzmann formula.

Chapter Two
Theory

A deep investigation and a more accurate knowledge of the electron distribution function is required for a proper understanding of various phenomena occurring in plasma, especially for those physical situations in which that distribution deviates appreciably from a Maxwillian.

1-Maxwell Distribution Function

The Maxwell distribution function is a probability distribution that describes the distribution of speeds of particles in a gas.

It is given by the equation $f(v) = \left(\frac{m}{2\pi KT}\right)^{\frac{3}{2}} * 4\pi v^2 * \exp\left(-\frac{mv^2}{2KT}\right)$, where m is the mass of the particle, k is the Boltzmann constant, T is the temperature of the gas, and v is the speed of the particle The distribution function is normalized such that the integral of, f(v) over all possible velocities is equal to 1.

The Maxwell distribution function is used in molecular dynamics simulations to initialize the velocities of particles. (Mohammad M. Othman, Saeed Rasoll Hussein,2020).

2-Boltzmann Distribution function

The Boltzmann distribution function, which describes the distribution of energies of particles in a gas.

Boltzmann distribution function The Boltzmann distribution function is a probability distribution that describes the distribution of energies of particles in a gas.

It is given by the equation $P(E) = \left(\frac{1}{Z}\right) * \exp\left(-\frac{E}{kT}\right)$

Where P(E) is the probability of finding a particle in a state with energy E, Z is the partition function, k is the Boltzmann constant, T is the temperature of the gas, and exp is the exponential function.

The partition function is given by $Z = \Sigma \exp\left(-\frac{Ei}{kT}\right)$, where the sum is taken over all possible energy states of the particles.

The Boltzmann distribution function is used to calculate the probability of finding a particle in a particular energy state, and it is used in statistical mechanics to calculate thermodynamic properties of a system.

The distribution function can be derived from the principle of maximum entropy, which states that the probability distribution that best represents the state of a system is the one that maximizes the entropy of the system. (Ibrahim KaittanFayyadh…. *etal* .2019)

3-MaxweII-Boltzmann Distribution

The widely used distribution function is the Maxwell-Boltzmann distribution function, which describes the equilibrium state that can be used in non-equilibrium situations as an approximation. This is because the system may be only slightly deviated from equilibrium and hence these of the Maxwell-Boltzmann distribution as first approximation. The exact distribution function of the system may be very difficult to determine and for this reason, the most common solutions for Boltzmann equation are approximate solution.

The system, in which the motion of the particles is perfectly random, can be described by the Maxwell-Boltzmann distribution function because it is impossible to reach thermal equilibrium even at ideal case .in this case effect of the particle interactions is to produce the random character of the system and this type of interaction does not affect the resultant equilibrium statistics (Alexander.A.S, 2020).in case where interaction particles are electrons, which interact with a gas in the presence of direct current electric filed, the system of electrons can be described by the Druyvesteyn distribution function.

The interacting particles behave like hard spheres and their interaction is described by the collision cross section which is a measure of the probability of an electron-gas atom collision. The Druyvesteyn distribution function drops off very faster at high kinetic; than the Maxwell-Boltzmann does. This means that there are few particles at high energy in a system which can be described by the Druyvesteyn distribution function than there are in the Maxwell-Boltzmann system (Kazunori.T....*etal*, 2011).

4-Druyvestun Distribution Function

The Druyvesteyn distribution function is a way to describe the electron energy distribution function (EEDF) in plasmas.
It is an extension of the Langmuir and Mott-Smith probe theory that allows the determination of the electron energy spectrum.
The Druyvesteyn formula is used to fit the EEDF data.

The Druyvesteyn-like distribution tends to a Maxwellian distribution and it is used to describe the bounded plasma, and the complex permittivity for the plasma with Druyvesteyn distribution is calculated. The Druyvesteyn theory is also used to study the electron energy distributions upstream of a current-free double layer (CFDL) contained. (N.A Dyatko,….*etal*1991).

Collision

Collisions occur when one object strikes another. Problems involving collisions are usually solved using conservation of momentum and conservation of energy.

Types of collisions

Types of collisions a collision is said to have taken place between two particles when any physical change can be detected after the distance between the two particles has first been decreased and then increased.

The probability that a given type of collision (reaction) will occur under given conditions is usually expressed in terms of a collision cross section. The collisions of electrons with atoms and molecules can be divided into three classes: elastic, inelastic, and super elastic

1- Elastic Collision

This is a collision where the total kinetic energy of the system is the same before and after the collision. Both momentum and kinetic energy are conserved in this type of collision.

2-Inelasic Collision

This is a collision where the total kinetic energy of the system is not conserved. Momentum is still conserved, but some of the kinetic energy is converted into other forms of energy, such as heat or sound. There are two types of inelastic collisions.

Partially inelastic and completely inelastic. In a partially inelastic collision, the objects separate after they collide, but are deformed in some way.

In a completely inelastic collision, the objects stick together after colliding

3-Superelastic Collision

This is a type of collision where the kinetic energy after the collision is greater than the kinetic energy before the collision. (N.A Dyatko....*etal*.1991)

Theory

Boltzmann equation

The behavior of electron interaction with gas molecules is governed by the distribution in space, energy and time of electrons in the pure gas or in a mixture of gases. The distribution function obeys a continuity equation which is known as the Boltzmann transport equation.

The general form of the Boltzmann equation is (W.L. Morgan,1995):

$$\left(\frac{\partial}{\partial t}+V.\nabla r-\frac{eE}{m}.\nabla_V\right)f(r,v,t)=\left(\frac{\delta}{\delta t}\right)_{coll.} \text{..........................(1)}$$

Where (f) is the electron velocity distribution function (EEDF), (V) the electron velocity, (∇_r) is the special gradient in r-dimension, while(e/m) is the ratio of electron charge to its mass which is refers to the acceleration due to applied electric field (E) (V.cm-1) and (∇_V) is the velocity-gradient operator. The term on the right-hand side of equation (1) is the collision integral, which accounts for electron energy transferred in elastic and inelastic collisions.

It is well known that the swarm parameters of electrons and collision cross-sections with molecules are related to each other through the medium of the velocity distribution function of the swarm. Therefore, the ionization coefficient can be calculated from. (Gulala. M.F ,2002)

Transport parameter

Electron-transport parameters in gases have long been studied and proved to be indispensable in determining appropriate cross sections of elastic and inelastic collisions between gases and slow electrons and the most transport parameter is the drift velocity.

The Drift Velocity

When electrons move through a gas in a uniform electric field E, their movement at moderate E is akin to that of a swarm of bees. Electrons in a swarm have a velocity distribution, move in random directions and have a small component of velocity. The drift velocity v_d is paralleled to the field direction. The essential difference between electron and ion swarms is the mass ratio and the possibility of charge exchange. Even in relativity moderate electric field the average energy, which an electron picks up along a mean free path, is large compared with the mean energy of the gas molecules ($eE\lambda_e > KT_g$ and $T_e >> T_g$) and therefore they acquire a random velocity v_e, which is considerably above that of v_d. This means that the mean collision time t depends on the energy gain $eE\lambda_e$ over a mean free path. Hence, a rise in $eE\lambda_e$ and T_e is the main cause of the rapid fall in electron mobility with increasing field per unit gas pressure, E/N. the electron drift velocity in larger.

For energies in the electron volt range, the electron passes by the molecule much too fast to allow sufficient energy transfer, and thus the electron must be temporarily bounded to the molecule in order to satisfy.

The drift velocity of electrons is calculated numerically as: -

$$V_d = -\frac{E}{3}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty \frac{\varepsilon}{N\sigma_m}\frac{\partial f(\varepsilon)}{\partial \varepsilon}d\varepsilon \text{ -------------- (2)}$$

Where E is electric field, (ε) is the electron energy in (eV), and (σ_m) is the momentum transfer cross-section for elastic collision of electron. (Gulala.M.F, 2002)

Chapter Three
Result and Discussion
Numerical solution method:

Equation (1) was solved numerically by iteration method omitting the details of this method usually, while solving the Boltzmann equation numerically a uniform grid in energy space is used.

According to the experimental data (V.Yu.Bazhenov…*et al*, 2001) the effective electron temperature Te is 0.3eV, the pressure P=0.2 torr.

In order to calculate the EEDF accurately, it is necessary to use a large number of grids point to make the energy interval Δu small with respect to Te.

Mixtures of Nitrogen and Carbon monoxide (N_2-CO) gas are taken as a symbol to calculate the electron energy distribution function with two different concentrations.

Two types of cross section are used for the analysis and these represent momentum transfer cross –section and ionization cross –sections these cross –section data are used as input data, therefore, Eq (1) was solved numerically for a wide range of E/N value were chosen to yield mean electron energies in the range (0.65-3.5) eV.

The calculate distribution function in N_2 –CO gas mixtures as a function is shown in fig (3.1) while fig (3.2) is representing the value of drift velocity as a function of E/N value in N_2-CO gas mixtures two different concentration.

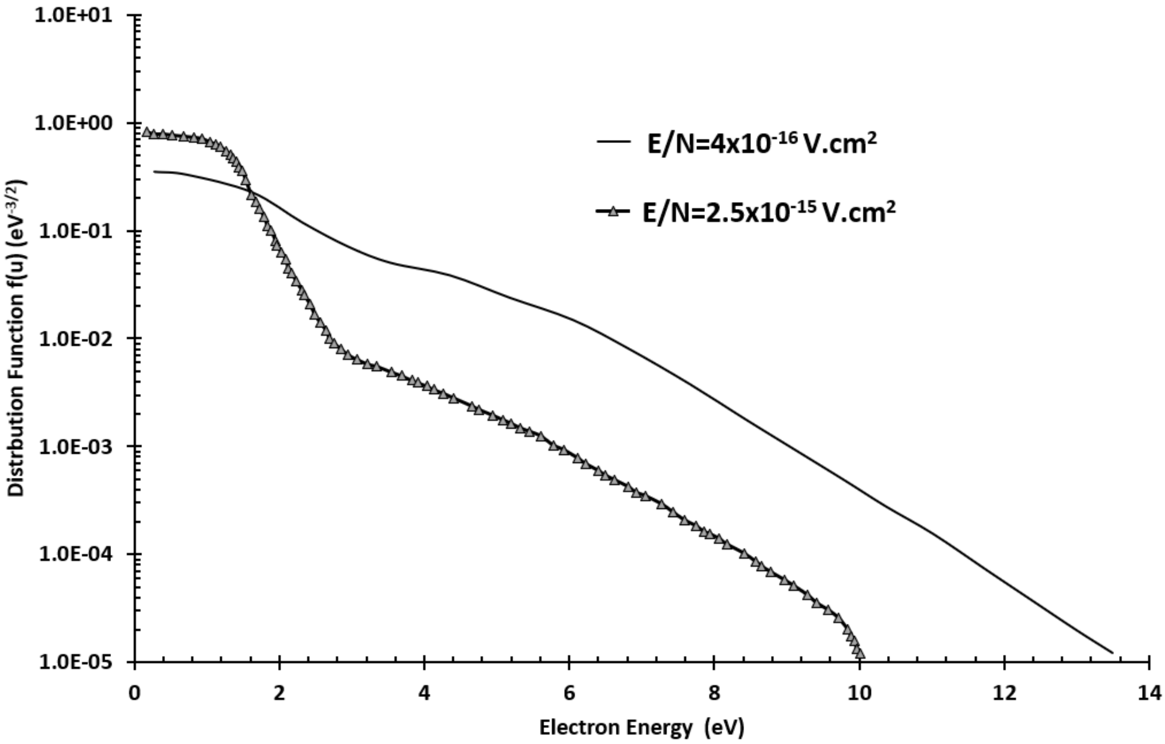

Figure (3.1): The Distribution Function as a function Electron Energy in N_2- CO gas mixtures for two different values of E/N.

In figure 3.1, the EEDF is strongly affected by changing the value of E/N and it can be note that the EEDF with (E/N=4×10^{-16} V.cm^2) had longer tail equal to (13.6eV) than the EEDF with (E/N=2.5×10^{-15}V.cm^2) which had tail equal to (10 eV).

In a matter of fact, calculation of the electron energy distribution function in N_2-CO gas mixtures have shown that the distribution is highly non-Maxwellian because the EEDF is decreased when E/N decreased which means that for higher value of E/N the EEDF shown an increase in its values.

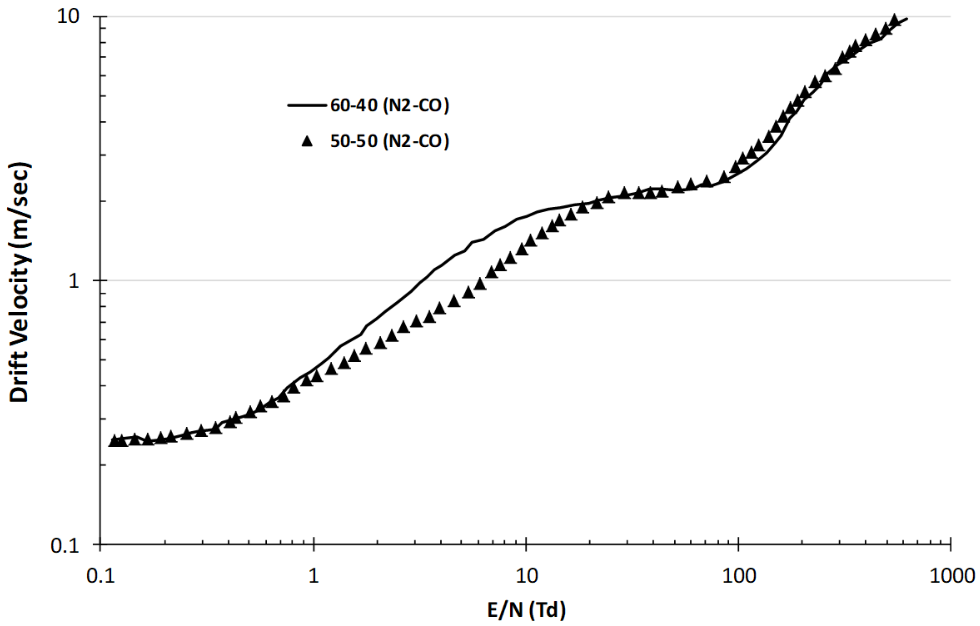

Figure (3.2): The Drift Velocity as a function of E/N values for N_2- CO for two different concentrations.

Electron is ordinary case have an ordinary movement which is called a thermal motion, but with increase E/N value the speed of electron will increase too and this will lead to another kind of motion named as drift velocity.

Fig (3.1) explains the effect of changing each gas concentration on the electron drift velocity for different mixing ratios, the computations between the two different concentrations are very sensitive to the magnitude and one can directly show the likely linear increase in the electron drift velocity for each mixing ratio.

Chapter four
Conclusion

The numerical solution of the Boltzmann equation in a-two-term spherical harmonic approximation using the numerical Boltz code and a set of cross sections for pure N_2 and CO gas mixtures have been used to investigate the behavior of the Electron energy distribution function and the electron swarm parameter (i.e. the drift velocity).

Generally, the accuracy of the calculations depends on the accuracy of the electron –molecule cross-section sets.

Calculation of the (EEDF) for discharge processes for N_2-CO gas mixtures with two different values of E/N have shown that the distribution function is highly non-Maxwellian.

It is observed that, mixing pure nitrogen and with carbon monoxide makes the electron to excite nitrogen atoms up to electronic levels at less E/N values.

On the other hand, the process of mixing N_2 -CO, causes a decrease in E/N value at the occurrence of the ionization state take place for nitrogen atoms, this is observed with the decrease of nitrogen and increase of carbon dioxide concentrations.

Finally, it can be interpreted that practically no one of the collision processes are neglected and also all the energy range are involved. Therefore, it needs to use different types of cross sections from many sets of published tables (as: electronic excitations, vibrations) In order to minimize the shift or the difference between the output values theoretically.

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نەخشەی دابەشبوونی ووزەی ئەلکترۆن و پارامیتەرەکانی گوژمە ئەلکترۆن بۆ تێکەڵەی غازی N_2-CO بە بەکارهێنانی پانە برگە ی گازە کان و هاوکێشەی بۆڵتزمان

تێزێکە
پێشکەشی ئەنجومەنی کۆلێژی پەروەردە کراوە لە زانکۆی سەلاحەدین-هەولێر
وەکو بەشێك لە پێداویستیەکانی بەدەستهێنانی پلەی بەکالۆریۆس لە فیزیك

لە لایەن
ئیلاف بهجت اسماعیل

بە سەرپەرشتی
پ .ی.م.گوڵاڵە محمد فرج

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