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FINAL REPORT

New model for the ion collection by cylindrical probes over a wide range of collisionality

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Introduction

The ion collection of probes immersed in a plasma has been studied for a long time, going back to the work of Mott-Smith and Langmuir [1]. However, even at low pressures of a few Pa, the ion current can be affected by collisions due to the large cross section for charge exchange, as is illustrated in Figure 1. At low pressure, ions perform an orbital motion around the probe, which is well described by the Bernstein-Rabinowitz-Laframboise (BRL) theory [2,3]. At increasing neutral gas pressures, collisions destroy this angular momentum, leading to an increased current collected by the probe (Figure 1, middle), as described by the Allen-Boyd and Reynolds (ABR) theory [4]. At even higher pressures, the current begins to decrease with increasing pressure, as the mobility of ions becomes small (Figure 1, right). However, while these general trends are well recognized in the literature, available theories for collisional or collision-enhanced ion currents onto probes are complex, not well validated, and often only valid for a certain range of probe sheath thickness or collisionality [5].

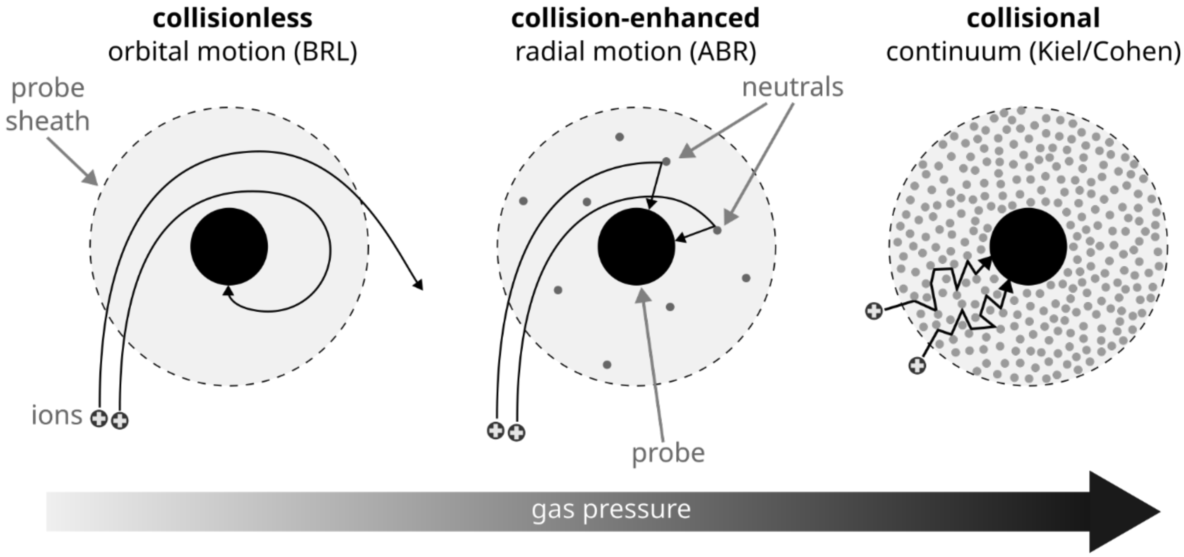

Figure 1: Illustration of the movement of ions attracted to a negatively biased probe for different neutral gas pressures.

To overcome this unsatisfactory situation, we proposed to modify the model of Gatti and Kortshagen, which describes the ion current onto a negatively charged spherical dust particle over a large range of collisionality [6]. The model treats the ion current onto the particle as the sum of collisionless, collision-enhanced and diffusion limited contributions, weighted by the probabilities for either none, one, or many collisions to occur within the sheath around the particle. This simple, intuitive, and fully analytical model yielded surprisingly good agreement with particle-in-cell (PIC) simulations over six orders of magnitude of collisionality [6].

The goal of this project was to modify the spherical Gatti and Kortshagen model to cylindrical probes and an arbitrary sheath thickness, using the same idea of expressing the ion current as a sum of multiple components with weight factors that “turn off” components when they are invalid. However, self-consistent PIC simulations are required to validate the model, as in [6]. Therefore, we proposed using the

2D particle-in-cell code EDIPIC maintained by the Princeton Collaborative Low Temperature Plasma Research Facility (PCRF) to compute ion currents onto probes of different radii over a large range of pressures, which are then compared to the results of the modified model.

Project Outcomes

Configuration and modification of the particle-in-cell code

Several modifications to the particle-in-cell (PIC) code EDIPIC were necessary to make it suitable for simulating a quasi-infinite plasma volume around a negatively biased, cylindrical probe. These modifications were identified and implemented together with the PCRF team, are publicly available on GitHub [7] , and will be discussed in an upcoming publication. Since the entire EDIPIC code is publicly available, other researchers will be able to use this code to test future probe models. Furthermore, we also implemented an advanced ion-neutral collision model [8] as part of this project that will make its way into the main EDIPIC code.

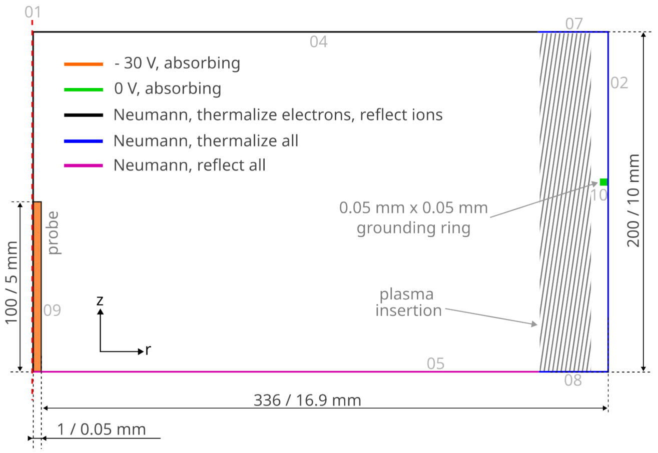

Figure 2: Simulation space in cylindrical geometry and boundary conditions for the particle-in-cell simulation of a quasi-infinite plasma surrounding the probe. The thickness of the probe as well as the ground ring dimensions are exaggerated to maintain visibility. The rest of the figure is true to scale. The dimensions in the figure show the number of cells in the simulation and the corresponding size in millimeter.

Figure 2 shows the configuration that was chosen for the simulation. The simulation is performed in two dimensions and in cylindrical coordinates, resolving the r-z plane. Argon was used as the gas at varying pressures.

Most of the edges of the simulation space are configured with Neumann boundary conditions with regard to the plasma potential, meaning that the electric field across the boundary is set to zero. This is in accordance with the idea that we simulate only a small section of a larger discharge volume, and that this larger volume is undisturbed by the probe. Some of the boundaries are adjusted to thermalize electrons, i.e., electrons hitting the boundary were reinserted with a random direction and velocity according to a Maxwell-Boltzmann distribution with a temperature of $T_e = 3$ eV. In this way, electrons are forced to follow a Maxwell distribution with a constant temperature, corresponding to the assumptions that probe models in the literature use, for comparison. Non-Maxwellian electron energy distribution functions (EEDFs) can easily be implemented and will be explored at a later date. Some of the boundaries are additionally set up to also thermalize ions. This is done to remove the excess energy that ions might have gained when being attracted by the probe, orbiting around it and then leaving again towards the further plasma volume, where we assume a low ion temperature.

Both electrons and ions are reinserted after interaction with most boundaries. The probe, however, needs to obviously act as an absorbing surface. The probe is set to a negative potential, according to the aims of the project to attract positive ions. This, however, necessitates another conductive/absorbing surface within the discharge volume. Otherwise, the plasma potential in the volume will simply adjust to a potential slightly above the probe potential to balance ion and electron fluxes towards the probe, which is undesired. To fix the plasma potential to the desired value, a second conductive object is inserted into the simulation: the grounding ring. Said ring is forced to a potential of 0 V and, due to it being much larger than the probe (cylindrical coordinates), will fix the plasma potential to 10 V – 12 V outside the probe sheath.

Electrons and ions absorbed by the probe or the grounding ring would cause the ion density to reduce over time. To prevent that from happening, a new electron-ion pair (mimicking ionization) is created whenever an ion is lost to any surface. The region of plasma insertion is shown in Figure 2.

The described simulation setup was successful in simulating a quasi-infinite plasma surrounding the probe, while keeping densities, temperatures, and the plasma potential constant in time and space outside of the sheath surrounding the probe and the grounding ring.

Simulation results

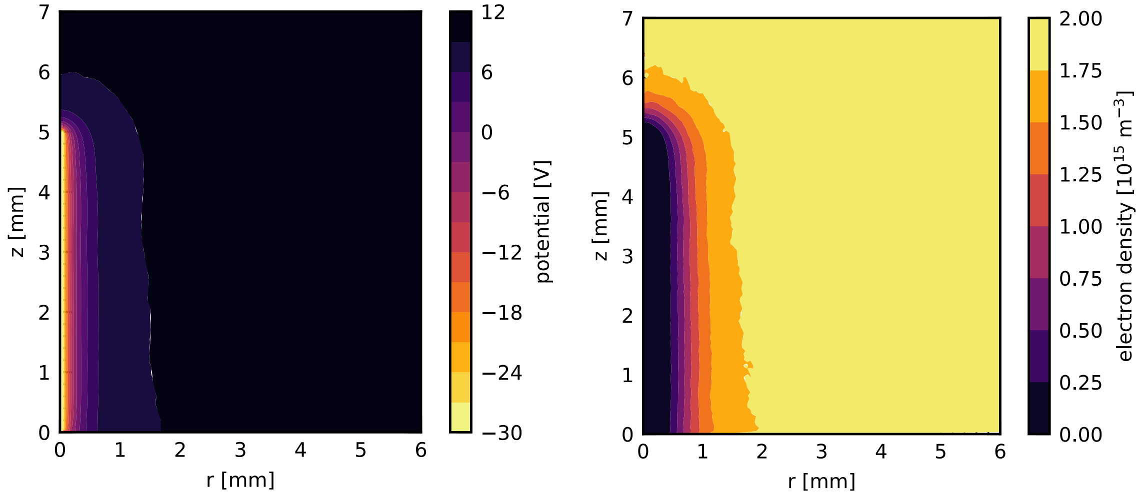

Figure 3: Plasma potential (left) and electron density (right) surrounding a cylindrical probe (located at r = 0) with a diameter of 100 µm, length of 5 mm and biased at -30 V. The simulation was performed with pure argon at a pressure of 3 Pa.

Figure 3 shows an enlarged view of the simulated region directly surrounding the probe. This example simulation was performed at a probe bias of -30 V relative to ground, or -42 V relative to the plasma potential. The argon pressure was set to 3 Pa, corresponding to the collision-enhanced regime (compare Figure 1). Both in the plasma potential surrounding the probe (Figure 3, left) as well as in the electron density (Figure 3, right), it becomes apparent that the region strongly disturbed by the probe extends roughly 2 mm. However, modest electric fields accelerating ions towards the probe can be observed to reach further into the wider plasma volume than that.

This observation underlines the importance of simulation the plasma in two dimensions: even a probe that is much longer (5 mm) than it is wide (100 µm diameter) cannot be modeled as an infinitely long cylinder, unless it's length also considerably exceeds the thickness of the sheath. For the very typical probe dimensions and electron densities we are studying here, this is not the case.

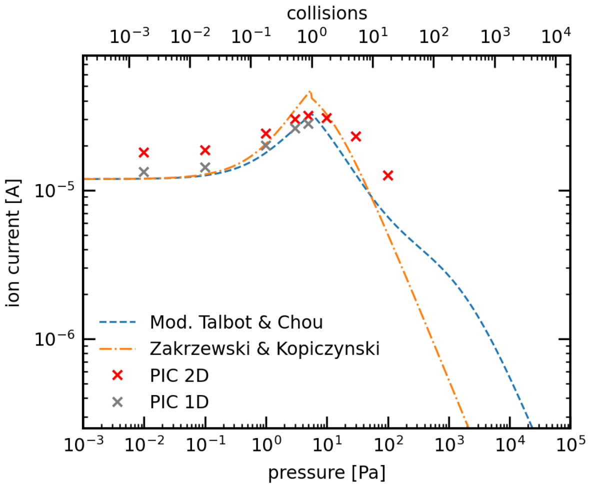

Figure 4: Ion current collected by the probe for different argon pressures for the simulation performed in 2D and pseudo-1D, as well as predicted by the modified Talbot & Chou model and the model of Zakrzewski and Kopiczynski. Probe voltage: -42 V. Ion density: $8 \times 10^{15}\ m^{-3}$.

This becomes clear from Figure 4, where the ion current collected by the probe is shown for different argon pressures at a probe bias voltage of -42 V (relative to the plasma potential) at an ion density of $n_i = 8 \times 10^{15}\ m^{-3}$. The figure shows results of the two-dimensional simulation shown in Figure 2, but also of a pseudo-1D version of the simulation, where the probe fills the entire simulation space in z-direction and all gradients in this direction are removed, leading the simulation to deliver results as if it was a 1D code. For comparison, the figure shows the ion currents predicted by the modified Talbot and Chou model by Tichy et al [9], as well as by the model of Zakrzewski and Kopiczynski [10]. These two models are the only prominent approaches in the literature that cover the entire pressure range, and will, thus, be employed for comparison.

Discussing first the collisionless limit for pressures of P ≤ 0.1 Pa (under these conditions), we see that both literature models agree well with the 1D simulation. This is expected since both models approach the collisionless BRL theory in this range [3], which is one-dimensional. However, we see that the 2D simulation predicts a considerably higher current in this range due to the additional current drawn to the tip of the probe. This illustrates that a one-dimensional approach is not appropriate for common probe dimensions and plasma densities, both when it comes to models used to determine densities from probe measurements and simulations that test these models. Since a large share of the validation studies in the literature compares these models to 1D PIC simulations, the reliability of these studies needs to be reconsidered. It should be noted that we are not the first to point out the influence of the finite probe length [11], but the extent of the problem is not well recognized in the literature.

In the collision-enhanced regime, here around 3 Pa, agreement of both simulation results and the modified Talbot and Chou model is considerably better. The theory of Zakrzewski and Kopiczynski predicts too high a current, but even here, the discrepancy is small. However, in the collisional regime (P > 50 Pa), we observe a strong discrepancy between both models and the simulation results. Here, both literature models demonstrate considerable differences in the simulation results. This is particularly interesting because this pressure range has become more important in recent years for plasma processing applications, and because no validation studies for the models exist in the literature in this range.

A new model

Given the unsatisfying agreement between our simulation results and the two most prominent models in the literature, we aim to introduce a more accurate and conceptually simpler model.

Following the approach of Gatti and Kortshagen, we combine the collisionless current and the collisional current, each multiplied with the respective probability of an ion to cross the probe sheath with (P_N) or without (P_0) collision at the given pressure. The current to the probe is then written as:

$$I = P_0 \left(I_{\mathrm{BRL,cyl}} + \frac{1}{2} I_{\mathrm{BRL,sph}} \right) + P_N I_{\mathrm{Bryant}} \tag{1}$$

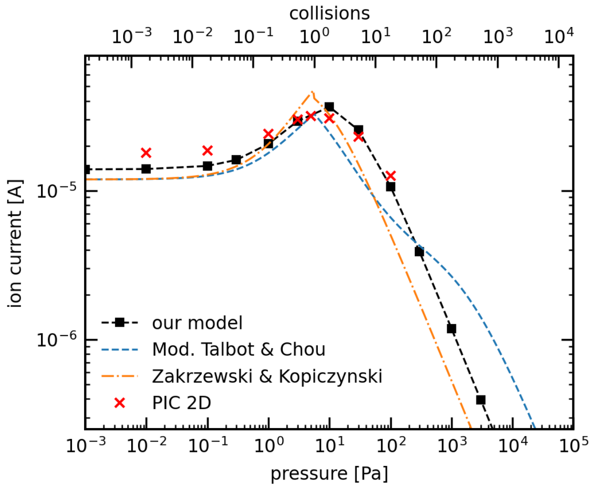

Figure 5: Comparison between the simulation, models from the literature and the new model proposed in this project. Probe voltage: -42 V. Ion density: $8 \times 10^{15}\ m^{-3}$.

Here, $I_{\mathrm{BRL,cyl}}$ and $I_{\mathrm{BRL,sph}}$ are the collisionless ion currents according to the BRL theory for a cylindrical and a spherical probe, respectively. This added term for the current attracted to a spherical probe is a simple and approximate approach from the literature to account for the current attracted to the probe endcap [11]. I_{Bryant} is the ion current according to the model by Bryant, which covers both the collision-enhanced and the highly collisional regime [12]. The model is also two-dimensional, thus, requiring no adjustments to account for the current drawn to the endcap.

The probability P_0 of an ion to cross the probe sheath without collisions depends on the ration of sheath thickness S and the mean free path for ion-neutral collisions λ_i as $P_0 = \exp\left(-\frac{S}{\lambda_i}\right)$. Correspondingly, $P_N = 1 - P_0$. For the sheath thickness S, we use the model of Basu and Sen [13], and the mean free path is calculated according to a constant cross-section of $1 \times 10^{18}\ \mathrm{m}^2$.

Figure 5 shows the ion current for different pressures according to the PIC simulation, the models from the literature and as calculated with our new model (eq. 1).

In the collisionless range (here: P ≤ 0.1 Pa), some discrepancies remain, presumably due to the approximate approach of taking the endcap current into account. However, our new model does perform better than the models from the literature.

Outside the collisionless regime, these discrepancies vanish, and we find excellent agreement between our model and the simulation results. Especially in the pressure range between 10 Pa and 100 Pa, our model produces much better agreement to the simulation than the literature models.

Parameterization

While the model described by equation 1 performs favorable compared to models from the literature in terms of accuracy and is conceptionally simple, it is not easy to use without further work. This is because the underlying models usually predict the probe potential V_{LP} as a function of probe current I, whereas for the analysis of probe measurements, it is necessary to calculate the probe current as a function of probe potential instead. Thus, $V_{LP}(I)$ needs to be inverted to obtain $I(V_{LP})$. In practice, this is done by pre-calculating V_{LP} values for a suitable range of currents, densities, and probe dimensions which can then be used to find an empirical equation to predict I for a given combination of probe bias, dimensions and plasma properties. For $I_{\mathrm{BRL,cyl}}$ such a parameterization already exists [14], but that is not the case for I_{Bryant}. For the spherical BRL current, $I_{\mathrm{BRL,sph}}$, available parameterizations [15] were found not to be precise enough over the entire parameter space.

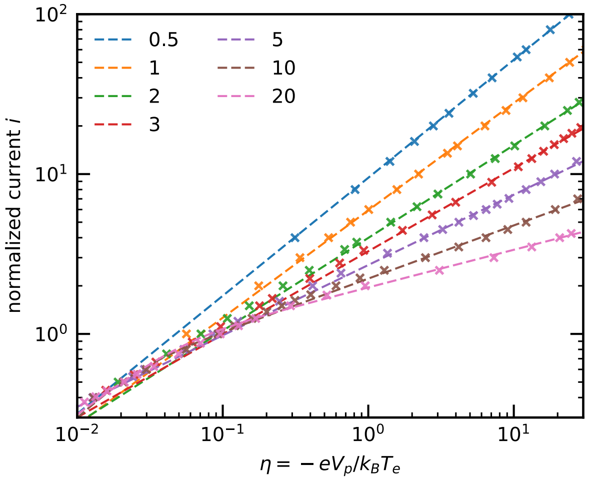

Figure 6: Normalized probe current i as a function of dimensionless probe potential $\eta = -e\frac{V_{LP}}{k_BT_e}$ *for different values of* R_P/λ_D *(probe radius over Debye length) between 0.5 and 20.*

Thus, a parameterization for the spherical BRL results was developed as part of the project. We used the original calculations by Laframboise [3], who provided a table of normalized currents *i* as a function of the dimensionless probe potential $\eta = -e\frac{V_{LP}}{k_B T_e}$, with the elementary charge *e*, and the electron temperature T_e. The model does not depend on the properties of the probe and the plasma density separately, but is instead described by the ratio of probe radius over Debye length R_P/λ_D. Laframboise's work tabulates *i* over η curves for a range of R_P/λ_D values, some of which are shown in Figure 6 as symbols. The figure also shows our parameterization as dotted lines, which obviously agrees well with the precalculated points.

This parameterization follows the approach of Chen for the cylindrical probe current [14], using the following equation for the normalized probe current *i*:

$$i = ((A\eta B)^{-4} + (C\eta D)^{-4})^{-1/4}$$

Where A, B, C and D are functions that depend only on R_P/λ_D. The full parameterization will be described in an upcoming publication.

The parameterization for the model by Bryant is underway, but has proven challenging, since the model depends on additional parameters describing the neutral gas pressure and the shape of the probe, which means that the complexity of the parameterization is considerably higher.

Publications and conference presentations

- Held J, Villafana W, Kaganovich I, and Kortshagen U 2025 *The importance of the finite probe length on the current attracted to a cylindrical probe* (in preparation)

- Held J, Villafana W, Kaganovich I, and Kortshagen U 2025 *Particle-in-cell simulation of the ion attraction by a cylindrical Langmuir probe at elevated pressures* (planned)

- Held J, Villafana W, Kaganovich I, and Kortshagen U 2025 *New model for the ion collection by cylindrical probes over a wide range of collisionality* (planned)

- Held J, Villafana W, Kaganovich I, and Kortshagen U, *New model for the ion collection by cylindrical probes over a wide range of collisionality*, ET2.00001, 2023 Annual Gaseous Electronics Conference, Ann Arbor, Michigan, Oct 9 – 13, 2023

- Held J, Villafana W, Kaganovich I, and Kortshagen U, *New model for the ion collection by cylindrical probes over a wide range of collisionality*, I.558, 2024 EPS Conference on Plasma Physics, Salamanca, Spain, Jul 8 – 12, 2024

- Held J, Villafana W, Kaganovich I, and Kortshagen U, *Validating and improving models for the ion collection by cylindrical probes*, EF1.00001, 2024 Annual Gaseous Electronics Conference, San Diego, California, Sep 30 – Oct 4, 2024

References

[1] Mott-Smith H M and Langmuir I 1926 The Theory of Collectors in Gaseous Discharges *Phys. Rev.* **28** 727–63

[2] Bernstein I B and Rabinowitz I N 1959 Theory of Electrostatic Probes in a Low-Density Plasma *The Physics of Fluids* **2** 112–21

[3] Laframboise J G 1966 *Theory of spherical and cylindrical Langmuir probes in a collisionless, Maxwellian plasma at rest* (University of Toronto Institute for Aerospace Studie)

[4] J E Allen, R L F Boyd, and P Reynolds 1957 The Collection of Positive Ions by a Probe Immersed in a Plasma *Proceedings of the Physical Society. Section B* **70** 297

[5] Bose S, Kaur M, Chattopadhyay P K, Ghosh J, Saxena Y C and Pal R 2017 Langmuir probe in collisionless and collisional plasma including dusty plasma *Journal of Plasma Physics* **83** 615830201

[6] Gatti M and Kortshagen U 2008 Analytical model of particle charging in plasmas over a wide range of collisionality *Phys. Rev. E* **78** 046402

[7] Held J 2025 https://github.com/Julian-Held/EDIPIC-2D/tree/WIP/Implement_cylindrical_coordinates

[8] Nanbu K and Kitatani Y 1995 An ion-neutral species collision model for particle simulation of glow discharge *J. Phys. D: Appl. Phys.* **28** 324

[9] Tichý M, Šícha M, David P and David T 1994 A Collisional Model of the Positive Ion Collection by a Cylindrical Langmuir Probe *Contrib. Plasma. Phys.* **34** 59–68

[10] Zakrzewski Z and Kopiczynski T 1974 Effect of collisions on positive ion collection by a cylindrical Langmuir probe *Plasma Physics* **16** 1195

[11] Jaeger E F, Berry L A and Batchelor D B 1991 Characteristics of a cylindrical Langmuir probe of finite length *Journal of Applied Physics* **69** 6918–22

[12] Bryant P M 2008 Theory of cylindrical Langmuir probes in weakly ionized, non-thermal, stationary and moderately collisional plasmas *Plasma Sources Sci. Technol.* **18** 014013

[13] Basu J and Sen C 1973 Sheath Thickness for a Cylindrical or Spherical Probe Placed in a Plasma *Jpn. J. Appl. Phys.* **12** 1081

[14] Chen F F 2001 Langmuir probe analysis for high density plasmas *Physics of Plasmas* **8** 3029–41

[15] Karamcheti A and Steinbrüchel Ch 1999 Parametrization of Laframboise's results for spherical and cylindrical Langmuir probes *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films* **17** 3051–6