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Collision chemistry impact on Townsend's avalanche development

Abstract. *This article explores the impact of collision chemistry on Townsend's avalanche development through an innovative computational approach. By combining the Particle-in-Cell algorithm and Monte Carlo Collisions, we determine the first Townsend coefficient for Helium gas. Further, we investigate the influence of a variable number of excitation collisions to achieve accurate compliance with experimental results. This work involves the use of a custom-built meta-programming library in the Julia programming language, enabling automatic code generation for enhanced efficiency and reproducibility.*

Streszczenie. *Artykuł bada wpływ chemii kolizji na rozwój lawiny Townsenda za pomocą innowacyjnego podejścia obliczeniowego. Poprzez połączenie algorytmu Particle-in-Cell i Monte Carlo Collision, wyznaczono pierwszy współczynnik jonizacji Townsenda dla helu. Zbadano wpływ zmiennej liczby kolizji wzbudzenia w celu uzyskania dokładnej zgodności z wynikami eksperymentalnymi. Do tych badań wykorzystano autorską bibliotekę metaprogramowania napisaną w języku programowania Julia, umożliwiającą automatyczną generację kodu w celu poprawy wydajności i reprodukowalności badań.* ***(Wpływ chemii kolizji na rozwój lawiny Townsenda)***

Keywords: Monte Carlo Collisions, Particle-in-Cell, Townsend's avalanche, Townsend coefficient, Julia programming language, metaprogramming, GPU programming
Słowa kluczowe: Monte Carlo Collisions, Particle-in-Cell, lawina Townsenda, współczynnik Townsenda, język programowania Julia, metaprogramowanie, karty graficzne

Introduction

In the world of gas discharge physics, Townsend's avalanche phenomenon has long been a focal point of study due to its fundamental significance in understanding electrical breakdown in gases. Although we know that Townsend's theory aligns with the experiments only under specific conditions, his proposed formulas still hold, especially when the electrode separation distance is small. The Townsend coefficient (α), quantifying the multiplication rate of charged particles in an avalanche, plays a crucial role in predicting and analyzing such plasma discharges. Traditional approaches to determining α rely on experimental measurements, which can be time-consuming, costly and often lack the necessary precision to understand the underlying collisional processes fully.

Conversely, simulation of plasma chemistry can be challenging due to high computational cost, especially when high number of collisions is considered. To address this challenge, we present an original implementation combining Particle-in-Cell (PIC) algorithm and Monte Carlo (MCC) collisions, enabling us to calculate the first Townsend coefficient (α) for various gas mixtures and pressure conditions. Further, we explore the influence of collision chemistry on Townsend avalanches development by experimenting with the number and type of collisions considered in our simulations.

A notable aspect of this research lies in the utilization of an original custom-built meta-programming library: Hennel.jl, written in Julia programming language. Our code is able to generate the simulation code automatically, basing on high level description. This approach not only simplifies the simulation process (especially when considering varying chemistry) but also ensures advanced code optimization and reproducibility.

In this article, we present the details of our PIC-MCC methodology and the parameters of the simulations. We discuss the impact of different collision setups on α and investigate the compliance of simulation results towards experimental findings.

Overall, the integration of PIC algorithm, MC collisions, and meta-programming in Julia offers a promising path for studying complex plasma phenomena and contributes to bridging the gap between experimental observations and theoretical predictions in gas discharge research.

Towsend avalanche

The study of Townsend avalanches and their coefficients has a rich history in the field of gas discharge physics. On the foundation of this area is J. S. Townsend's book [1], which provided essential insights into the fundamental nature of electron avalanches and their relevance in electrical breakdown phenomena. First of two coefficients: α plays a critical role in characterizing the phenomenon of electron multiplication within a gas medium under the influence of an applied electric field. When an electron acquires sufficient energy from the electric field, it undergoes a collision with gas molecules. When the energy of the electron is high enough, it can result in ionization and the generation of secondary electrons. These secondary electrons, in turn, gain energy from the electric field and initiate additional ionization events, creating a chain reaction known as the electron avalanche. The first Townsend coefficient quantifies the rate of this electron multiplication process. Mathematically, it can be defined as the ratio of the number of electrons produced by ionization to the number of electrons initially present in the gas volume per unit length of the discharge path (Eq. 1).

$$\alpha = \frac{N_i}{N_0 \cdot d} \tag{1}$$

Following the findings of Townsend's work, Chanin and Rork conducted experimental investigations to determine the first Townsend coefficient specifically for helium gas [3]. This study focused on empirical measurements to establish α and boasts results consistent with various theoretical studies.

However, such experimental approaches often have limitations in precision and applicability to various gas mixtures and pressure conditions. Therefore, along with the development of computers, scientists in this area of research quickly became interested in computer simulations, allowing them to reproduce such results faster, cheaper, and more repeatable.

Determination of first Townsend coefficient through simulation

One of the methodologies that can be employed to simulate the evolution of the Townsend electron avalanche involves the utilization of the Particle-in-Cell (PIC) algorithm in conjunction with the Monte Carlo Collisions (MCC) algorithm. The application of these two algorithms to model gas

discharges is explicated in the renowned paper authored by Birdsall [5]

Building upon these foundational works, Crosette et al. employed these simulation techniques to calculate the first Townsend ionization coefficient in Helium [2]. The simulation software utilized in this study was VSim, a multiphysics simulation software developed by Tech-X. To validate the accuracy of their simulations, the authors compare their results with experimental results from Chanin and Rork[3]. This comparison establishes the reliability of their simulation approach and demonstrates its capability to replicate experimental observations.

Julia programming language

Nowadays, the field of scientific computing is experiencing rapid advancements, leading to the emergence new tools and technologies. One of the significant outcomes of this trend is the Julia programming language. Julia is a high-level, high-performance programming language designed for scientific computing, numerical analysis, and data science tasks. It was first introduced in 2012 and has gained significant popularity in the computational science community due to its ease of use and remarkable speed. Julia is renowned for its powerful metaprogramming capabilities, which allow developers to perform tasks such as code generation, optimization, and customization. This allows for creating efficient and highly specialized code tailored to specific use cases, improving performance and maintainability.

Motivation

This research endeavor is greatly inspired by the work of Crosette et al., whose article showed the methodology for computational investigations into determining the first Townsend ionization coefficient. Although their study exhibited commendable congruence with both experimental and analytical findings, the alignment between their results and empirical data demonstrated a very good alignment only at a specific ratio of electric field to pressure ($E/p_0 = 100\frac{V}{cm \cdot Torr}$). However, when exploring regimes with smaller or larger values of E/p_0, a discernible trend emerged wherein the estimated coefficient values either exceeded (for lower E/p_0) or fell short of the anticipated values (for higher E/p_0). To address that, Crosette et al. suggested that augmenting the number of excitation collision processes within the simulations might produce a more accurate representation of the Townsend coefficient's behavior in smaller E/p_0.

The reasoning behind this prediction appears to be quite straightforward. As the number of excitation processes incorporated into the simulation increases, the likelihood of an electron "selecting" an excitation event over ionization or elastic collision during the Monte Carlo Collisions iteration also rises. Within the MCC method, when an electron undergoes an excitation collision with the background gas, it loses a portion of its energy. With an escalation in the count of excitation processes, the overall energy of the electrons diminishes. This reduction in energy makes electrons less prone to ionize the background gas, consequently leading to a lower value for the first Townsend coefficient.

In this research, we harness the capabilities of our novel meta programming library to produce highly optimized simulation code. In this case, we generated code tailored for Nvidia GPUs. The library's ability to do so, has notably expedited our simulations, allowing us to complete this extensive study within a more manageable timeframe. We undertake an extensive exploration, employing an increased number of excitation processes. We aim to validate the assertions by Crosette et al. and determine if the incorporation of additional excitation collision processes indeed reduces the Townsend coefficient values in weaker electric fields, consequently enhancing the agreement between simulations and experimental data.

Simulation parameters

In this study, our focus revolves around replicating the essential physical parameters featured in the experiments conducted by Chanin and Rork, employing the methodology elucidated by Crosette et al. Specifically, our simulation is conducted within a one-dimensional, three-velocity (1D3V) domain. To establish an appropriate grid discretization, we employed a method akin to that utilized by the VSim software and, presumably, Crosette et al. This method calculates the grid cell size based on the value of mean free path. The formula for obtaining mean free path (λ) is presented in Eq. 2

$$\lambda = \frac{1}{\max(\sigma_{total})/p_0/T} \tag{2}$$

, where $max(\sigma_{total})$ represents maximal collission crosssection (m^2), p_0 represents background gas pressure (Pa) and T background gas temparature (J). The number of grid points (N) is derived from Eq. 2 as follows:

$$N = \text{int}\Big(\frac{L}{\lambda/4} + 0.5\Big) \tag{3}$$

, where L is a distance between electrodes.

In their research, Crosette et al. employed a simulation setup involving 100,000 electrons to model the phenomena of interest. Because of relatively high computational cost of performing such simulation, we performed repeated series of simulations with different numbers of particles consisting of 10,000, 100,000 and 1,000,000. Our investigations showed that although it is possible to achieve satisfactory results with 10,000 particles, the variance in results between individual runs is much higher. on the other hand, increasing number of particles to 1,000,000 lowered the variance even more, but didn't improve the general results, so was not worth the increased computational cost. This observation prompted our decision to utilize the same number of electrons as in Crosette et al. study (100,000). Alongside the electrons, the simulation domain is populated with neutral helium gas, mirroring the experimental conditions.

For boundary conditions within the simulation domain, we implemented an absorbing boundary configuration at its ends. This configuration entails that particles reaching the boundaries at the cathode (ions) or anode (electrons) are effectively removed from the simulation. The simulation proceeds until all electrons exit the computational domain, with a constant timestep of 0.1 picoseconds employed throughout the simulation duration.

For collisional events, we employed cross-sectional data sourced from the Biagi 8.97 database[8]. Throughout all simulation scenarios, we considered electron-neutral collisions exclusively; no ion-neutral collisions were modeled. We accounted for elastic collisions featuring Vahedi scattering [9], ionization collisions incorporating energy-based scattering mechanisms [10][11], and varying sets of excitation collisions paired with isotropic scattering. We have experimented with different configurations of scattering models used. Our final conclusion aligns with a critical observation made by both

Crosette et al. regarding the importance of the Vahedi scattering model which plays the crucial role in achieving accurate results.

Methodology of Townsend coefficient determination

The concept underlying the process of determining the Townsend coefficient involves quantifying the count of ionization events for various static voltages applied to the boundaries of the simulation domain. This sequence of simulations maintains a consistent E/p_0 ratio at a predefined level. To achieve that, the length of the computational domain varies to balance changes of applied voltage. One can deduce the normalized current by correlating the initial electron count and the cumulative ionization events (Eq. 4).

$$\frac{I(x)}{I_0} = 1 + \frac{2N_i}{N_0} \tag{4}$$

Subsequently, discrete outcomes of normalized current can be utilized, along with an alternate normalized current formula, to extract values for α and x_0 (Eq. 5). This is achieved by applying the least squares method, where our research deviated by directly fitting to this formula. Example of resulting fits are presented on Fig. 1

$$\frac{I(x)}{I_0} = e^{\alpha(x-x_0)} \tag{5}$$

An alternative approach introduced by Crosette involves employing log-linear fits. At last, the derived value of α - the first Townsend coefficient - must be divided by p_0, which allows us to compare the results with reference studies ([3] and [4]) with both presented values of α/p_0 rather than measuring/calculating the coefficient directly.

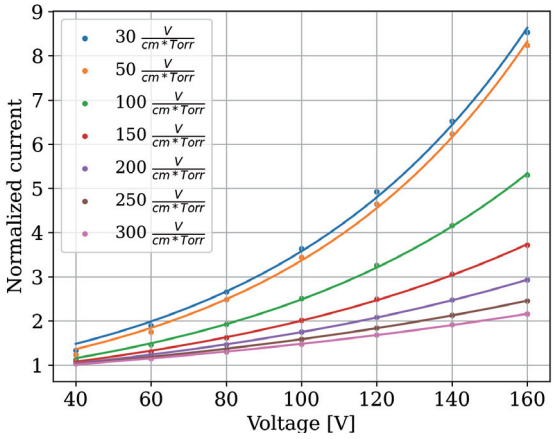

Fig. 1. Results of fitting Eq. 5 to data gathered from simulation with 5 excitation processes, for all values of E/p_0.

Hennel.jl - code validation

Initially, we replicated the simulation configuration outlined by Crosette et al. to ascertain the congruity of our code with their findings. Regrettably, precise results were not presented in their publication. However, since Crosette et al. elucidated the capabilities of the VSim software, supplementary results are available on the Tech-X website [12], serving as a valuable reference for validation purposes. Comaparison of achieved results can be seen in Figure 2. In this investigation, we employed an identical set of five excitation collision processes at energies of 19.82 eV, 20.62 eV, 20.96 eV, 21.22 eV, and 23.09 eV, mirroring the approach of Crosette et al. in their work.

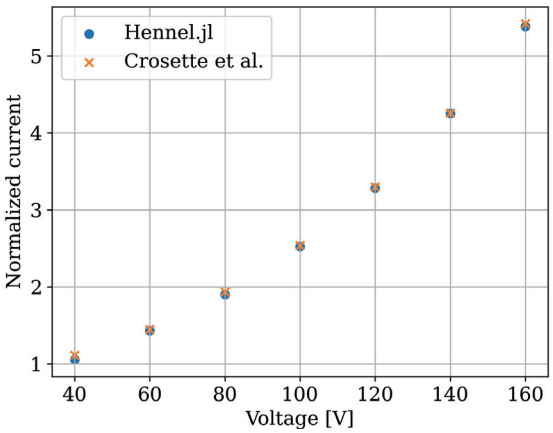

Fig. 2. Normalized current results comparison between Hennel.jl and VSim (Crosette et al.) for $E/p_0 = 100\frac{V}{cm \cdot Torr}$

The computed α/p_0 value reported in [12] for the normalized current vaules from Figure 2 stands at 1.3295, showcasing remarkable proximity to the experimental outcome documented in [3], which stands at 1.31. It should be noted that our code achieved an even higher level of concordance, yielding a value of 1.3092. As evident, the outcomes from our code and those presented by Crosette exhibit an almost indistinguishable similarity. This agreement marked the essential first step in advancing our study.

Subsequently, we replicated the sequence of simulations for a range of E/p_0 values, namely 30, 50, 100, 150, 200, 250, and 300 $\frac{V}{cm \cdot Torr}$. This allowed us to comprehensively compare the outcomes against both experimental data from Chanin and the analytical formula proposed by Lieberman. These results can be seen among others in Figure 3.

Much akin to the observations in the work by Crosette et al., the calculated Townsend coefficient demonstrates excellent concordance at $E/p_0 = 100\frac{V}{cm \cdot Torr}$, while displaying underestimation at higher E/p_0 values and overestimation at lower E/p_0 values.

Results

In their original study, Crossette et al. selected a set of five excitation processes without explicitly providing a rationale behind that choice. Nearly 50 cross-sections for excitation collisions across various energies are available within the Biagi dataset utilized in their study. Among these picked by Crosette, the first four processes correspond to the ones with the lowest energies, with the fifth process ranked tenth in terms of energy. In our investigation, we explored four additional distinct sets of excitation collisions comprising the first 10, 20, 30 processes with the lowest energies and the one incorporating all 49 available excitation processes. The resulting Townsend coefficients are presented in Figure 3.

Summary

Although it is true that increasing the number of particles did lead to a systematic reduction in the disparity between measurements and simulations at E/p_0 values below 100 $\frac{V}{cm \cdot Torr}$ (see Fig. 4), this improvement was rather modest. It's also important to highlight that the resulting value of α/p_0 for 100 $\frac{V}{cm \cdot Torr}$ also decreased, which, in contrast, diminished the previously achieved agreement. Interestingly, the values of α/p_0 for E/p_0 over 100 $\frac{V}{cm \cdot Torr}$ remained rela-

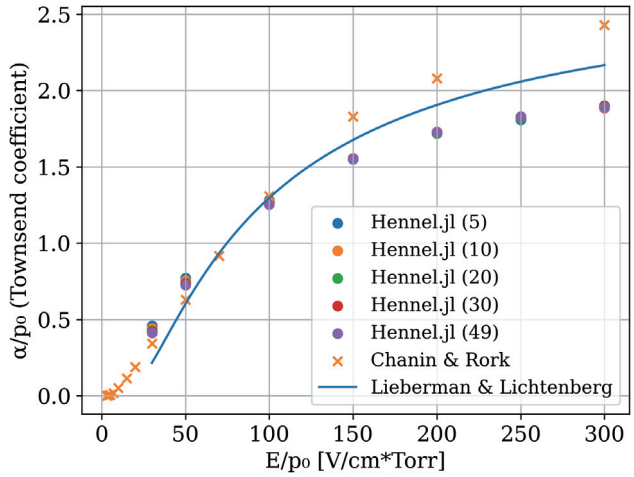

Fig. 3. Townsend coefficient comparison between Hennel.jl (5, 10, 20, 30 and 49 excitation processes), Chanin & Rork and Lieberman & Lichtenberg for various E/p_0

tively unaffected. This could be attributed to the fact that the ratio between energy loss resulting from excitations and the energy stemming from the higher velocity of electrons was significantly smaller in a stronger electric fields.

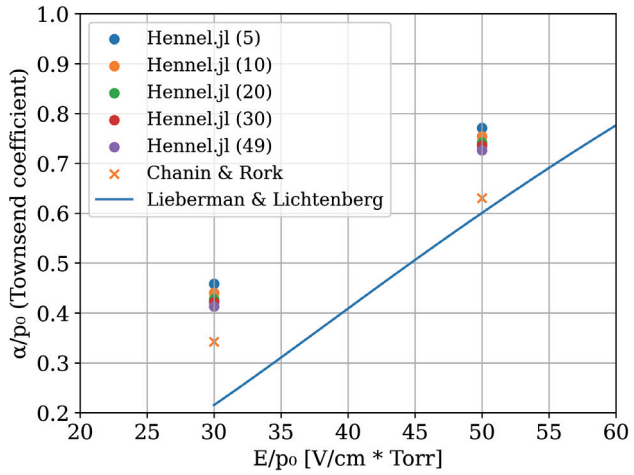

Fig. 4. Townsend coefficient comparison between Hennel.jl (5,10,20,30, 49 excitation processes), Chanin & Rork and Lieberman & Lichtenberg for $E/p_0 = 30\frac{V}{cm \cdot Torr}$ and $E/p_0 = 50\frac{V}{cm \cdot Torr}$

The overall effectiveness of this endeavor hinges on the trade-off between computational and development costs required to incorporate numerous processes into the simulation. In our particular case, the architecture of our library allowed us to circumvent any development costs, and the computational expenses remained minimal.

It appears that achieving precise simulations of the first Townsend coefficient across the entire spectrum of E/p_0 values remains a challenge awaiting further exploration by researchers. As suggested by Crosette et al., a potential path involves the refinement or incorporation of more advanced particle scattering methodologies. Such enhancements have the potential to better capture the intricacies of underlying physics, thereby contributing to more accurate simulation outcomes.

This investigation has demonstrated the capability of our library, Hennel.jl. It underscored the library's effectiveness in simulating the Townsend avalanche phenomenon comparably well to the commercial software. By utilizing the potential of meta-programming, we achieved easy and repetitive generation of optimized code, enabling the computation of results for nearly 200 simulated cases, including scenarios involving 51 collisional processes. Without the library's adeptness, conducting such a comprehensive study would have entailed substantial effort.

We firmly assert that the incorporation of meta-programming and code generation holds significant promise in computational physics. This approach streamlines and expedites research processes, offering a potent avenue for advancing our understanding of complex physical phenomena.

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REFERENCES

[1] J. Townsend: Electricity in gases Oxford: Clarendon press, 1915
[2] N. Crossette, T. G. Jenkins, J. R. Cary, J. Leddy, and D. N. Smithe: Determination of First Townsend Ionization Coefficient by Simulation, 2019 IEEE Pulsed Power & Plasma Science (PPPS), Orlando, FL, USA: IEEE, Jun. 2019, pp. 1–3.
[3] L. M. Chanin and G. D. Rork: Experimental Determinations of the First Townsend Ionization Coefficient in Helium, Phys. Rev., vol. 133, no. 4A, pp. 1005-A1009, Feb. 1964
[4] M. A. Lieberman and A. J. Lichtenberg: Principles of Plasma Discharges and Materials Processing, Lieberman/Plasma 2e. Hoboken, NJ, USA: John Wiley & Sons, Inc., 2005
[5] C. K. Birdsall: Particle-in-cell charged-particle simulations, plus Monte Carlo collisions with neutral atoms, PIC-MCC, IEEE Trans. Plasma Sci., vol. 19, no. 2, pp. 65–85, Apr. 1991
[6] C. Nieter and J. R. Cary: VORPAL: a versatile plasma simulation code, Journal of Computational Physics, vol. 196, no. 2, pp. 448–473, May 2004
[7] J. Bezanson, A. Edelman, S. Karpinski, and V. B. Shah: Julia: A Fresh Approach to Numerical Computing, SIAM Rev., vol. 59, no. 1, pp. 65–98, Jan. 2017
[8] S. Pancheshnyi, S. Biagi, M. Bordage, G. Hagelaar, W. Morgan, A. Phelps, L. Pitchford: The LXCat project: Electron scattering cross sections and swarm parameters for low temperature plasma modeling, Chem. Phys. (2012) 398, 148–153
[9] V. Vahedi, C. K. Birdsall, M. A. Lieberman, G. DiPeso, and T. D. Ronhlien: Capacitive RF discharges modelled by particle-in-cell Monte Carlo simulation. II. Comparisons with laboratory measurements of electron energy distribution functions, Plasma Sources Sci. Technol., vol. 2, no. 4, pp. 273–278, Nov. 1993
[10] Z. Donko et al.: eduPIC: an introductory particle based code for radio-frequency plasma simulation, Plasma Sources Sci. Technol., vol. 30, no. 9, p. 095017, Sep. 2021
[11] C. B. Opal, W. K. Peterson, and E. C. Beaty: Measurements of Secondary-Electron Spectra Produced by Electron Impact Ionization of a Number of Simple Gases The Journal of Chemical Physics, vol. 55, no. 8, pp. 4100–4106, Oct. 1971
[12] VSim Documentation 12.0.3 -r169, VSimExamples: Townsend, [web page] `https://txcorp.com` [Accessed on 25 Jul. 2023.].