

GLIDING ARC DISCHARGE MODEL IN EJECTOR FLOW

Table of Contents

Problem Statement	3
Power Supply Configuration.....	3
Resonance Parameter Calculation	4
Discharge Model	9
Influence of Water Droplets	10
Concentration of Water Droplets and Medium Velocity	10
Absorption of Electrons and Ions by Water Droplets	11
Elastic Scattering by Water Droplets	13
Collision Integral.....	13
Ionization	14
Attachment.....	15
Elastic scattering.....	15
Elastic scattering.....	16
Electron-Ion Recombination	16
Plasma-Fluid and Drift-Diffusion Approximation.....	16
First momentum – the mass conservation law	17
Second momentum – the conservation of momentum law	17
Third momentum – the energy conservation law	18
Final Equations	18
Electrons:.....	19
Positive ions i^+ :.....	19
Negative ions i^- :	19
Analysis of reaction cross-sections	20
Boundary conditions.....	24
Field enhancement at the conductor boundary	24
Secondary electron emission	24
Formal boundary conditions	25
Final equations for numerical solution	26
Vectorization of equations for heavy particles	26
Final vectorized equations	28
Numerical solution.....	30
Finite difference scheme	30
Reaction database and input matrix calculations.....	30
Code optimization and parallelization.....	30
How to use code	30

Problem Statement

We are developing a two-dimensional model of a low-temperature gas discharge powered by a resonant H-bridge.

Several key assumptions are made for this model:

1. The potential difference between the electrodes changes significantly more slowly than the characteristic time for a substantial change in electron energy.
2. The characteristic spatial scale of field variation is much larger than the mean free path of an electron (except within the cathode layer).

These assumptions allow us to assert that the electron energy distribution function depends on the local electromagnetic field, and thus we can employ the drift-diffusion approximation. While this approximation is not valid within the cathode layer, it is fully applicable in the rest of the spatial domain.

The task is reduced to solving the plasma hydrodynamic equations along with Poisson's equation, subject to given boundary conditions.

In the literature on gas discharge modeling, researchers often focus on one specific aspect—either solving the Boltzmann equations under certain approximations or studying and approximating the voltage-current characteristics of the discharge. This specialization, while useful for advancing particular areas of study, often creates a disconnect between the fundamental physics and the practical implementation of discharge systems.

For an engineer or a researcher working on practical solutions, bridging these two domains can be challenging. Understanding how to integrate both the fundamental theoretical aspects and the applied electrical characteristics is crucial for effective system design. In this document, we aim to guide the reader through the complete process of designing and calculating a discharge chamber from the ground up. We will break down each stage step-by-step, from designing and calculating the power circuit to directly modeling the gas discharge itself.

Our goal is to provide a holistic view that connects the theoretical underpinnings with practical engineering decisions, offering an accessible pathway for those looking to combine both aspects in their work.

Power Supply Configuration

The model assumes a power supply based on a resonant H-bridge circuit (an equivalent circuit is provided [here](#)).

From a modeling perspective, it is more convenient to work with the T-equivalent circuit of the transformer rather than the transformer itself. The equivalent circuit is shown in Figure 1.

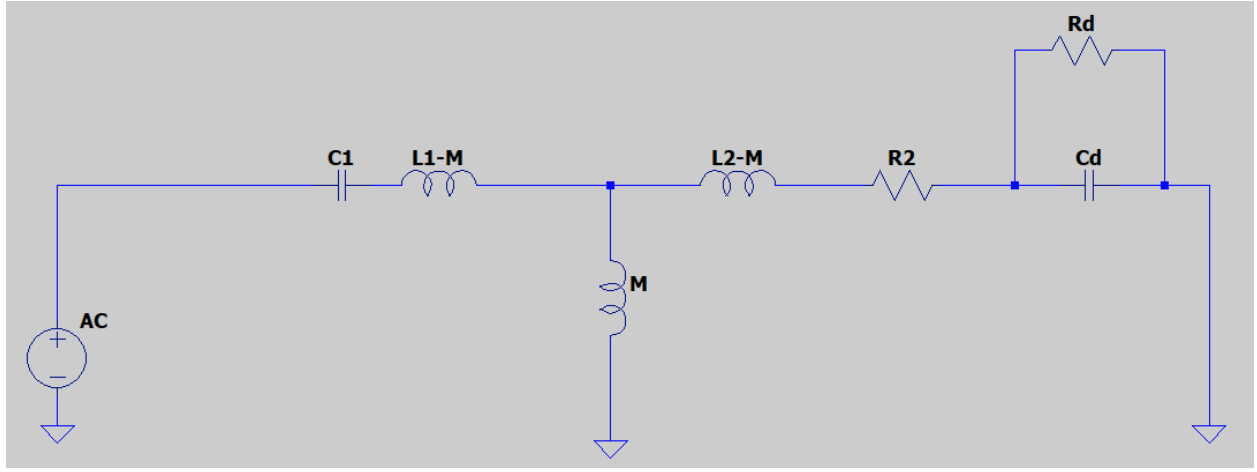


Figure 1. T-equivalent circuit

$M = k\sqrt{L_1 L_2}$ – Mutual inductance, with k – being the coupling coefficient, which depends on the coil design.

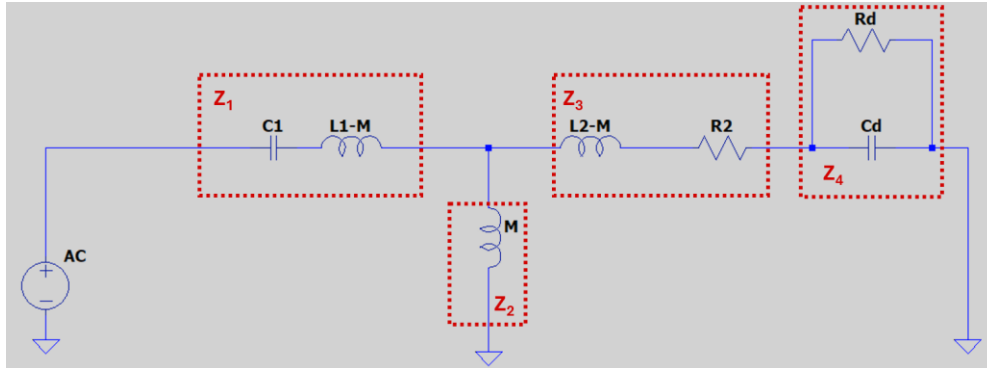
The coupling coefficient, k , is considered known. In practice, for high-voltage high-frequency transformers, values of k around 0.5 to 0.6 can be easily achieved. Example of high-frequency resonant power transformer can be found [here](#).

It is technically extremely challenging to build a high-voltage transformer with a turns ratio in the hundreds or thousands. Therefore, it is more convenient to work with a resonant circuit, which increases the voltage between the electrodes through both resonance and the turns ratio.

Resonance Parameter Calculation

$$\text{Im}(Z) = 0 \quad (1)$$

where Z – complex impedance



$$Z = Z_1 + \frac{Z_2 \cdot (Z_3 + Z_4)}{Z_2 + Z_3 + Z_4}$$

$$Z_1 = -\frac{i}{\omega C_1} + i\omega(L_1 - M)$$

$$Z_2 = i\omega M$$

$$Z_3 = R_2 + i\omega(L_2 - M)$$

$$Z_4 = \frac{-R_d \cdot i / \omega C_d}{R_d - i / \omega C_d}$$

An analytical expression for Z can be derived, but the resulting formulas are quite cumbersome. As can be seen, all parameters are known except for R_d . The resistance of the discharge gap depends on the applied voltage, ranging from infinity (when there is no breakdown) to nearly zero when the discharge transitions to an arc.

To begin, we will analyze the behavior of the circuit under no-load conditions, i.e., in the absence of discharge, where $R_d = \infty$. Our primary interest is the quality factor Q of the resonant circuit, which indicates how much the voltage is amplified at resonance. By knowing Q , we can easily estimate the amplitude of the voltage across the discharge gap U_d .

$$U_d = U_0 \cdot Q \cdot k \cdot N$$

$$\Gamma \text{де } N = \sqrt{\frac{L_2}{L_1}}$$

$$Q = \frac{f}{2} \left| \frac{dZ}{df} \frac{1}{Z} \right|$$

$\omega = 2\pi f$, f – switching frequency of the keys (transistors).

Figure 2 shows the result of the quality factor calculation for the following parameters (I have conducted the initial measurements of the future coil and know its characteristics):

$$C_1 = 50 \text{ nF}$$

$$L_1 = 1.531 \text{ uH}$$

$$L_2 = 1,522 \text{ uH}$$

$$R_2 = 0.12 \text{ Oh}$$

$$C_d = 1.6 \text{ pF}$$

$$R_d = \infty \text{ Oh}$$

$$k = 0.5$$

It is customary to express the quality factor in decibels.

$$Q [\text{db}] = 20 \cdot \log_{10} Q$$

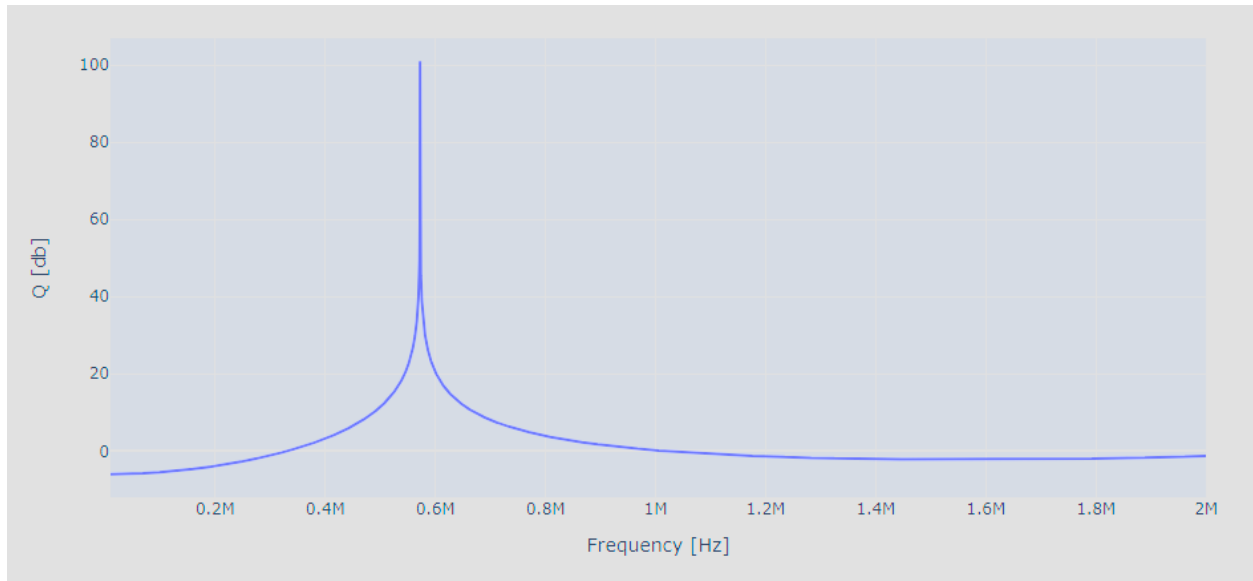


Fig 2. Quality factor modeling.

The resonant frequencies for the given discharge chamber and coil parameters can be controlled using the balancing capacitor C_1 . By adjusting C_1 it is possible to shift the resonant frequencies to the left or right.

Next, let's examine how R_d affects the behavior of the circuit. Suppose we are operating at the first resonant frequency $f_1 = 572$ kHz. We will analyze how the quality factor depends on R_d .

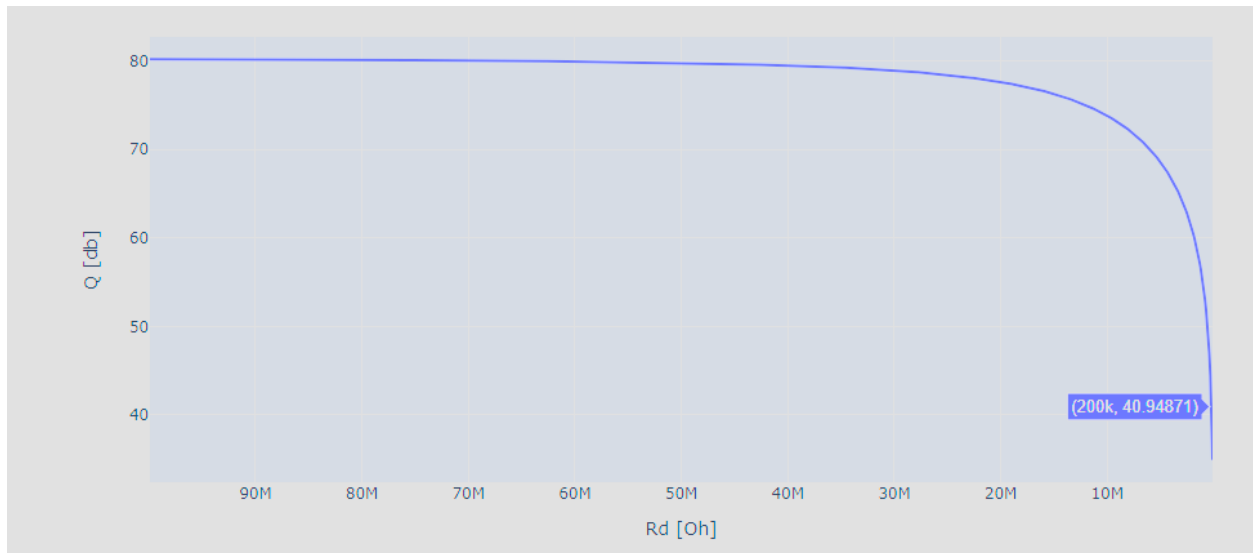


Fig 3. The dependence of the quality factor at the first resonant frequency on the resistance of the discharge gap.

As can be seen, the quality factor starts to drop significantly only when the resistance is below 10 M Ω , and, for example, at a resistance of ~ 200 k Ω , it reaches approximately 40 dB (which corresponds to a voltage amplification of ~ 100 times).

Now, let's try to determine the steady-state active voltage across the discharge gap.

A typical voltage-current characteristic of the gas discharge is shown in Figure 4.

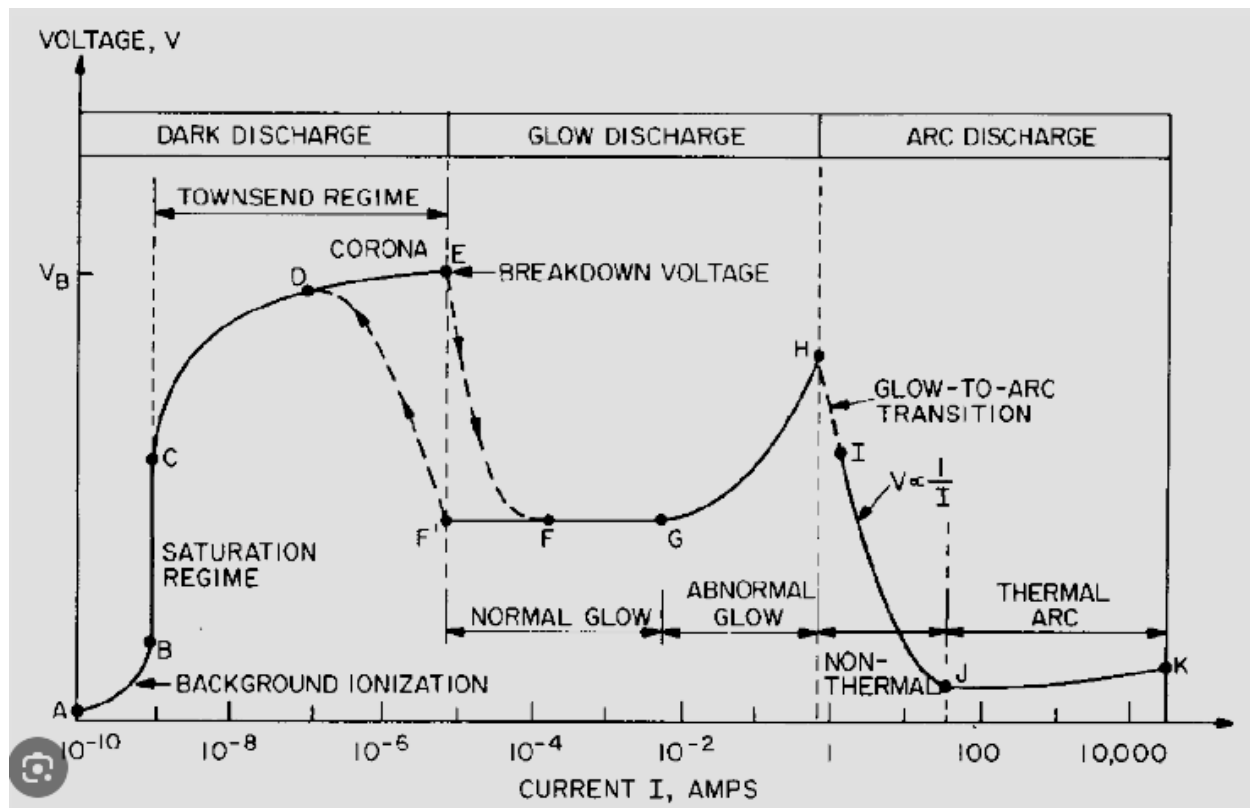


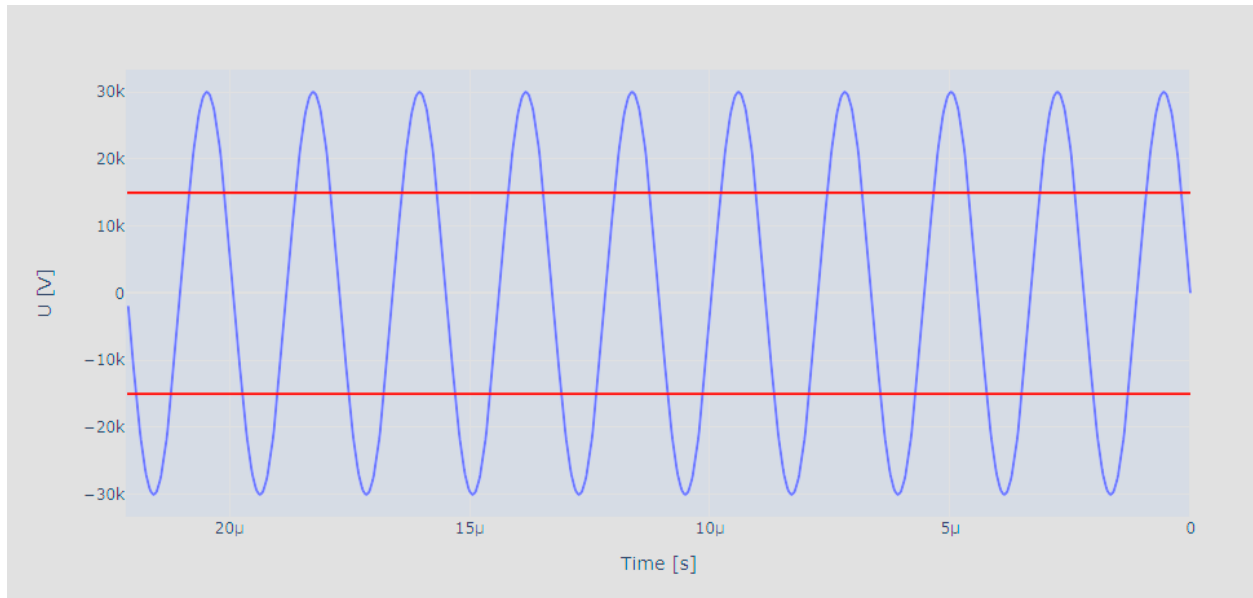
Figure 4. Qualitative voltage-current characteristic of the gas discharge

At low voltage, the current through the discharge gap is zero. As the breakdown voltage is reached (triggering the electron avalanche), a corona discharge ignites first, which then transitions to a glow discharge, and eventually to an arc. At this point, the resistance drops to very low values, and the discharge can be maintained with relatively low external voltage. This occurs when an arc forms in a localized area, making further spatial propagation of the discharge impossible, as it stabilizes in this narrow spatial zone, and resonant processes are no longer needed to sustain it.

We see that it is not necessary to apply a voltage between the electrodes much higher than the breakdown voltage. This is a crucial observation, as once the breakdown voltage is reached, all the power from the source is used to increase the current (i.e., to sustain and grow the electron avalanche).

In other words, we should maintain the voltage between the electrodes close to the breakdown voltage most of the time.

Consider a discharge chamber with a breakdown voltage of about 15 kV. Geometrically, this corresponds to approximately 5 mm between the electrodes (which is roughly typical setup). Since we want the voltage to exceed the breakdown voltage for most of the period, we will set a target amplitude of 30 kV.



Assume that the power of the DC source is known and is approximately 500 watts (again, typical for small experimental setups). Let us also assume that other circuit losses are negligible, and all the power from the source is used to sustain the discharge.

$$P = \frac{U_d^2}{2R_d}$$

Thus, the resistance $R_d \approx 200 \text{ k}\Omega$, and as can be seen from Figure 3, the quality factor remains high even at this resistance, with the current through the discharge gap being approximately 30-40 mA.

In other words, we observe that under power limitation and high breakdown voltage conditions (tens of kilovolts), the discharge behavior does not affect the resonant frequencies, provided that the discharge does not transition to an arc. If the discharge transitions to an arc, high voltage is no longer required to sustain it, and even a detuning from resonance with a drop in voltage to the hundreds of volts range would be sufficient to maintain the arc.

In practice, this means that the DC source amplitude and the geometry of the discharge gap should be chosen such that:

1. The voltage between the electrodes exceeds the breakdown voltage for most of the period.
2. The discharge chamber design prevents the formation of a stable but geometrically small arc.

If both of these conditions are met, the discharge gap will still have a significant resistance, ensuring that it does not affect the resonant processes of the power circuit.

Let's take a moment to reflect on this point. We have significantly simplified the model by removing the feedback loop between the power electronics and the discharge model. We also recognized the importance of preventing the discharge from transitioning to a stable arc, which can be sustained with relatively low power but is, due to its limited geometry, largely useless for our purposes.

Discharge Model

Before proceeding to the plasma equations, it is necessary to formulate the problem and clarify some important parameters.

We are modeling a gliding arc discharge. The overall design of the device is shown in Figure 5.

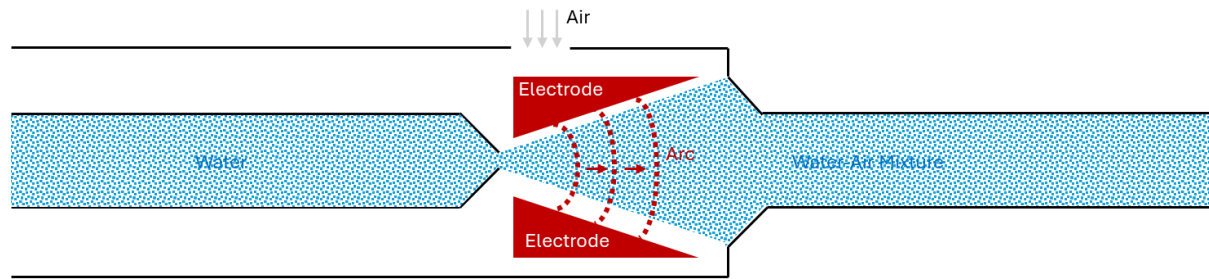


Figure 5. Gliding Arc in Ejector Flow

Water under pressure p_p enters through the ejector nozzle, and due to the narrowing of the nozzle, the water flow velocity increases, creating a region of reduced pressure in the discharge chamber p_n , after which it exits into the external environment at pressure p_c . Due to the pressure difference, air is drawn into the discharge chamber and mixes with the water in a volume ratio of air-to-water ψ . This is a classical water-air ejector setup. All parameters p_p, p_c, p_n, ψ are considered known. For details, see [ejector model](#).

At the nozzle exit, two electrodes are positioned, supplied with power from the circuit described in the previous chapter. The electrodes are designed in a diverging geometry, meaning the distance between them increases as one moves away from the ejector nozzle.

A few words about the gliding arc discharge:

The gliding arc discharge forms in a system of diverging electrodes. The arc ignites at the narrowest point and moves slowly (at a rate comparable to the medium's velocity) into the expansion zone of the gap between the electrodes (i.e., from left to right in Figure 5). At a certain distance, where the field strength is insufficient to sustain the discharge, the arc extinguishes. Thus, the arc seems to glide between the electrodes in the direction of the medium's flow. Importantly, a gliding discharge only occurs in a moving medium. This means that if the medium between the electrodes is stationary, a gliding discharge will not occur, and we will observe a stationary arc at the point of minimum distance between the electrodes. The mechanism behind the arc's gliding behavior is not fully understood, but it likely involves two factors:

1. The moving medium "disrupts" the stationary arc, imparting some velocity to the electrons and ions in the direction of the medium's movement.
2. The electrode geometry creates a potential gradient in the direction of the electrode divergence.

In other words, we are modeling a discharge in a moving medium consisting of oxygen molecules, nitrogen, vapor, and macro-particles (droplets) of liquid water.

Let's consider the main classes of particles:

1. Electrons
2. Positive ions of oxygen, nitrogen, and water
3. Negative ions of oxygen and water, formed through electron attachment reactions
4. Neutral molecules of oxygen, nitrogen, and water
5. Macro-particles of liquid water

There are practical engineering implementations of water spray into the discharge zone. However, it is important to note that the above setup is quite different from typical spraying. We are dealing with a continuous ejector jet, which, at some distance from the nozzle, begins to break into large droplets due to airflow and turbulent effects. Therefore, we have a medium consisting of very humid air and large (0.5-1 mm in diameter) water droplets in the jet.

Points 1-4 are more or less straightforward and are considered in all hydrodynamic plasma models, so we will focus particularly on the macro-particles of water.

Influence of Water Droplets

Consider a water droplet of radius r_d moving at velocity \mathbf{u}_g in a medium with concentrations and average energies of electrons and ions, $n_e, \bar{\epsilon}_e$ and $n_i, \bar{\epsilon}_i$, respectively. Let us analyze the processes of absorption and scattering of charged particles by the droplet.

Concentration of Water Droplets and Medium Velocity

Next, we derive the velocity of the medium and the concentration of water molecules. We assume that the volumetric mixing coefficient of air and water ψ , the saturated vapor pressure p_s , the pressure inside the discharge chamber p_n , and the temperature inside the chamber T , are known.

The mass of water in the discharge chamber is given by $\frac{\rho V}{1+\psi}$, where ρ is the density of water, and is the V volume of the discharge chamber.

On the other hand, the mass of water in the discharge chamber is equal to the sum of the mass of liquid water droplets and the mass of water in vapor form.

$$\frac{\rho V}{1+\psi} = \underbrace{\frac{\widehat{A}_w}{N_A}}_{\text{Mass of water molecule}} \cdot \underbrace{\frac{\widehat{p_s V}}{k_b T}}_{\text{Number of vapor molecules}} + \underbrace{\widehat{N}_d}_{\text{Number of droplets}} \cdot \underbrace{\frac{\widehat{\rho V_d} N_A}{A_w}}_{\text{Number of molecules in one drop}} \cdot \underbrace{\frac{\widehat{A}_w}{N_A}}_{\text{Mass of water molecule}}$$

N_A – Avogadro constant

$$V_d = \frac{4}{3} \pi r_d^3 - \text{water drop volume}$$

From this equation, the concentration of water droplets can be determined.

$$n_d = \frac{N_d}{V} = \frac{1}{V_d(1+\psi)} - \frac{p_s A_w}{N_A k_b T} \frac{1}{\rho V_d} \quad (1)$$

The concentration of vapor molecules is calculated using the ideal gas equation of state.

$$n_s = \frac{p_s}{k_b T} \quad (2)$$

Concentration of oxygen and nitrogen molecules

$$n_{O_2} = 0.21 \cdot \frac{p_n - p_s}{k_b T} \quad (3)$$

$$n_{N_2} = 0.79 \cdot \frac{p_n - p_s}{k_b T} \quad (4)$$

Now, let's consider the overall flow pattern of the jet.

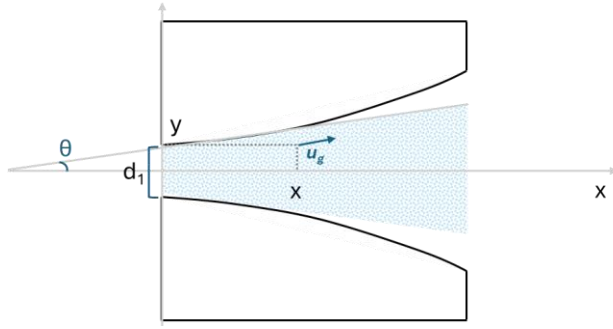


Fig 6. Ejector water flow

[TBD] Provide a particular solution of the Navier-Stokes equation for a free laminar jet.

Absorption of Electrons and Ions by Water Droplets

A droplet absorbs electrons and ions, acquiring a certain charge. The charge cannot be infinite, as a negatively charged droplet, for instance, will begin to repel electrons and attract ions. The equilibrium charge can be estimated by balancing the fluxes of electrons and ions onto the droplet's surface. We will disregard quantum mechanical tunneling effects and consider a classical approximation. Additionally, we assume that the electron energy distribution follows Maxwellian statistics. In a gas discharge, this is generally not true, but for estimating the droplet charge, the Maxwellian assumption provides acceptable accuracy.

Number of electron absorptions of the drop per unit time:

$$\frac{dN_e^d}{dt} = n_e \cdot \bar{v}_e \cdot \pi r_d^2 \cdot \left(1 - \frac{e \cdot \varphi_d}{\bar{\varepsilon}_e}\right) e^{-e \varphi_d / \bar{\varepsilon}_e}, \text{ where } \bar{v}_e = \sqrt{\frac{2 \bar{\varepsilon}_e}{m_e}} - \text{average electron velocity} \quad (5)$$

Let's go through the formula in detail:

$n_e \cdot \bar{v}_e$ the electron flux multiplied by the absorption cross-section $\pi r_d^2 \cdot \left(1 - \frac{e \varphi_d}{\bar{\varepsilon}_e}\right)$, which equals the droplet's surface area multiplied by the probability of overcoming the Coulomb barrier $\left(1 - \frac{e \varphi_d}{\bar{\varepsilon}_e}\right)$. φ_d here, is the potential on the droplet surface, and $e^{-e \varphi_d / \bar{\varepsilon}_e}$ represents the fraction of electrons that have energy greater than the Coulomb barrier.

The number of positive ion absorptions by the droplet per unit time:

$$\frac{dN_i^d}{dt} = n_i \cdot \bar{v}_i \cdot \pi r_d^2 \cdot \left(1 + \frac{e \cdot \varphi_d}{\bar{\varepsilon}_i}\right)$$

Since ions are attracted to the negatively charged droplet, the sign in the coefficient for overcoming the barrier is reversed, and the Maxwellian distribution exponent is absent.

Let us find the equilibrium potential φ_d , assuming quasi-neutral plasma where $n_i = n_e$.

$$\frac{dN_i^d}{dt} = \frac{dN_e^d}{dt}$$

Omitting the mathematical derivation under the assumption that $\bar{\varepsilon}_e \gg \bar{\varepsilon}_i$ and $m_i \gg m_e$:

$$\frac{e\varphi_d}{\bar{\varepsilon}_e} \sim 1 - e \cdot \sqrt{\frac{\bar{\varepsilon}_e}{\bar{\varepsilon}_i}} \Big/ \sqrt{\frac{m_i}{m_e}} \sim 1$$

In other words, the equilibrium potential on the droplet accumulates a very large charge, effectively blocking further electron flux onto the droplet surface due to Coulomb repulsion. Such a result is evident even from simple considerations without requiring mathematical calculations. The average velocity of electrons in non-equilibrium plasma is orders of magnitude higher than that of ions, and therefore, to "balance" the difference in fluxes, the droplet must accumulate a very large charge.

Now, let us estimate how much time is required to reach this equilibrium. Let us return to equation (5).

The potential of the droplet can be expressed in terms of the number of absorbed electrons.

$$\varphi_d = \frac{1}{4\pi\varepsilon_0} \frac{N_e^d e}{r_d}$$

Then

$$\frac{dN_e^d}{dt} = n_e \cdot \bar{v}_e \cdot \pi r_d^2 \cdot \left(1 - \frac{1}{4\pi\varepsilon_0} \frac{N_e^d e^2}{r_d \bar{\varepsilon}_e}\right) e^{-\frac{1}{4\pi\varepsilon_0} \frac{N_e^d e^2}{r_d \bar{\varepsilon}_e}} \quad (6)$$

Integrating equation (6) from 0 to N_e^d (maximum possible charge of the droplet):

$$N_e^d = N_{eq}^d \cdot \zeta, \text{ где } N_{eq}^d = \frac{4\pi\varepsilon_0 r_d \bar{\varepsilon}_e}{e^2}, \zeta = 1 - e \cdot \sqrt{\frac{\bar{\varepsilon}_e}{\bar{\varepsilon}_i}} \Big/ \sqrt{\frac{m_i}{m_e}}$$

We obtain the time required for the droplet to absorb the maximum possible charge.

$$t = \tau_s \int_0^\zeta \frac{e^u}{1-u} du, \tau_s = \frac{1}{n_e \cdot \sqrt{\frac{2\bar{\varepsilon}_e}{m_e}} \cdot \pi r_d^2} \quad (7)$$

Unfortunately, integral (7) can only be solved numerically. To proceed, we will substitute typical energy and concentration values for the gas discharge.

$$\frac{\varepsilon_e}{\varepsilon_i} \sim 50, \varepsilon_e \sim 4 \text{ эВ}, \frac{m_i}{m_e} \sim 60\,000 \text{ (O}_2 \text{ or N}_2 \text{ ions)}, r_d \sim 800 \text{ }\mu\text{m}, \bar{\varepsilon}_e \sim 4 \text{ eV}$$

We obtain $t \sim 10^{-19} \text{ s}$, which means that a water droplet, upon entering the active discharge zone, absorbs a large charge almost instantaneously, and the absorption cross-section of the droplet can be calculated using the formula:

$$\sigma_d^{e-att}(\varepsilon_e, \bar{\varepsilon}_e) \approx \pi r_d^2 \cdot \left[1 - \frac{\bar{\varepsilon}_e}{\varepsilon_e}\right], \varepsilon_e > \bar{\varepsilon}_e \quad (8a)$$

For ions:

$$\sigma_d^{i-att}(\varepsilon_i, \bar{\varepsilon}_e) \approx \pi r_d^2 \cdot \left[1 + \frac{\bar{\varepsilon}_e}{\varepsilon_i}\right] \quad (8b)$$

For ions, we can directly calculate the average absorption frequency by droplets, assuming a Maxwellian distribution function.

$$\nu_d^{i-att} \approx 2 \cdot r_d^2 \cdot \sqrt{\frac{\pi}{k_b T_i m_i}} \cdot \bar{\varepsilon}_e \quad (8c)$$

Elastic Scattering by Water Droplets

Elastic scattering of charges in plasma is derived using Rutherford's formula

$$\sigma_d^{el}(\varepsilon_e) = 4\pi \cdot \left(\frac{N_d^d e^2}{4\pi\epsilon_0 2\varepsilon_e} \right)^2 \ln\Lambda \quad (9)$$

$\ln\Lambda$ here, is the Coulomb logarithm, obtained by integrating Rutherford's formula over scattering angles related to Debye and Coulomb radii. Generally, without going into details, for plasma it can be considered a dimensionless constant approximately equal to 10-12

Substituting the maximum possible charge into (10), we get:

$$\sigma_d^{att} = \pi r_d^2 \left(\frac{\varepsilon_e}{\varepsilon_e} \right)^2 \ln\Lambda \quad (10)$$

Below, we will show that elastic scattering by droplets plays no significant role.

Collision Integral

Important Note: Below, I break down the simplification of the Boltzmann collision integral step-by-step by integrating it over momentums. There is nothing particularly novel or noteworthy here — this is an entirely standard technique described in all plasma physics textbooks. Anyone who has studied plasma physics has almost certainly done this exercise during lectures or seminars. Below, I provide the standard method of simplifying the collision integral for those who want to refresh their knowledge or are unfamiliar with hydrodynamic plasma modeling. You may skip this part and go directly to the final equations in the last section (but if you are not familiar with the plasma-fluid approximation, skipping this section will make it difficult to understand why the equations of motion are formulated as they are).

In general, the particle distribution function in plasma is described by the Boltzmann equation.

$$\frac{\partial f}{\partial t} + \vec{\partial} \nabla f - \frac{e}{m_e} \left[\vec{E} + \frac{\vec{B} \times \vec{\partial}}{c} \right] \nabla f = \left. \frac{\delta f}{\delta t} \right|_{collision} \quad (11)$$

Before simplifying this rather complicated equation, let's take a closer look at the right-hand side $\left. \frac{\delta f}{\delta t} \right|_{collision}$, which is referred to as the collision integral.

In general, the collision integral can be expressed as:

$$\left. \frac{\delta f}{\delta t} \right|_{collision} = \sum_k N \chi_k \int [f(\mathbf{v}') - f(\mathbf{v})] \omega(\mathbf{v} \rightarrow \mathbf{v}') d^3 v'$$

Where N is the total concentration of scattering particles, χ_k is the molar fraction of reactant particles, and is a scalar function $\omega(\mathbf{v} \rightarrow \mathbf{v}')$ representing the probability of transition from state \mathbf{v} to state \mathbf{v}' . The relationship between $\omega(\mathbf{v} \rightarrow \mathbf{v}')$ and the reaction cross-section can be expressed as follows:

$$\omega(\mathbf{v} \rightarrow \mathbf{v}') d^3 v' = v \cdot d\sigma$$

We will also use a simple identity (which can be easily derived by swapping indices during integration).

$$\int \varphi(\mathbf{v}) [\alpha f(\mathbf{v}') - \beta f(\mathbf{v})] \omega(\mathbf{v} \rightarrow \mathbf{v}') d^3 v' d^3 v = \int f(\mathbf{v}) [\alpha \varphi(\mathbf{v}') - \beta \varphi(\mathbf{v})] \omega(\mathbf{v} \rightarrow \mathbf{v}') d^3 v' d^3 v \quad (12)$$

Where α, β are some numbers and $\varphi(\mathbf{v})$ is a scalar function.

Now, let's return to our problem and consider all possible reactions:

- Ionization
- Attachment
- Elastic scattering
- Inelastic scattering (excitation, dissociation)
- Neutralization

For each type of reaction, we will calculate three moments (integration is carried out over the entire velocity space). These moments will be needed for the hydrodynamic equations of plasma.

$$M[0] = \frac{1}{n} \int \frac{\delta f}{\delta t} \Big|_{\text{collision}} d^3v$$

$$M[1] = \frac{1}{n} \int \mathbf{v} \frac{\delta f}{\delta t} \Big|_{\text{collision}} d^3v$$

$$M[2] = \frac{1}{n} \int \frac{mv^2}{2} \frac{\delta f}{\delta t} \Big|_{\text{collision}} d^3v$$

Ionization

Here and in the following sections, we will assume that the function can be represented as the product of two factors: $f(\mathbf{v}, \mathbf{r}, t) = n(\mathbf{r}, t) \cdot F(\mathbf{v}, t)$.

This is the first and very important simplification. In the general case, this is quite a strict condition and is not applicable to all plasmas. For this approximation to be valid, the plasma must be in a state close to local thermodynamic equilibrium, with small spatial gradients of external fields and a high collision frequency between particles. As we can see, all these conditions are satisfied in a wide range of gas discharges (how fortunate for us!).

Now let's calculate moment $M[0]$ using (12)

$$\varphi(\mathbf{v}) = \varphi(\mathbf{v}') = 1, \alpha = 2, \beta = 1$$

$$M[0] = -Nn_e \sum_k \chi_k \int F(\mathbf{v}) v \sigma_k^{ion} d^3v$$

The integral represents the frequency of collisions leading to ionization. To calculate the integral, one must explicitly know the energy distribution function and the reaction cross-sections. Reaction cross-sections can be found in specialized databases such as LxCat. The energy distribution function, however, is more complex. This topic will be discussed in more detail in the section on the hydrodynamic description of plasma.

Thus

$$M[0] = Nn_e v^{ion}, \text{ где } v^{ion} = \sum_k \chi_k \int F(\mathbf{v}) v \sigma_k^{ion} d^3v$$

Now let's calculate $M[1]$

$$\varphi(\mathbf{v}) = \varphi(\mathbf{v}') = 1, \alpha = 2, \beta = 1$$

$$M[1] = Nn_e \sum_k \chi_k [\int \mathbf{v}' v \sigma_k^{ion} d^3v - \int \mathbf{v} v \sigma_k^{ion} d^3v]$$

The first term becomes zero because \mathbf{v}' is isotropic relative to \mathbf{v} , meaning that after ionization, the electrons scatter isotopically.

$$M[1] = -Nn_e \sum_k \chi_k \int \mathbf{v} v \sigma_k^{ion} F(v) d^3v$$

Let us represent $\mathbf{v} = \mathbf{u} + \delta\mathbf{v}$, where \mathbf{u} is the average electron velocity, and $\delta\mathbf{v}$ is the thermal random velocity. Assuming local near-thermodynamic equilibrium, $\delta\mathbf{v}$ is directed isotropically.

So integral over $\delta\mathbf{v}$ will be zero. Therefore:

$$M[1] = -\mathbf{u}Nn_e v^{ion}$$

Let's calculate $M[2]$

$$\varphi(\mathbf{v}) = \frac{mv^2}{2}, \varphi(\mathbf{v}') = \frac{mv'^2}{2}, \alpha = 2, \beta = 1, \frac{mv'^2}{2} - \frac{mv^2}{2} = -\varepsilon_{ion}, \text{ where } \varepsilon_{ion} - \text{ionization energy}$$

$$M[2] = -\varepsilon_{ion}Nn_e v^{ion}$$

Attachment

$$M[0] = -Nn_e v^{att}$$

$$M[1] = -\mathbf{u}Nn_e v^{att}$$

$M[2]$ is a bit difference as electron lost all their energy:

$$\varphi(\mathbf{v}) = \frac{mv^2}{2}, \varphi(\mathbf{v}') = 0, \alpha = 0, \beta = 1$$

$$M[2] = -L_{ext}Nn_e$$

where

$$L_{ext} = \int \frac{mv^2}{2} v \sigma_k^{ext} F(\mathbf{v}) d^3v - \text{average energy lost due to attachments}$$

Elastic scattering

Let's calculate $M[0]$

$$\varphi(\mathbf{v}) = \varphi(\mathbf{v}') = 1, \alpha = 1, \beta = 1$$

$$M[0] = 0$$

Let's calculate $M[1]$

$$\varphi(\mathbf{v}) = \mathbf{v}, \varphi(\mathbf{v}') = \mathbf{v}', \alpha = 1, \beta = 1$$

$$M[1] = Nn_e \sum_k \chi_k [\int \mathbf{v}' \cdot \mathbf{v} d\sigma_k^{sc}(\theta) d^3v - \int \mathbf{v} \cdot \mathbf{v} d\sigma_k^{sc}(\theta) d^3v]$$

Represent $\mathbf{v}' = \mathbf{v} \cdot \cos(\theta) + \mathbf{v}_\perp$ where θ – scattering angle. Integral over \mathbf{v}_\perp becomes zero, as we consider isotropic scattering over \mathbf{v} . Again taking into account $\mathbf{v} = \mathbf{u} + \delta\mathbf{v}$

$$M[1] = -\mathbf{u}Nn_e v^{sc}$$

where $v^{sc} = \sum_k \chi_k \int \mathbf{v} \cdot \mathbf{v} \sigma_k^{total sc} (1 - \overline{\cos(\theta)}) d^3v$, a $\overline{\cos(\theta)}$ – cosine averaging over the differential scattering cross section, $\sigma_k^{total sc}$ – total scattering cross section.

Note: Usually in databases and in literature, when data on elastic scattering cross-sections are given, they usually mean $\sigma_k^{total sc} (1 - \overline{\cos(\theta)})$.

Now $M[2]$

$$\varphi(\mathbf{v}) = \varphi(\mathbf{v}') = \frac{mv^2}{2}, \alpha = 1, \beta = 1$$

We neglect energy losses in elastic scattering due to the large mass of molecules and electrons

$$M[2] = 0$$

Elastic scattering

Calculating $M[0]$

$$\varphi(\mathbf{v}) = \varphi(\mathbf{v}') = 1, \alpha = 1, \beta = 1$$

$$M[0] = 0$$

Now $M[1]$

Similarly, we assume that for inelastic scattering the remaining velocity scatters isotopically.

$$M[1] = -\mathbf{u}Nn_e v^{sc}$$

and $M[2]$

$$\varphi(\mathbf{v}) = \frac{mv^2}{2}, \varphi(\mathbf{v}') = \frac{mv'^2}{2}, \alpha = 2, \beta = 1, \frac{mv'^2}{2} - \frac{mv^2}{2} = -\varepsilon_{ext}, \text{ где } \varepsilon_{ext} - \text{excitation energy}$$

$$M[2] = -\varepsilon_{ext}Nn_e v^{ext}$$

Electron-Ion Recombination

For recombination, the electron/ion disappear, so similar to attachment

$$M[0] = -n_i n_{e/i} v^{rec}$$

$$M[1] = -\mathbf{u}n_i n_{e/i} v^{rec}$$

$$M[2] = -\overline{\varepsilon_{e/i}}n_i n_{e/i} v^{rec}$$

Typically, recombination rates for the ions of interest can be found in reference books or publications.

Plasma-Fluid and Drift-Diffusion Approximation

Coming back to Boltzmann Equation

$$\frac{\partial f}{\partial t} + \vec{\vartheta} \nabla f - \frac{e}{m_e} \left[\vec{E} + \frac{\vec{B} \times \vec{\vartheta}}{c} \right] \nabla f = \frac{\delta f}{\delta t} \Big|_{collision} \quad (13)$$

Equation (13) is not a piece of cake, as f is a seven-dimensional function for each particle species, and the equation itself is both an integral (due to collisions) and a differential equation with two gradients. Solving it directly is challenging or even impossible. Therefore, certain simplifications are used, one of which is the fluid model of plasma. The idea is that for a large class of problems, it is not necessary to know the full velocity distribution function (in case know diffusion and mobility coefficients), but it is enough. Fortunately, our problem falls into this category.

The fluid description of plasma is obtained by integrating equation (13) over velocity space, multiplying by $1, \mathbf{v}, \varepsilon$, resulting in equations similar to those in hydrodynamics (which is why we spent so much time dealing with collision integrals in the previous chapter). First, we will write them in general form, and then specify them for each particle species.

First momentum – the mass conservation law

$$\frac{\partial n}{\partial t} + \nabla \mathbf{G} = M[0] \quad (14)$$

where $\mathbf{G} = n \cdot \mathbf{u}$ particles flow.

Second momentum – the conservation of momentum law

$$\frac{\partial}{\partial t} \int f \vec{v} + \int f \vec{v} (\vec{v} \nabla f) - \frac{e}{m_e} \int \left[\vec{E} + \frac{\vec{B} \times \vec{v}}{c} \right] \nabla_v f = M[1]$$

The calculations for this integral are quite cumbersome, but they are often provided in the literature (for example [here](#)), so I will only present the results here, once again assuming local thermodynamic equilibrium.

If we honestly carry out the integration, considering the above assumption, we obtain:

$$n \frac{d\mathbf{u}}{dt} + \nabla P = \frac{q}{m} \left[\mathbf{E} + \frac{\mathbf{B} \times \mathbf{u} n}{c} \right] - nN[2v^{ion} + v^{sc} + v^{ext}]$$

P – pressure tensor.

$$P = \int \delta \mathbf{v} \times \delta \mathbf{v} f d^3v, \delta \mathbf{v} \times \delta \mathbf{v} - \text{tensor multiplication}$$

P can be represented as:

$$P = p\mathbf{I} + \boldsymbol{\pi}, \text{ where } p - \text{scalar pressure, a } \boldsymbol{\pi} - \text{viscosity tensor}$$

We also assume.

1. Neglecting viscosity
2. \mathbf{u} changing very slow, so $\frac{d\mathbf{u}}{dt} = 0$

While the first assumption is fairly straightforward, the second requires a more detailed discussion. In the assumption of near-local thermodynamic equilibrium, the average velocity will be a function of the electromagnetic field strength. This field is, of course, not constant, and as shown in Chapter 1, it varies at a frequency of hundreds of kilohertz. However, the propagation time of the electron avalanche on our scale is tens of nanoseconds, which is orders of magnitude shorter than the frequency of field variation. In other words, during the breakdown process, the field remains nearly unchanged, making the quasi-stationary approximation more than justified.

Thus, pressure becomes:

$$\nabla p = \frac{q}{m} \left[\mathbf{E} n + \frac{\mathbf{B} \times \mathbf{u} n}{c} \right] - n\mathbf{u}N[2v^{ion} + v^{sc} + v^{ext}]$$

Also taking into account, that $p = nkT$ and

3. The average temperature in space changes more slowly than the concentration (the same logic as in 2)

$$\nabla p = kT \nabla n$$

$$n\mathbf{u} = \mathbf{G} = -D \nabla n + \frac{q}{|q|} \mu \left[n\mathbf{E} + \frac{\mathbf{B} \times \mathbf{G}}{c} \right] \quad (15a)$$

$$D = \frac{kT}{vN}, \mu = \frac{|q|}{mNv} \quad (15b)$$

Thus, we have just derived the well-known drift-diffusion approximation, which is commonly presented in the literature on discharge physics.

However, it can be noted that modern approaches (e.g., the "gold standard" for calculating coefficients in gas discharge models — [Hagelaar 2005](#)) for calculating the coefficients D and μ differ somewhat from those given above. The discrepancy begins with the assumption of local thermodynamic equilibrium. Using the H-theorem, it can be shown that for local thermodynamic equilibrium, the most probable distribution is the Maxwellian distribution with an average velocity \mathbf{u} , also known as the local Maxwell-Boltzmann distribution. In other words, formulas (15b) implicitly assume a local Maxwellian distribution of electrons.

Nevertheless, the drift-diffusion approximation can also be derived without the assumption of local thermodynamic equilibrium. Formally, the expression (15a) can be derived only by assuming quasi-stationarity (zeroing out the total time derivative of the average velocity) and the absence of viscosity. However, in such a case, the values of the diffusion and mobility coefficients will no longer be trivial. In particular, [Hagelaar 2005](#) explicitly derives these coefficients by solving the Boltzmann equation through an expansion of the distribution function in Legendre polynomials. The difference in the coefficients reaches 10-30%, which is significant. Therefore, we will use data from [BOLSIG+](#) (a free software based on Hagelaar's 2005 publication) for the drift-diffusion equations.

Someone might ask — why did we struggle through all these formulas for the past few pages if, in the end, we use a slightly different approach? Nonetheless, it was important to show where the hydrodynamic plasma equations fundamentally come from, especially since we derived them without assuming local thermodynamic equilibrium. Furthermore, it was crucial for me to demonstrate the simple physical meaning of the diffusion and mobility coefficients, which is of great value to engineers and experimentalists.

Additionally, the derivations above make the BOLSIG+ program and its output parameters a bit more comprehensible.

Third momentum – the energy conservation law

$$\frac{\partial n\bar{\varepsilon}}{\partial t} + \nabla \mathbf{G}_\varepsilon = q\mathbf{E}\mathbf{G} + \sum M[2] \quad (16)$$

where $\mathbf{G}_\varepsilon \equiv n \int \mathbf{v} \varepsilon F(\mathbf{v}) d^3v$ – energy flux

In the simplest case of local equilibrium (local Maxwell-Boltzmann distribution), the equation for the average energy is simply given by $\bar{\varepsilon} = \frac{mu^2}{2}$, and there is no need to solve equation (16). However, this approach provides completely unacceptable accuracy for the average energy, so solving equation (16) is still necessary. To do this, one must determine \mathbf{G}_ε . As I mentioned earlier, deriving it from simple considerations is not possible, as an acceptable level of accuracy is only achieved by accounting for the anisotropy of the distribution function. This is exactly what Hagelaar (2005) does in his paper, providing us with the following equation for the energy flux.

$$\mathbf{G}_\varepsilon = -D_\varepsilon \nabla n + \frac{q}{|q|} \mu_\varepsilon \left[n\mathbf{E} + \frac{\mathbf{B} \times \mathbf{G}}{c} \right] \quad (17)$$

Where D_ε and μ_ε are the energy mobility and diffusion coefficients, which are also output parameters of the BOLSIG+ program.

Final Equations

Now, let's bring all the equations together. Up to this point, we have considered the motion of electrons in a stationary medium, so we will also introduce \mathbf{u}_g — the velocity of the medium. The velocity \mathbf{u}_g is 5–6 orders of magnitude lower than the velocity of electron motion in the field, meaning \mathbf{u}_g only affects the spatial distribution of electrons. We also assume $\nabla \mathbf{u}_g \sim 0$, as the velocity of the medium changes more slowly in space compared to particle concentrations.

Electrons:

$$\frac{\partial n_e}{\partial t} + \nabla \mathbf{G}_e + \mathbf{u}_g \nabla n_e = N n_e v^{ion}(\bar{\varepsilon}) - N n_e v^{att}(\bar{\varepsilon}) - \sum_{i+} n_{i+} n_e v_{rec}^{e-i}(\bar{\varepsilon}) + IonRec \quad (18a)$$

$$\mathbf{G}_e = -D_e(\bar{\varepsilon}) \nabla n - \mu_e(\bar{\varepsilon}) \left[n_e \mathbf{E} + \frac{\mathbf{B} \times \mathbf{G}_e}{c} \right] \quad (18b)$$

$$\frac{\partial n_{e,\varepsilon}}{\partial t} + \nabla \mathbf{G}_{e,\varepsilon} + \mathbf{u}_g \nabla n_{e,\varepsilon} = -e \mathbf{E} \mathbf{G}_e - n_e P_e, P_e = -\sum M[2]/n_e \quad (18c)$$

$$\mathbf{G}_{e,\varepsilon} = -D_{e,\varepsilon}(\bar{\varepsilon}) \nabla n_{e,\varepsilon} - \mu_{e,\varepsilon}(\bar{\varepsilon}) \left[n_{e,\varepsilon} \mathbf{E} + \frac{\mathbf{B} \times \mathbf{G}}{c} \right] \quad (18d)$$

$$\bar{\varepsilon} = \frac{n_{e,\varepsilon}}{n_e} \quad (18e)$$

As seen in equation (18a), there is an additional term, *IonRec*, which we haven't previously discussed. It is related to the fact that negative ions, when colliding with neutral atoms, can release electrons. In the next section, we will discuss this term in more detail.

Positive ions $i +$:

$$\frac{\partial n_{i+}}{\partial t} + \nabla \mathbf{G}_{i+} + \nabla(n_{i+} \mathbf{u}_g) = N n_e v_{i+}^{ion} - \sum_{i-} n_{i-} n_{i+} v_{rec}^{ion+ - ion-} - N \chi_d n_{i+} v_d^{i-att}(\bar{\varepsilon}_i, \bar{\varepsilon}_e) + R \quad (19a)$$

$$\mathbf{G}_{i+} = -D_{i+}(\varepsilon) (\nabla n_{i+})^T + \mu_{i+} \left[n_{i+} \mathbf{E} + \frac{\mathbf{B} \times \mathbf{G}_{i+}}{c} \right] \quad (19b)$$

χ_d – concentration of water droplets

In equation (19a), a new term, *R*, has appeared—this represents the interaction of ions with neutral particles. In the final vectorized-form equations, we will examine this term in detail.

Negative ions $i -$:

$$\frac{\partial n_{i-}}{\partial t} + \nabla \mathbf{G}_{i-} + \nabla(n_{i-} \mathbf{u}_g) = N n_e v_{i-}^{att} - \sum_{i+=N_2^+, O_2^+, H_2O^+} n_{i-} n_{i+} v_{rec}^{ion+ - ion-} + R \quad (20a)$$

$$\mathbf{G}_{i-} = -D_{i-}(\varepsilon) \nabla n + \mu_{i-} \left[n_{i-} \mathbf{E} + \frac{\mathbf{B} \times \mathbf{G}_{i-}}{c} \right] \quad (20b)$$

It can be noted that we explicitly account for droplets only for positive ions, but in reality, we also consider them for electrons. This is done by including the droplet absorption cross-sections and their concentration as input parameters when calculating the coefficients in BOLSIG+.

Now, a few words about the data sources. All the electron data is taken from the BOLSIG+ program. For ions, we only need the diffusion and mobility coefficients. The formula for electron mobility is given by [Raizer \(1987\)](#).

$$\mu_i = \frac{q_i}{|q_i|} \frac{36 \sqrt{1 + \frac{A_i}{A_g}}}{\sqrt{\left(\frac{\alpha}{a_0}\right)^3 A_i p}} \cdot 10^{-4} \frac{\text{m}^2}{\text{V} \cdot \text{s}} \quad (21)$$

where

A_i – ion mass

A_g – average mass of medium molecules

$\left(\frac{\alpha}{a_0}\right)^3$ – dimensionless polarization constant for the gas mixture

p – pressure in the gas chamber in bars (input parameter)

The ion temperature can be determined by the formula

$$T_i = T_g + \frac{A_i + A_g}{5A_i + 3A_g} A_g m_a \frac{(\mu_i E)^2}{k_b} \quad (22)$$

where

$m_a = 1.66^{-27} \text{ kg}$ – atomic mass

k_b – Boltzman constant

The diffusion coefficient can be found using the Einstein relation.

$$D_i = \mu_i \cdot k_b T_i \quad (23)$$

Analysis of reaction cross-sections

As input parameters, BOLSIG+ uses electron reaction cross-sections, which are typically taken from the public LXCat database. LXCat contains various datasets; I analyzed them all and chose the most comprehensive ones.

So, we use the following data:

Molecule	LXCat DataBase
O ₂	IST-Lisbon database
N ₂	IST-Lisbon database
H ₂ O	Itikawa database

Below are comparison graphs of reactions with and without droplets.

Input data for the calculation:

- Volume ratio of water/air: $u = 2.7$
- Average electron energy (needed for droplet cross-section calculation): 3 eV
- Droplet diameter: 400 μm
- Saturated vapor pressure (needed for calculating the concentration of water vapor and liquid droplets): 7,381 Pa
- Pressure in the discharge chamber (needed for calculating the concentration of water vapor and liquid droplets): 55,000 kPa
- Coulomb logarithm: 12

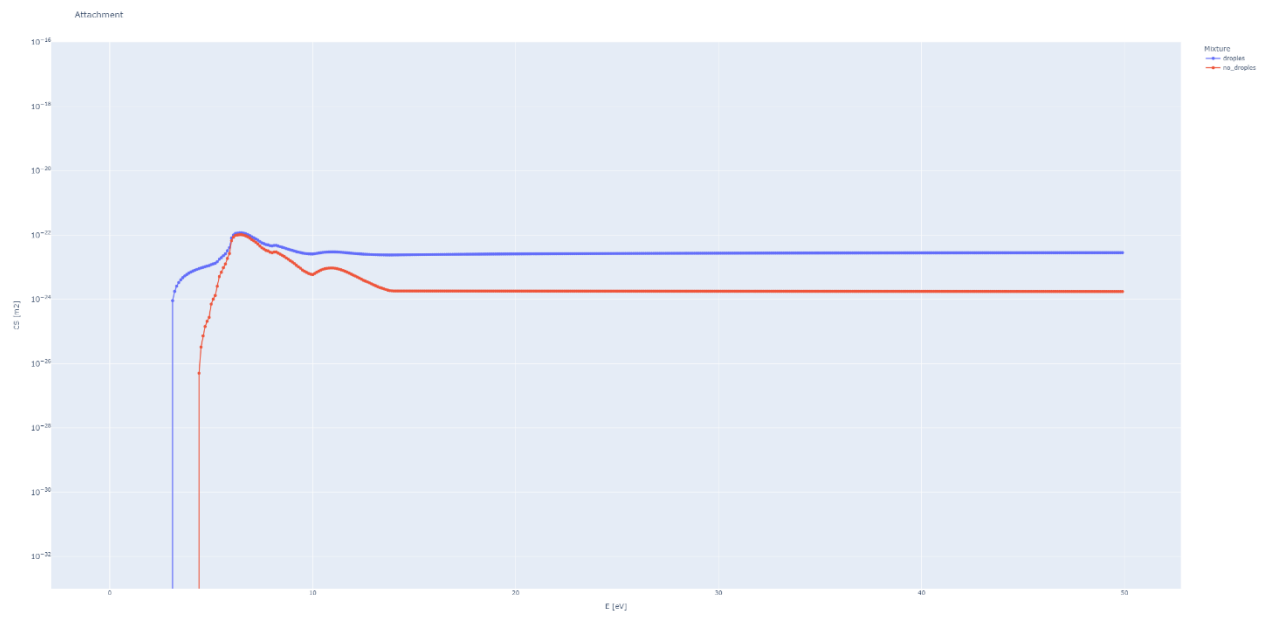


Fig 7. Attachment cross-sections

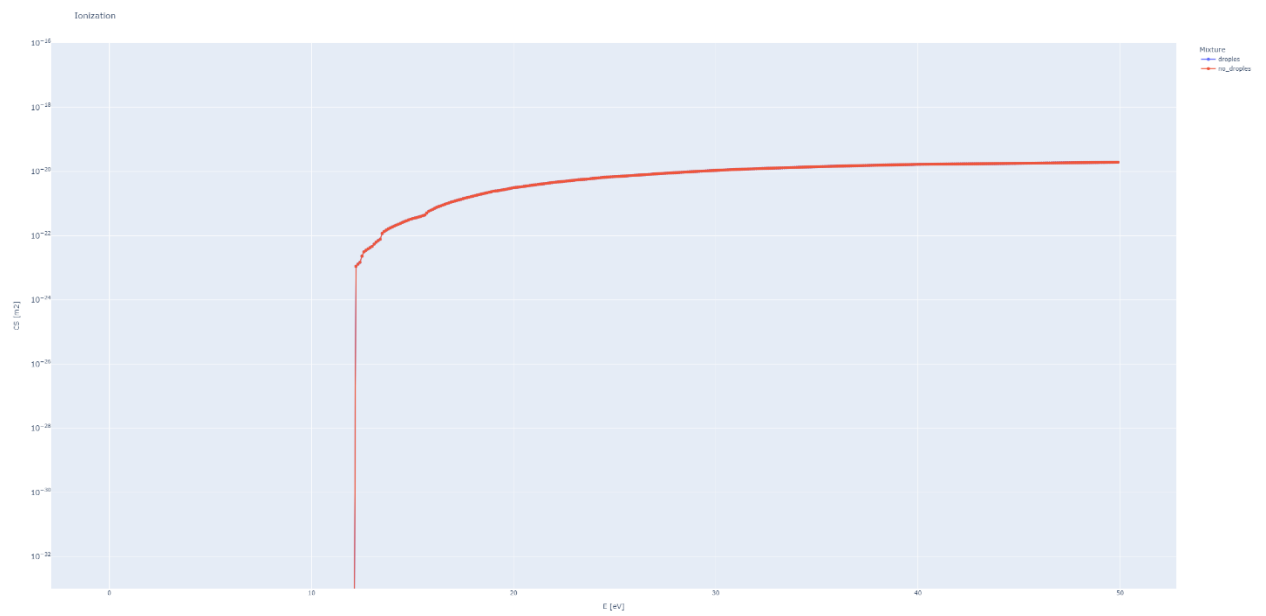


Fig 8. Ionization cross-section.

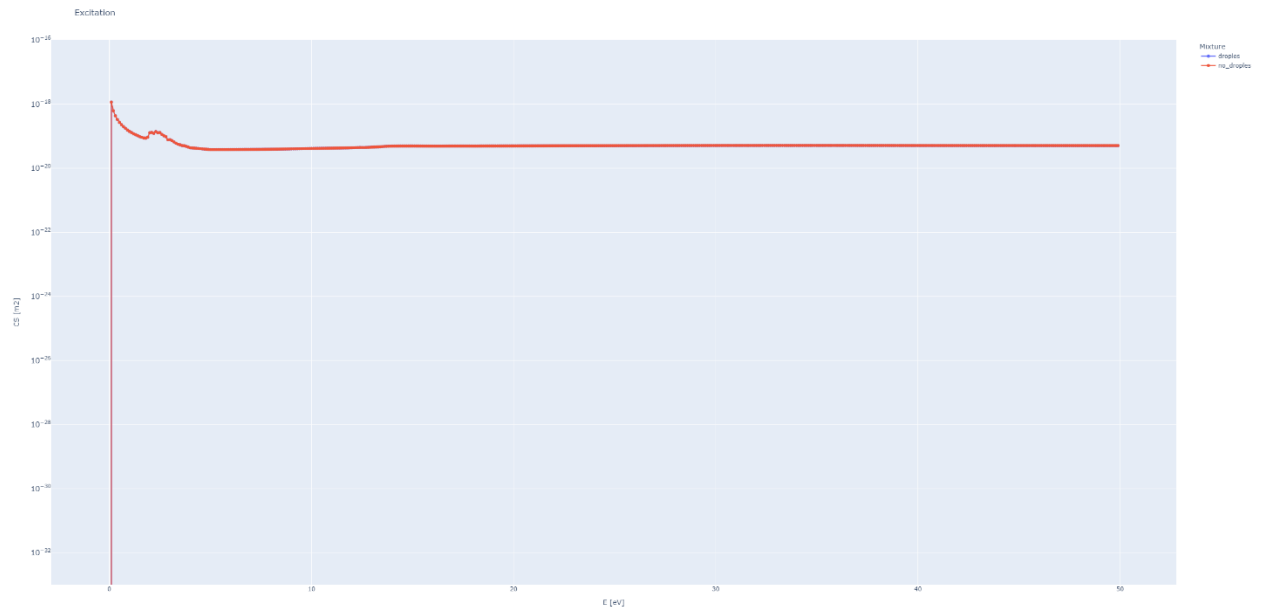


Fig 9. Inelastic Scattering cross-section

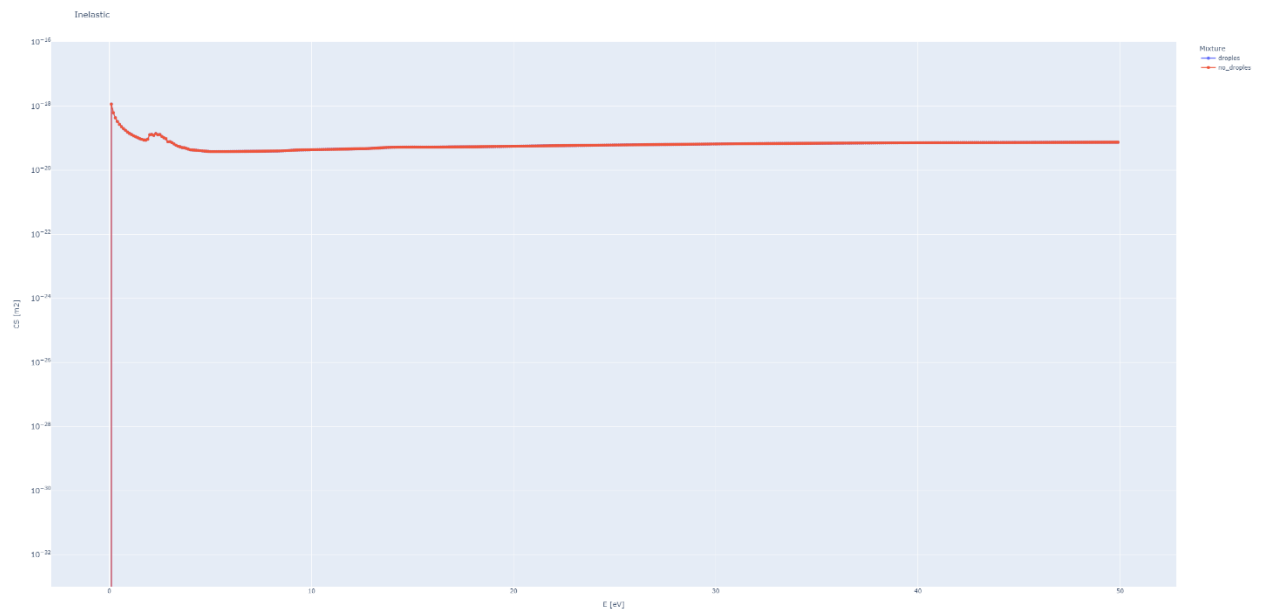


Fig 10. Total inelastic collisions – ionization, attachment, scattering

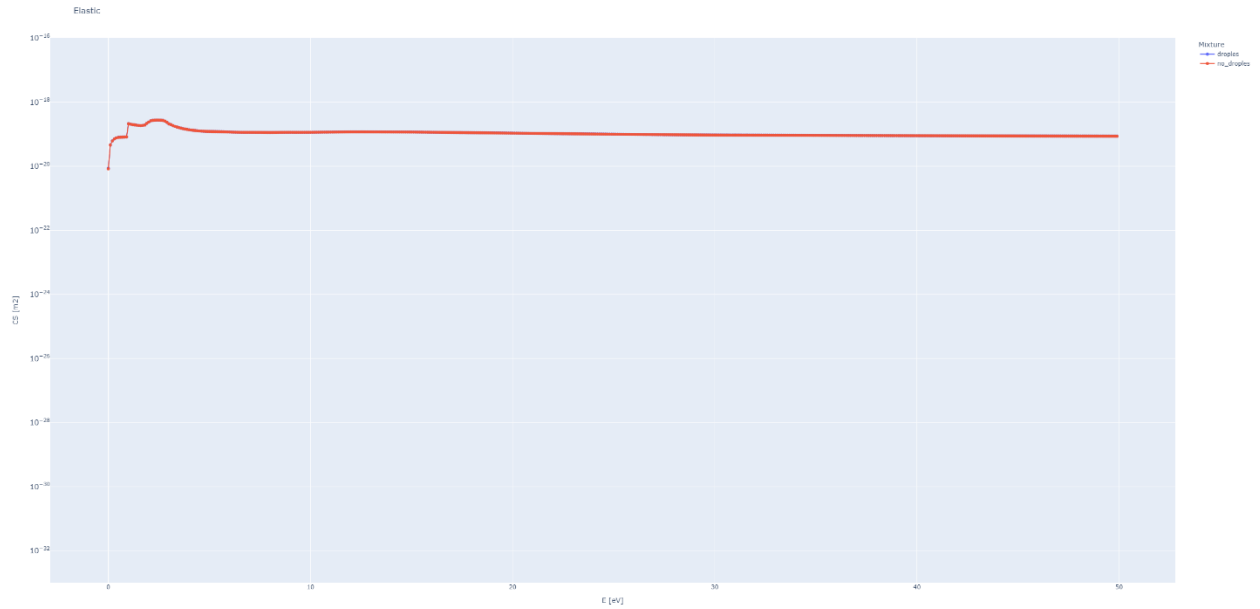


Fig 11. Elastic Scattering cross section

What can we conclude from these graphs? Significant differences are only observed in attachment reactions, but even with consideration of inelastic reactions, the overall contribution is practically zero (the blue line is not even visible under the red one). In elastic scattering reactions, there are also no differences.

All this suggests that the differences in diffusion and mobility coefficients will be practically negligible. This is indeed the case, as seen in the BOLSIG+ calculations of electron mobility and diffusion coefficients with and without droplets (Figures 12 and 13).

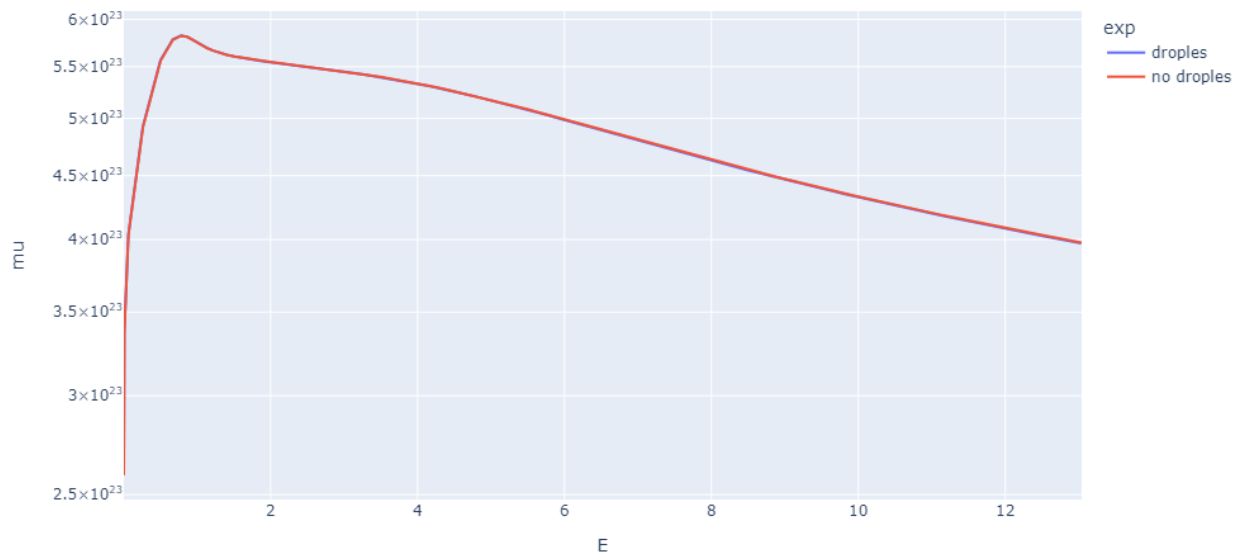


Fig 12. BOLSIG+ calculations - mobility

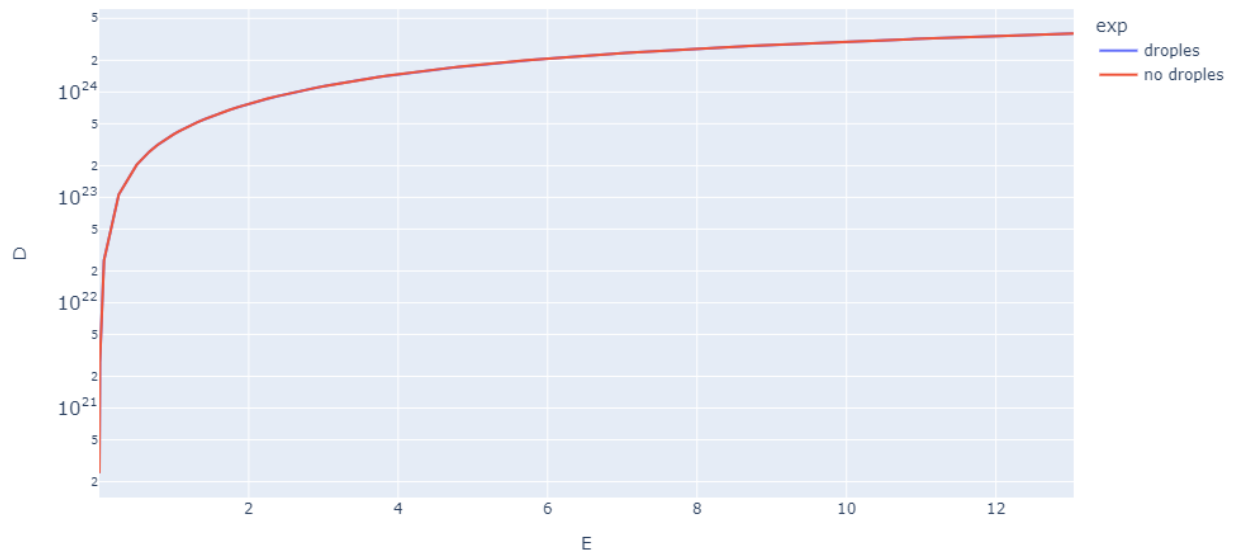


Fig 13. BOLSIG+ calculations - Diffusion

Thus, the presence of water droplets may affect the electron concentration (we will verify this when we develop the discharge model), but they have virtually no effect on mobility coefficients, diffusion coefficients, or, apparently, the average energy.

Boundary conditions

In the work [Hageelar 2000](#), the boundary conditions for gas discharge problems are carefully derived. Like the authors of the paper, we neglect thermionic emission of electrons, as it is practically zero for electrodes that are not made of special materials taking into account electrode temperature of several hundred kelvins.

Before writing these equations, it is necessary to discuss several important processes.

Field enhancement at the conductor boundary

The surface of a conductor is not perfectly smooth and consists of numerous microcracks and roughness. As a result, the field near the conductor is greatly amplified. Therefore, at the boundary, we will use $E_f = FEF \cdot E$, where FEF is the Field Enhancement Factor, a dimensionless coefficient that accounts for field enhancement due to surface irregularities. For steel without special polishing, it is typically around 100.

Secondary electron emission

There are two processes of secondary electron emission:

- **Thermionic emission:** Emission of electrons by conductors heated to high temperatures.
- **Secondary emission:** Ejection of electrons from the conductor's surface by positive and negative ions.

Thermionic emission can be neglected, as noticeable thermionic emission requires special materials (which, obviously, we do not have).

For estimating secondary emission, the secondary emission coefficient γ is used—a dimensionless parameter that indicates how many electrons are ejected by one ion hitting the

conductor's surface. γ depends on the ion's energy or the field strength and is measured experimentally. In our case, considering the FEF, it will be approximately $\gamma \sim 0.1$ (Figure 14).

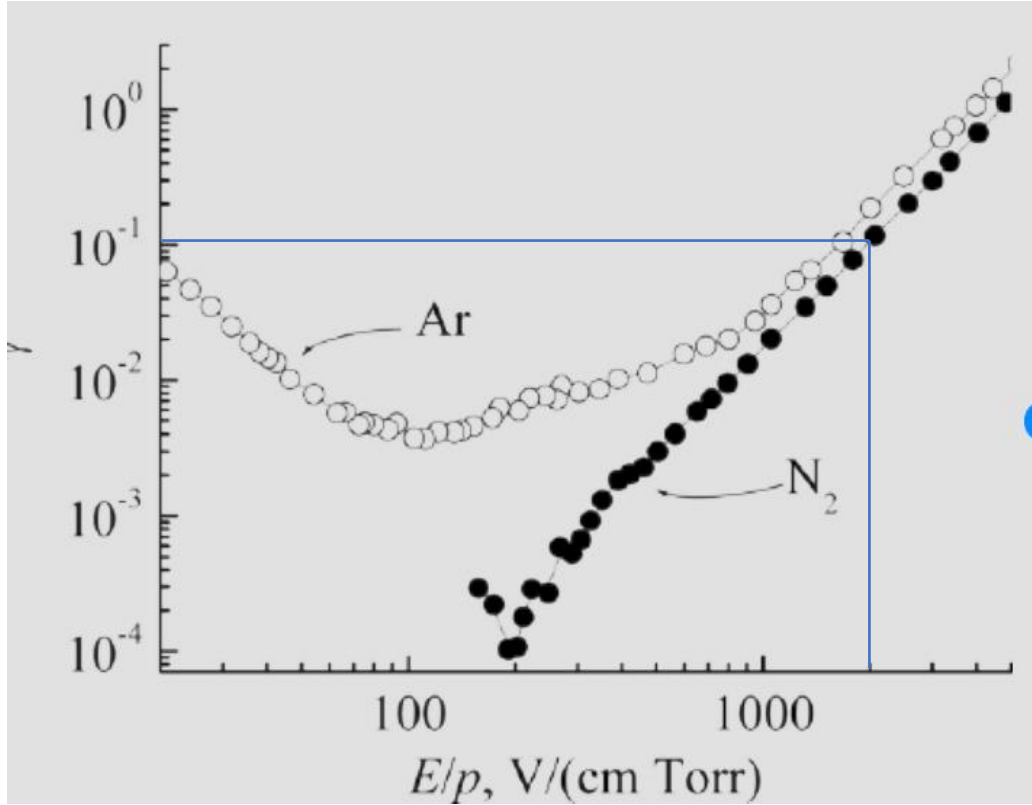


Fig 14. Secondary emission coefficient

Formal boundary conditions

[Hagelaar](#) provides the following boundary conditions

Electrons

$$\boldsymbol{\eta} \cdot \mathbf{G}_e = \frac{1}{2} \left[-(2a_e - 1) \mu_e n_e FEF \cdot \mathbf{E} \cdot \boldsymbol{\eta} + \frac{1}{2} v_{th,e} n_e - \frac{1}{2} v_{th,e} n_\gamma \right] - (1 - a_e) \gamma \sum_i \mathbf{G}_i \cdot \boldsymbol{\eta}$$

Ions

$$\boldsymbol{\eta} \cdot \mathbf{G}_i = \frac{1}{2} \left[-(2a_i - 1) \mu_i n_i FEF \cdot \mathbf{E} \cdot \boldsymbol{\eta} + \frac{1}{2} v_{th,i} n_i \right]$$

Where

$\boldsymbol{\eta}$ – boundary normal vector

$$v_{th,e} = \sqrt{\frac{16 \epsilon_e}{3 \pi m_e}}$$

$$v_{th,i} = \sqrt{\frac{8 k_b T_i}{\pi A_i m_a}}$$

$$a_{e,i} = \begin{cases} 1, & \text{sgn}(e,i) \mathbf{E} \cdot \mathbf{n} > 0 \\ 0, & \text{sgn}(e,i) \mathbf{E} \cdot \mathbf{n} \leq 0 \end{cases}$$

$$n_Y = (1 - a_e) \frac{1}{\mu_e} \frac{\gamma}{2} \sum_i [(2a_i - 1) \cdot \text{sgn}(q_i) + \frac{1}{2} \left(\frac{8(A_i + A_g)}{\pi(5A_i + 3A_g)} \frac{A_g}{A_i} \right)^{1/2}] \mu_i n_i$$

Final equations for numerical solution

Before writing the final equations, let's discuss an important point regarding heavy particles that we haven't addressed before.

Comment – vectorized equations to be checked for misspelling and mistakes

Vectorization of equations for heavy particles

In a discharge involving water vapor, many types of ions are produced—approximately 23 types. Only six of them are formed directly due to attachment and ionization reactions. The rest are generated when ions collide with neutral particles, forming new classes of ions. For example, $N_2^+ + O \rightarrow NO^+ + N(2D)$, and there are many such reactions.

Moreover, in plasma discharge, a large number of new neutral particles are generated, which are of great interest. For instance, $N(2D) + H_2O \rightarrow NH + OH$. Ideally, we would also include these in the model. After all, the concentrations of chemically active radicals are the main focus of all calculations. Fortunately, the reaction rates for all these processes are known and do not require additional calculations. All of this suggests that it would be beneficial to extend equations (19,20) to neutral particles and rewrite them in a unified matrix form for all classes of heavy particles, which is not very difficult.

Another point is that, given the large number of particles, the problem becomes quite resource-intensive. Additional complexity will be introduced by the term $\frac{\mathbf{B} \times \mathbf{G}}{c}$, which will require additional iterations at each step of the flux calculation. Therefore, to simplify the problem, we assume $\mathbf{B} = \mathbf{0}$

Now, let us define:

\mathbf{n} – $n \times 1$ vector representing the concentrations of all heavy particles, including positive ions, negative ions, and chemical radicals. The dimension of vector \mathbf{n} is the number of heavy particles considered in the model.

\mathbf{D} – an $n \times 1$ vector containing the diffusion coefficients. The diffusion coefficient for ions is calculated using formula (21), while for neutral particles, the diffusion is equal to

$$D_m = \frac{1}{3\sqrt{2}n_m\sigma_m} \sqrt{\frac{8k_bT}{\pi m_m}}$$

$$\sigma = \pi(r_m^2 + r_g^2)$$

r_m, r_g – effective radii of radicals and molecules

n_m – particles concentration

$m_m = A_m m_a$ – heavy particle mass (A_m - molar mass, $m_a = 1.66 \cdot 10^{-27}$ kg atomic mass)

T – environment temperature

The vector is tied to the computational grid because \mathbf{D} depends on the ion temperature, which in turn depends on the field strength.

$\boldsymbol{\mu}$ – an $n \times 1$ mobility vector. The mobility for ions is calculated using formula (21), while for neutral particles, it is equal to 0. This vector is constant and is calculated once.

$\nabla \mathbf{n}$ – gradient matrix $n \times 2$, $(\nabla \mathbf{n})_{i,j} = \frac{\partial n_i}{\partial x_j}$

\mathbf{Z} – an $n \times 1$ charge vector, representing the values of elementary charges for ions and 0 for neutral particles.

\mathbf{Z}_{abs} – an $n \times 1$ charge vector, representing binary values of particles: 1 if the particle is an ion and 0 if it is neutral.

\odot – element-wise multiplication

$\mathbf{R}^e(\bar{\varepsilon}_e)$ – An $n \times n$ matrix containing the reaction rates for interactions between electrons, ions, and neutral atoms. It includes all ionization, attachment, excitation, elastic collision, and neutralization coefficients. Some reactions depend on the average electron energy, meaning we will technically have a set of such matrices for each average electron energy. Most of the information in this matrix is obtained from the results of BOLSIG+.

The situation is more complex with interactions between particles themselves. For example, $N_2^+ + O \rightarrow NO^+ + N(2D)$. Fully linearizing such a system is not feasible, so we will use a few tricks.

First, we introduce the stoichiometric matrix \mathbf{S}^{rec} of dimensions $n \times r$, where r - is the number of reactions. Each column represents a reaction, with +1 or +2 or -1 indicating the addition or depletion of the corresponding particle from the respective row as a result of the reaction.

Second, we now need to link this matrix with the concentrations of the particles and the reaction constant (the reaction constant has units of m^3s^{-1} ; by multiplying it by the concentrations, we obtain units of $m^{-3}s^{-1}$, i.e., the rate of change in the number of particles per unit time). Thus, we need two factors—the reaction constants and the product of two concentrations $n_i n_j$. In other words, $\mathbf{K}^{rec} \odot \mathbf{N}^{rec}$, where \mathbf{K}^{rec} is an $r \times 1$ vector consisting of reaction constants, and \mathbf{N}^{rec} is a vector consisting of the products $n_i n_j$ for the reacting particles.

*Comments for efficient computations: I suggest introducing and storing this information in a vector structure $\xi^k = \{i, j\}^k$, indicating which particles are involved in each reaction. Then we can redefine the multiplication function as $\xi * \mathbf{n} \equiv \{n_i n_j\}$.*

Thus, the reaction rate vector can be written as $\mathbf{K}^{rec} \odot (\xi * \mathbf{n})$, and the change in concentration as $\mathbf{S}^{rec} \cdot (\mathbf{K}^{rec} \odot (\xi * \mathbf{n}))$.

Now, let's write the reactions for heavy particles in vectorized form

$$\frac{\partial \mathbf{n}}{\partial t} + \mathbf{G} \cdot \nabla + \nabla \mathbf{n} \cdot \mathbf{u}_g = n_e \mathbf{n} \mathbf{R}^e(\bar{\varepsilon}_e) + \mathbf{S}^{rec} \cdot (\mathbf{K}^{rec} \odot (\xi * \mathbf{n}))$$

$$\mathbf{G} = -\mathbf{D}(\mathbf{E}) \odot \nabla \mathbf{n} + \boldsymbol{\mu} \odot (\mathbf{n} \cdot \mathbf{E}^T)$$

Such a vector form will also affect the equations for electrons, specifically in terms of electron neutralization by ions and electron production due to collisions of ions with neutral atoms.

Therefore, we need two more matrices:

$\mathbf{R}_{NEU}^e(\bar{\varepsilon}_e)$ – an $n \times 1$ vector containing the rates of electron neutralization reactions by heavy particles (obviously, for negative ions and neutral atoms, the values will be zero). This vector is tied to the computational grid.

R_e^s – an $n \times n$ matrix responsible for electron production due to interactions of ions with neutral molecules. $\{R_e^s\}_{i,j} = k_{i,j}$, where $k_{i,j}$ is the reaction constant for particle i interacting with particle j , resulting in electron emission.

Final vectorized equations

The geometry of the problem is shown in Figure 15.

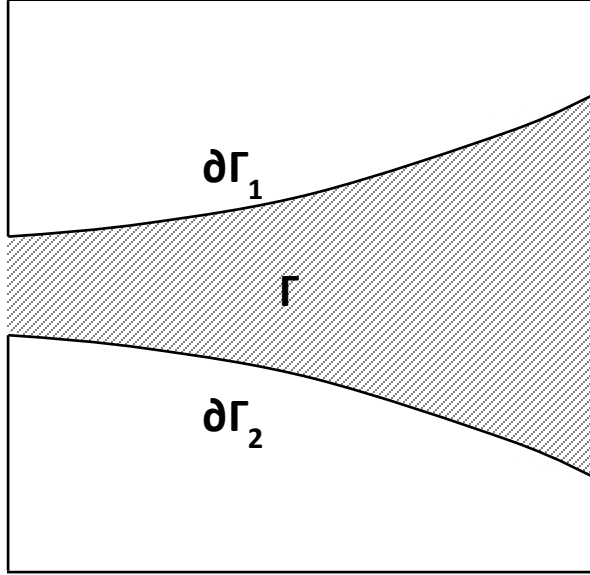


Fig 15. Problem geometry

A two-dimensional problem solved in the domain Γ with boundary conditions on the boundaries $\partial\Gamma_1, \partial\Gamma_2$.

Electrons

$$\frac{\partial n_e}{\partial t} + \nabla \mathbf{G}_e + \mathbf{u}_g \nabla n_e = N n_e \nu^{ion}(\bar{\varepsilon}) - N n_e \nu^{att}(\bar{\varepsilon}) - n_e \mathbf{n}^T \mathbf{R}_{NEU}^e(\bar{\varepsilon}_e) + \mathbf{n}^T \mathbf{R}_e^s \mathbf{n} \quad (24a)$$

$$\mathbf{G}_e = -D_e(\bar{\varepsilon}_e) \nabla n_e - \mu_e(\bar{\varepsilon}_e) n_e \mathbf{E} \quad (24b)$$

$$\frac{\partial n_{e,\varepsilon}}{\partial t} + \nabla \mathbf{G}_{e,\varepsilon} + \mathbf{u}_g \nabla n_{e,\varepsilon} = -e \mathbf{E} \mathbf{G}_e - n_e P_e \quad (24c)$$

$$\mathbf{G}_{e,\varepsilon} = -D_{e,\varepsilon}(\bar{\varepsilon}_e) \nabla n_{e,\varepsilon} - \mu_{e,\varepsilon}(\bar{\varepsilon}_e) n_{e,\varepsilon} \mathbf{E} \quad (24d)$$

$$\bar{\varepsilon} = \frac{n_{e,\varepsilon}}{n_e} \quad (24e)$$

$R_{NEU}^e(\bar{\varepsilon}_e), R_e^s, D_e(\bar{\varepsilon}_e), \mu_e(\bar{\varepsilon}_e), D_{e,\varepsilon}(\bar{\varepsilon}_e), \mu_{e,\varepsilon}(\bar{\varepsilon}_e)$ – input parameters based

\mathbf{u}_g – Input parameter: we know the velocity of the medium at each point of the grid

Heavy Particles

$$\frac{\partial \mathbf{n}}{\partial t} + \mathbf{G} \cdot \nabla + \mathbf{u}_g \odot \nabla \mathbf{n} = n_e \mathbf{R}^e(\bar{\varepsilon}_e) + \mathbf{S}^{rec} \cdot (\mathbf{K}^{rec} \odot (\boldsymbol{\xi} * \mathbf{n})) \quad (25a)$$

$$\mathbf{G} = -\mathbf{D}(\mathbf{E}) \odot \nabla \mathbf{n} + \boldsymbol{\mu} \odot (\mathbf{n} \cdot \mathbf{E}^T) \quad (25b)$$

$$D(E)_i = \begin{cases} \mu_i \cdot k_b T_i, & T_i = T + \frac{A_i + A_g}{5A_i + 3A_g} A_g m_a \frac{(\mu_i E)^2}{k_b}, i - ion \\ \frac{1}{3\sqrt{2}N\pi(r_i^2 + r_g^2)} \sqrt{\frac{8k_b T}{\pi A_i m_a}}, & i - neutral molecule \end{cases} \quad (25c)$$

$$\mu_i = Z_i \frac{36 \sqrt{1 + \frac{A_i}{A_g}}}{\sqrt{(\frac{\alpha}{a_0})_i^3 A_i \cdot p}} \cdot 10^{-4}, \quad Z_i - particle's charge \quad (25d)$$

$R^e(\bar{\varepsilon}_e)$, S^{rec} , K^{rec} , ξ , r_g , A_i , r_i – input parameters

\mathbf{u}_g – Input parameter: we know the velocity of the medium at each point of the grid

N – total particles concentration (depends on pressure in discharge chamber) – input parameter

Poisson equation

$$\Delta \varphi = -\frac{e}{\varepsilon_0} [-n_e + \mathbf{Z}^T \mathbf{n}] \quad (26a)$$

$$\mathbf{E} = -\nabla \varphi \quad (26b)$$

$$\varphi = 0|_{\partial\Gamma_1}$$

$$\varphi = U_0 \sin \omega t|_{\partial\Gamma_2}$$

Boundary conditions ($\partial\Gamma_1, \partial\Gamma_2$)

$$\boldsymbol{\eta} \cdot \mathbf{G}_e = \frac{1}{2} \left[-(2a_e - 1) \mu_e n_e \mathbf{E} \cdot \boldsymbol{\eta} + \frac{1}{2} v_{th,e} n_e - \frac{1}{2} v_{th,e} n_\gamma \right] - (1 - a_e) \gamma (\mathbf{Z}_{abs}^T \cdot \mathbf{G}) \cdot \boldsymbol{\eta} \quad (27a)$$

$$\boldsymbol{\eta} \cdot \mathbf{G}_{e,\varepsilon} = \frac{1}{2} \left[-(2a_e - 1) \mu_{e,\varepsilon} n_{e,\varepsilon} \mathbf{E} \cdot \boldsymbol{\eta} + \frac{1}{2} v_{th,e} n_{e,\varepsilon} - \frac{1}{2} v_{th,e} n_{\gamma,\varepsilon} \right] \quad (27b)$$

$$\mathbf{G} \cdot \boldsymbol{\eta} = \frac{1}{2} \left[-(2\alpha - 1) \odot abs(\boldsymbol{\mu}) \odot \mathbf{n} \cdot (\mathbf{E} \cdot \boldsymbol{\eta}) + \frac{1}{2} \mathbf{V}_{th} \odot \mathbf{n} \right] \quad (27c)$$

Where

$$n_\gamma = (1 - a_e) \frac{1}{\mu_e} \frac{\gamma}{2} \cdot [((2\alpha - 1) \odot \boldsymbol{\mu})^T \cdot \mathbf{n} + (\boldsymbol{\beta} \odot abs(\boldsymbol{\mu}))^T \cdot \mathbf{n}]$$

$$\alpha_i = \begin{cases} 1, & sign(Z_i) \cdot (\mathbf{E} \cdot \boldsymbol{\eta}) > 0 \\ 0, & sign(Z_i) \cdot (\mathbf{E} \cdot \boldsymbol{\eta}) \leq 0 \end{cases}$$

$$\beta_i = \begin{cases} \frac{1}{2} \left(\frac{8(A_i + A_g)}{\pi(5A_i + 3A_g)} \frac{A_g}{A_i} \right)^{1/2}, & Z_i \neq 0 \\ 0, & Z_i = 0 \end{cases}$$

$$a_e = \begin{cases} 1, & -\mathbf{E} \cdot \mathbf{n} > 0 \\ 0, & -\mathbf{E} \cdot \mathbf{n} \leq 0 \end{cases}$$

$$v_{th,e} = \sqrt{\frac{16\bar{\varepsilon}_e}{3\pi m_e}}$$

$$V_{th} = \begin{cases} \sqrt{\frac{8k_b T_i}{\pi A_i m_a}}, T_i = T + \frac{A_i + A_g}{5A_i + 3A_g} A_g m_a \frac{(\mu_i E)^2}{k_b}, & i - ion \\ \sqrt{\frac{8k_b T_i}{\pi A_i m_a}}, T_i = T, & i - neutral particle \end{cases}$$

γ, Z_{abs}^T, A_g - input parameter

Numerical solution

Coming soon ...

Finite difference scheme

Coming soon ...

Reaction database and input matrix calculations

Coming soon ...

Code optimization and parallelization

Coming soon ...

How to use code

Coming soon ...