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Benchmarking SEDCS and Maxwellian Distribution subroutines in the GPT Ionization Routine

1 Purpose

To benchmark the secondary electron differential cross section (SEDCS) and Maxwellian distribution subroutines for the secondary electron and ion energies respectively in the GPT ionization routine. Both subroutines use known distribution functions and a Monte Carlo routine to assign the energies to the secondary electron and ion. To check the accuracy of these subroutines, we can run a GPT ionization simulation to generate ionization data and then check that the histograms of secondary electron and ion energies follow the shape of the corresponding distribution functions.

2 Benchmarking the SEDCS and Maxwellian Distribution Subroutines

2.1 SEDCS Equation

The equation for the SEDCS used by the ionization routine is from the binary encounter dipole model [1]. Let T be the incident electron energy, B be the binding energy of the secondary electron (i.e. ionization energy), and $U = \left\langle \vec{p}^2 \right\rangle / 2m$ be the average kinetic energy of electrons in the subshell (from which the secondary electron was ejected). Note that $T \geq B + W$. Define energy ratios t, w and u by

$$t = \frac{T}{B}$$
$$w = \frac{W}{B}$$
$$u = \frac{U}{B}$$

Using these definitions, the SEDCS in the Binary Encounter Dipole model is

$$\begin{aligned} \frac{d\sigma}{dW}(T,W) = \frac{4\pi a_0^2 R^2 N}{B^3 (t+u+1)} & \left[\frac{(N_i/N)-2}{t+1} \left(\frac{1}{w+1} + \frac{1}{t-w} \right) \right. \\ & \left. + \left(2 - \frac{N_i}{N} \right) \left[\frac{1}{(w+1)^2} + \frac{1}{(t-w)^2} \right] + \frac{\ln t}{N(w+1)} \frac{df}{dw} \right] \\ N_i \equiv & \int_0^\infty \frac{df(w)}{dw} dw \end{aligned} \tag{1}$$

where $R = 13.6\text{eV}$ is the Rydberg energy, a_0 is the Bohr radius, N is the number of electrons in the orbital, and the term $\frac{df}{dw}$ differential oscillator strength. Using values for B, U, N, and $\frac{df}{dw}$ for H_2 gas given in Ref. [2], we can plot $\frac{d\sigma}{dW}$ (eq. (1)) as a function of secondary electron energy W (i.e. the energy distribution of secondary electrons) for an incident electron energy of $T = 130$ keV below in Figure 1. Clearly the secondary electron will most likely have a much lower energy than the primary electron.

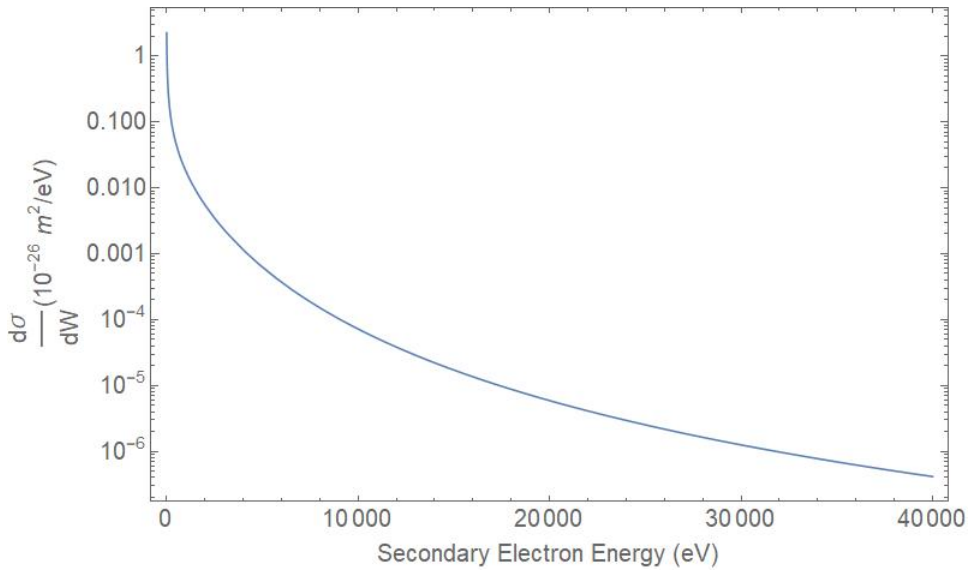

Figure 1: Log plot of the SEDCS $\dfrac{d\sigma}{dW}$ as a function of W, for $T = 130$ keV using eq. (1).

2.2 Maxwellian Distribution Function

The speeds of molecules v in an ideal gas follow a Maxwellian distribution. The probability distribution function for a Maxwellian distribution of particles with density n can be written as:

$$F(v)\,dv \equiv n\sqrt{\frac{2}{\pi}}\frac{v^2 \exp\left(-\dfrac{v^2}{2a^2}\right)}{a^3}dv \tag{2}$$
$$a = \left(\frac{kT}{m}\right)^{\frac{1}{2}}$$

where k is the Boltzmann constant, T is the temperature and m is the mass of a given particle in the distribution.

Let $n = 1$ (i.e. we have a maxwellian "distribution" with only one molecule). We can plot $F(v)\,dv$ for different a:

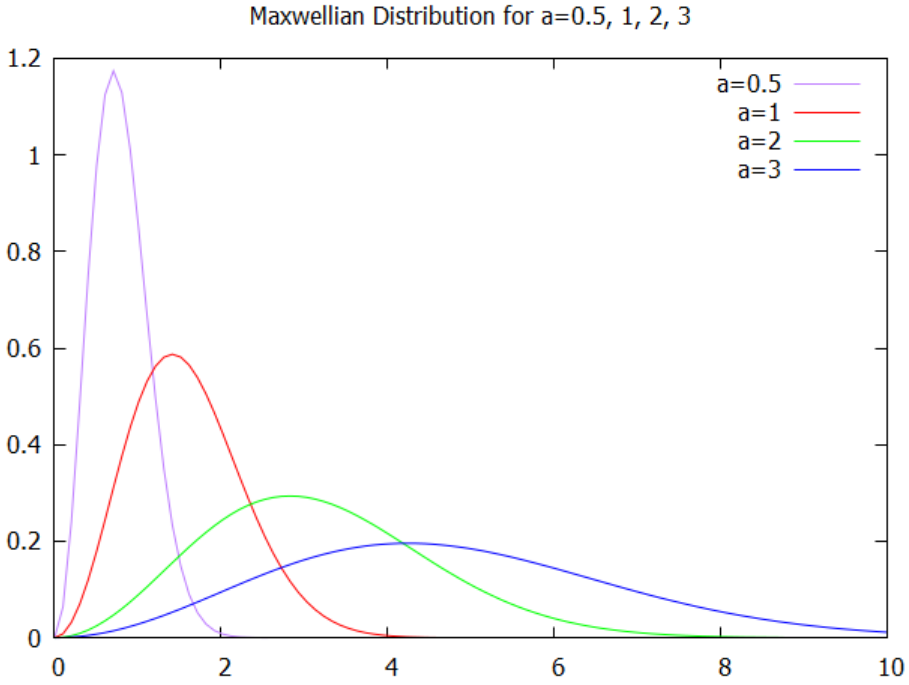

Figure 2: Plots of the Maxwellian probability distribution function for $a = 0.5, 1, 2, 3$

2.3 GPT Simulations

For benchmarking purposes, two GPT electron simulations were created using the ionization custom element. Both simulations involved a uniform "pancake" distribution (1 mm in radius with no longitudinal distribution) of 10^4 electron macro-particles with 130 keV of kinetic energy travelling in the $z-$direction for 0.5 m. The number of electrons each macro-particle in the distribution was set such that the total charge of the distribution was 1 nC for one simulation and 5 nC for the other. In both simulations, the electrons pass through H_2 gas with density 10^{16} m^{-3} with the probability of ionization given by the ionization cross section σ. The form of σ used in the custom element is from Reiser [3] and is not shown here.

Whenever an H_2^+ ion is created in the GPT simulations, a secondary electron is also created. The directions of the H_2 gas molecule, the H_2^+ ion, and secondary electron are random. However, for the purposes of benchmarking, the primary electron's energy and momentum before and after ionization are the same. This ensures that all primary electrons ionize with the same kinetic energy. (Note: the term "primary electron" is taken to mean both the electron macro particles and the secondary electrons. However, since the secondary electrons each represent one electron while the electron macro particles represent billions of electrons, it is highly unlikely that a secondary electron will ionize in the simulation, even though the ionization cross section for a secondary electron is roughly two orders of magnitude higher than that of the electron macro-particles). The energies of the secondary electron and ion are determined based on the SEDCS and Maxwellian distribution functions respectively, the algorithms of which are described in the next section. Note that while the secondary electron energy is based on the primary electron energy T, the ion energy is based on a Maxwellian distribution with the most probable energy set at 4 eV.

2.4 Monte-Carlo Algorithm to Determine Secondary Electron and Ion Energies

The purpose of using a Monte-Carlo algorithm to assigning energies to the secondary electrons and ions is to ensure that the energy chosen is not deterministic. The algorithm involves mapping a random number between 0 and 1 onto a unique E given by the corresponding probability distribution. This ensures that the energy chosen is not deterministic. However, because neither the SEDCS nor the Maxwellian dsitribution are uniform, the following method is used:

Let $p(E)$ be the probability distribution function (representing either the SEDCS or the Maxwellian distribution). We can take a discrete integral of the probability distribution using the trapezoidal approximation up to an energy E_N with the

function:

$$F(E_N) = \frac{1}{2}\sum_{i=1}^{N}(E_i - E_{i-1})\,(p(E_i) + p(E_{i-1})) \tag{3}$$

The stepsize $E_i - E_{i-1}$ is chosen to be very small in order to ensure precision. In this case, the stepsize is $W_N/5000$.

The function $g(N)$ is defined as the ratio between the p integrated up to E_N and the p integrated up to a maximum (cutoff) energy $E_{N_{max}}$:

$$g(N) = \frac{F(E_N)}{F(E_{N_{max}})} \tag{4}$$

Since the SEDCS becomes starts to become unphysical as E approaches the primary electron energy T, the cutoff for the SEDCS is set at $E_{N_{max}} = 0.75(T - I_{H_2})$ where I_{H_2} is the ionization energy of H_2. The cutoff for the Mawellian distribution is taken to be five times the most probable speed, or $v_{cutoff} = 5\sqrt{2}a$. Clearly the range of $g(N)$ is between 0 and 1.

The routine calculates 5000 values of g and stores them in an array G to be used by the Monte Carlo approach:

$$G = \{g(E_{max}/5000), g(E_{max}/5000 + E_{max}/5000), g(E_{max}/5000 + 2E_{max}/5000), \ldots, g(E_{max})\} \tag{5}$$

Note that the elements of G are in ascending order and are between 0 and 1. From here, a random number x is generated and is matched to the closest element of G. The routine finds this value by looping through successive elements of G until x is less than or equal to the element, at which point E is assigned this value. The routine uses a do-while loop that will loop over all secondary electrons and ions produced in this timestep and calculates E for each ion and secondary electron.

2.5 Simulation Results

During each simulation, whenever an ionization occurs, the energies of the secondary electron and ion are written to a text file. These energies can then be tallied in histograms and compared with the theoretical distribution functions. Table 1 below shows the simulation parameters and number of ions created in each simulation.

	Simulation 1	Simulation 2
Total charge of electron macro-particles	1 nC	5 nC
Kinetic energy of electron macro-particles	130 keV	130 keV
H_2 density	10^{16} m^{-3}	10^{16} m^{-3}
Distance travelled by electron macro-particles	0.5 m	0.5 m
Total # H_2^+ ions produced (= # secondary electrons)	1212	6015

Table 1: GPT simulation parameters and results

Figures 3 and 4 below show histograms of secondary electron and ion energies for both simulations. Recall that the ion energies are chosen to follow a Maxwellian distribution with the most probable energy set at 4 eV.

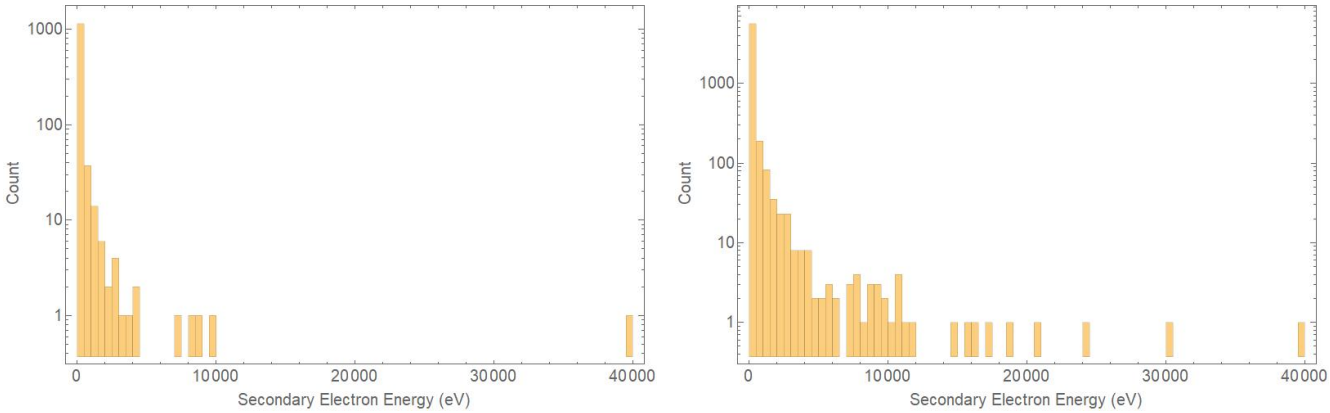

Figure 3: Histograms of secondary electron energies for the 1 nC simulation (left) and 5 nC simulation (right).

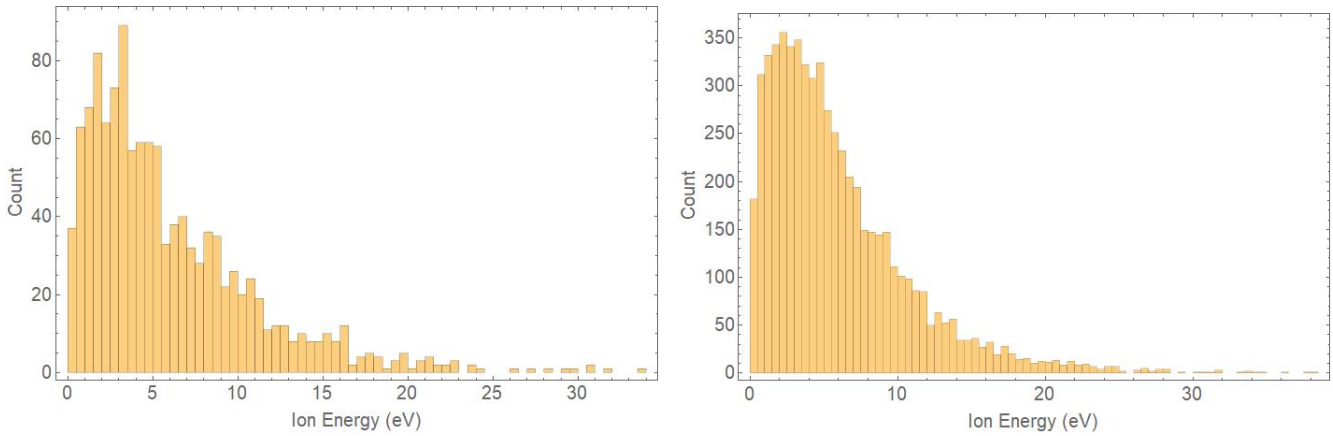

Figure 4: Histograms of ion energies for the 1 nC simulation (left) and 5 nC simulation (right).

Since the form of the Maxwellian distribution function in (2) is a function of the particle *speed*, not energy, the ion energies were converted to speeds based the relativistic kinetic energy equation:

$$v = c\sqrt{1 - \frac{1}{\left(\frac{T}{mc^2} + 1\right)^2}} \tag{6}$$

Figure 5 below shows histograms of ion speeds for both simulations:

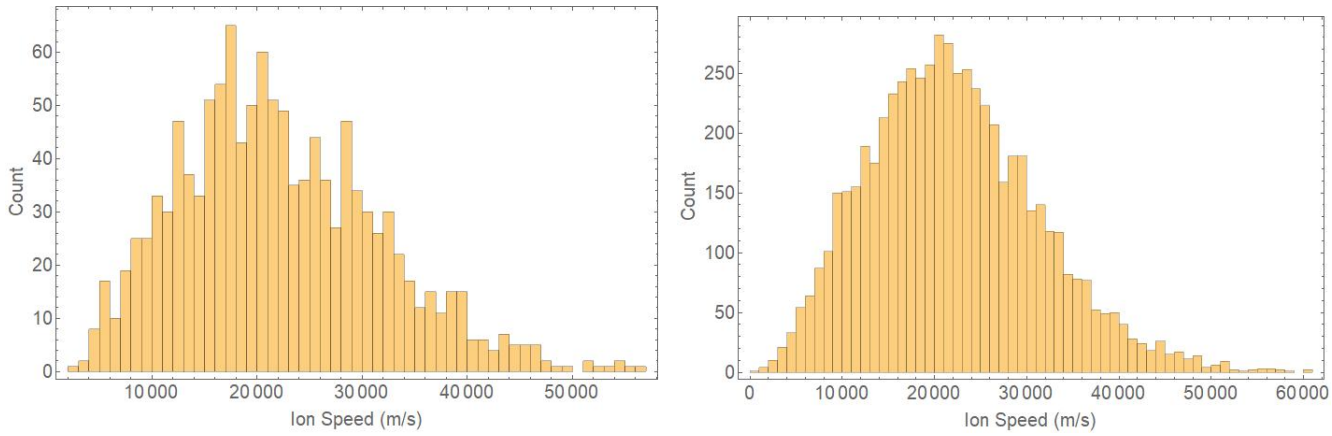

Figure 5: Histograms of ion speeds for the 1 nC simulation (left) and 5 nC simulation (right).

We can compare the histograms in Figures 3 and 5 with their respective distribution functions (eq. (1) and (2)). However, in order to do so, we have to normalize the histograms and distribution functions. The Maxwellian distribution function (2) is already normalized. To normalize the SEDCS, we integrate it from $E = 0$ to $E = E_{N_{max}}$ for $T = 130$ keV. We then set the result equal to $1/A$ where A is the normalization constant:

$$\int_0^{E_{N_{max}}} \frac{d\sigma}{dW}(T, W)\, dW = \frac{1}{A} \tag{7}$$

Using Mathematica, the numerical value for the normalization constant is $A \approx 7.40 \times 10^{23}$. We can "normalize" the histograms in a similar way, where instead of each bar representing the total amount, it represents the relative probability, such that the sum of all relative probabilities equals one. Figures 6 and below show the normalized histograms overlayed with their respective normalized distribution functions:

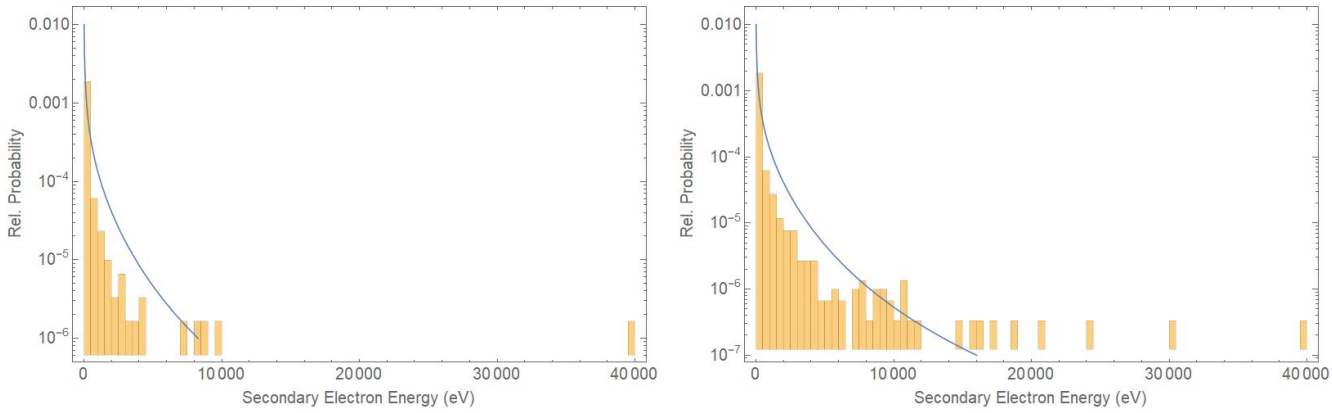

Figure 6: Normalized histograms of secondary electron energies overlayed with the normalized SEDCS for the 1 nC simulation (left) and 5 nC (right).

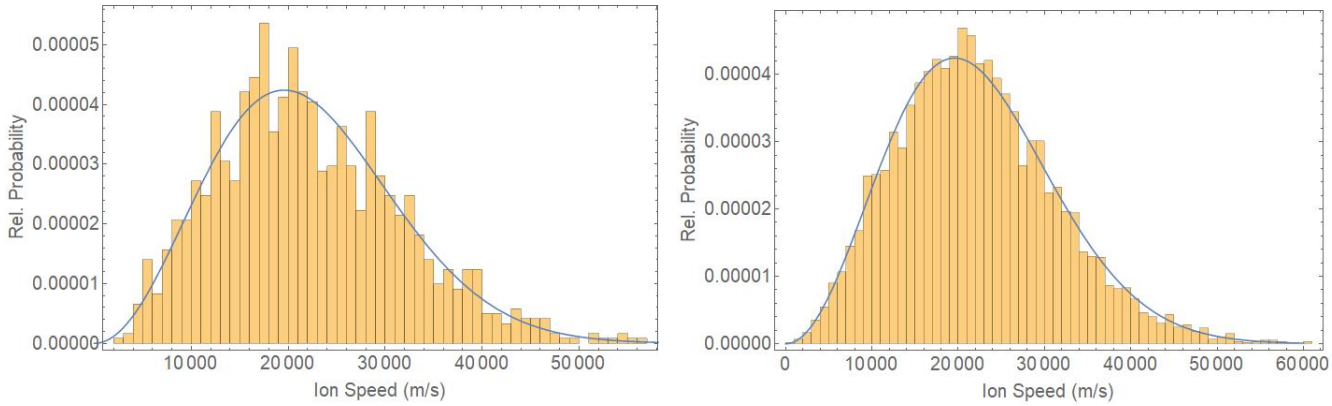

Figure 7: Normalized histograms of ion speeds overlayed with the normalized Maxwellian distribution for the 1 nC simulation (left) and 5 nC (right).

Both sets of histograms show excellent agreement with the theoretical distribution functions, indicating that the SEDCS and Maxwellian distribution subroutines in the GPT custom element are accurate and working correctly.

References

[1] Yong-Ki Kim and M. Eugene Rudd. Binary-encounter-dipole model for electron-impact ionization. *Physical Review A*, 50(5):3954–3967, nov 1994. doi: 10.1103/physreva.50.3954.

[2] Ratko Janev, editor. *Atomic and Molecular Processes in Fusion Edge Plasmas*. Springer US, 1 edition, 1995. ISBN 0-306-45043-7.

[3] Martin Reiser. *Theory and Design of Charged Particle Beams*. Wiley VCH Verlag GmbH, 2008. ISBN 3527407413.