ELEC 4700 Assignment 1: Monte-Carlo Modeling of Electron Transport

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Contents

1 Part 1: Electron Modelling

1. In this problem, the system is 2 dimensional (has 2 degrees of freedom). The thermal velocity is calculated as follows;

$$v_{th} = \sqrt{\frac{2k_B T}{m_e}} \tag{1}$$

where k_B is Boltzmann's constant, T is the temperature and m_e is the effective mass of an electron. The thermal velocity was calculated to be;

$$\boxed{\mathrm{v}_{th} = 1.870\text{e-}5 \text{ m/s}}$$

2. The mean free path is the average distance travelled before a collision. It is calculated as;

$$MFP = v_{th}\tau_{min} \tag{2}$$

where τ_{min} is the mean time between collisions. The mean free path is

$$\boxed{MFP = 3.74e - 8m}$$

3. The code was developed as instructed. The value of Δt was chose to be 0.2e-12 seconds. The simulation was run for 100 time steps and 20 particles were plotted. A plot of the particle trajectory and temperature is shown in Figures 1 and 2, respectively;

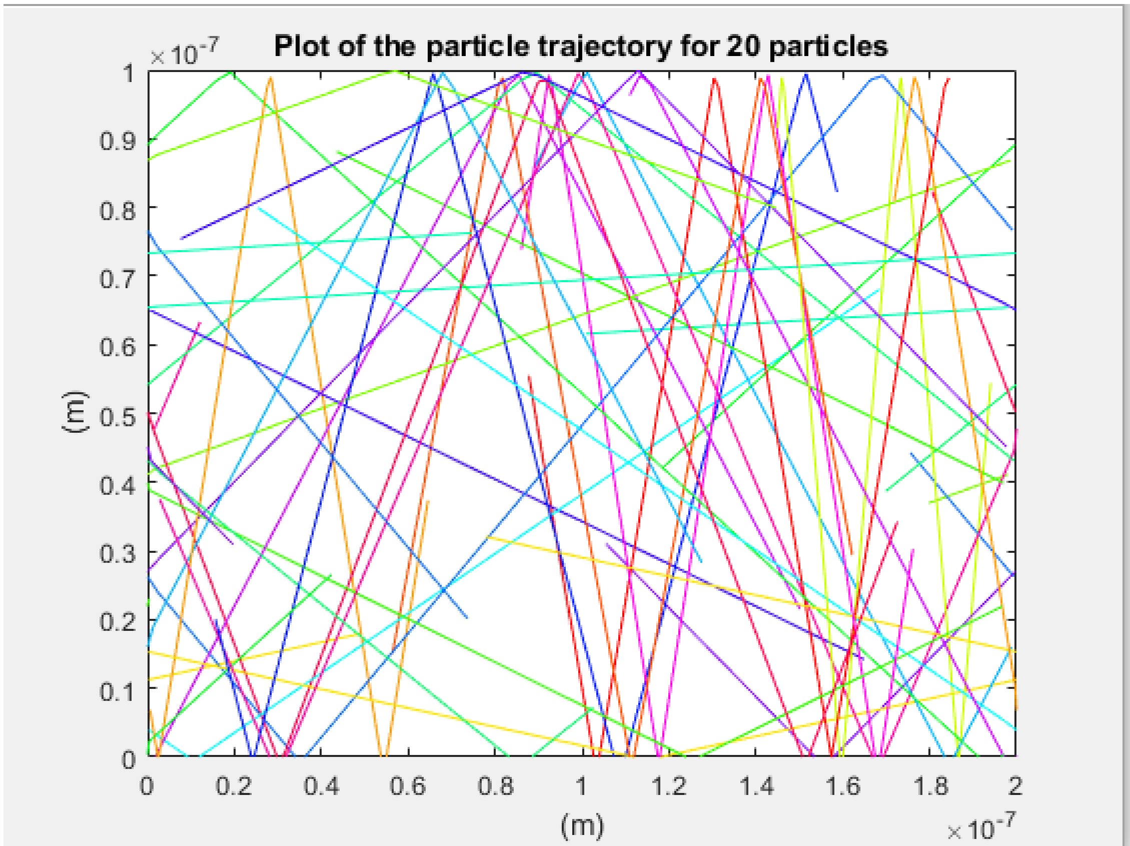

Figure 1: Trajectory plot of the particles

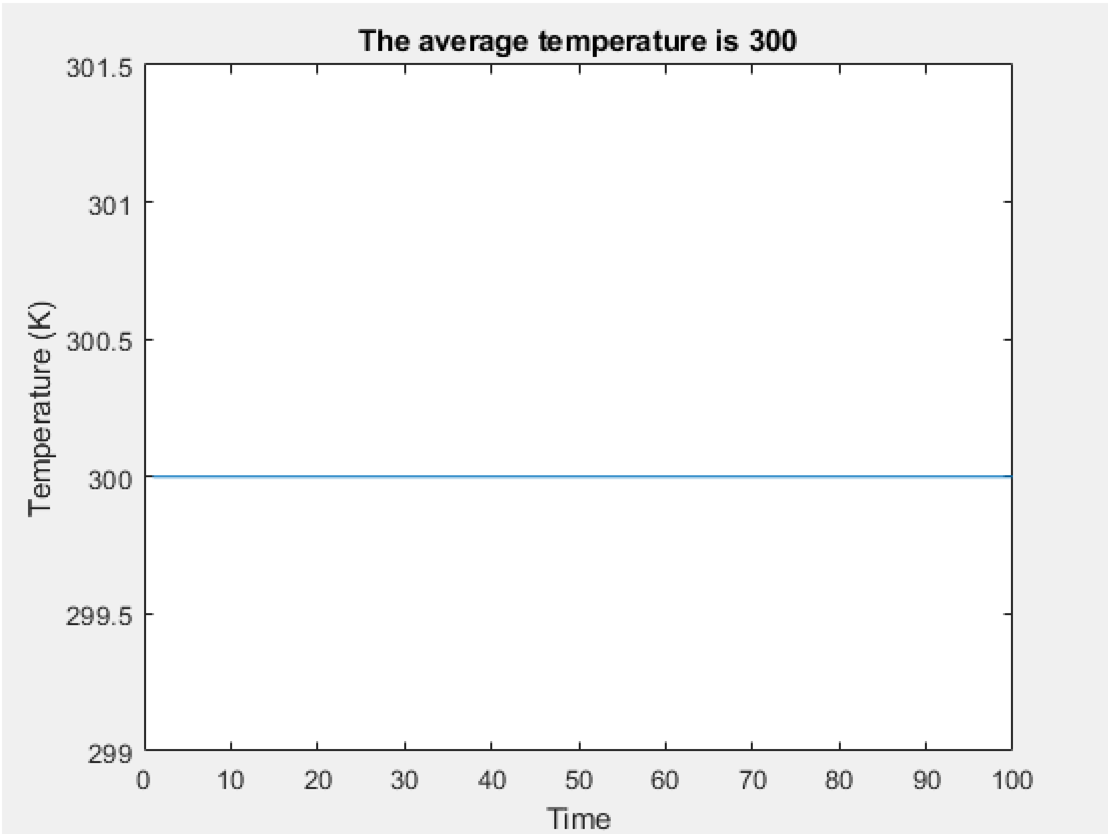

Figure 2: Temperature plot of the particles

As expected, the temperature remains constant at 300K throughout the entire simulation.

2 Part 2: Collisions with Mean Free Path

The code for collisions with mean free path was developed. The average temperature was calculated as;

$$T_{avg} = \frac{V_{avg} m_e}{2k_b} \tag{3}$$

where V_{avg} is the sum of the squared x and y velocity components. Compared to Part 1, the average temperature is no longer constant over time. This is because the scattering of electrons changes the average velocity and in turn changes the temperature.

A histogram of the initial velocity is show below;

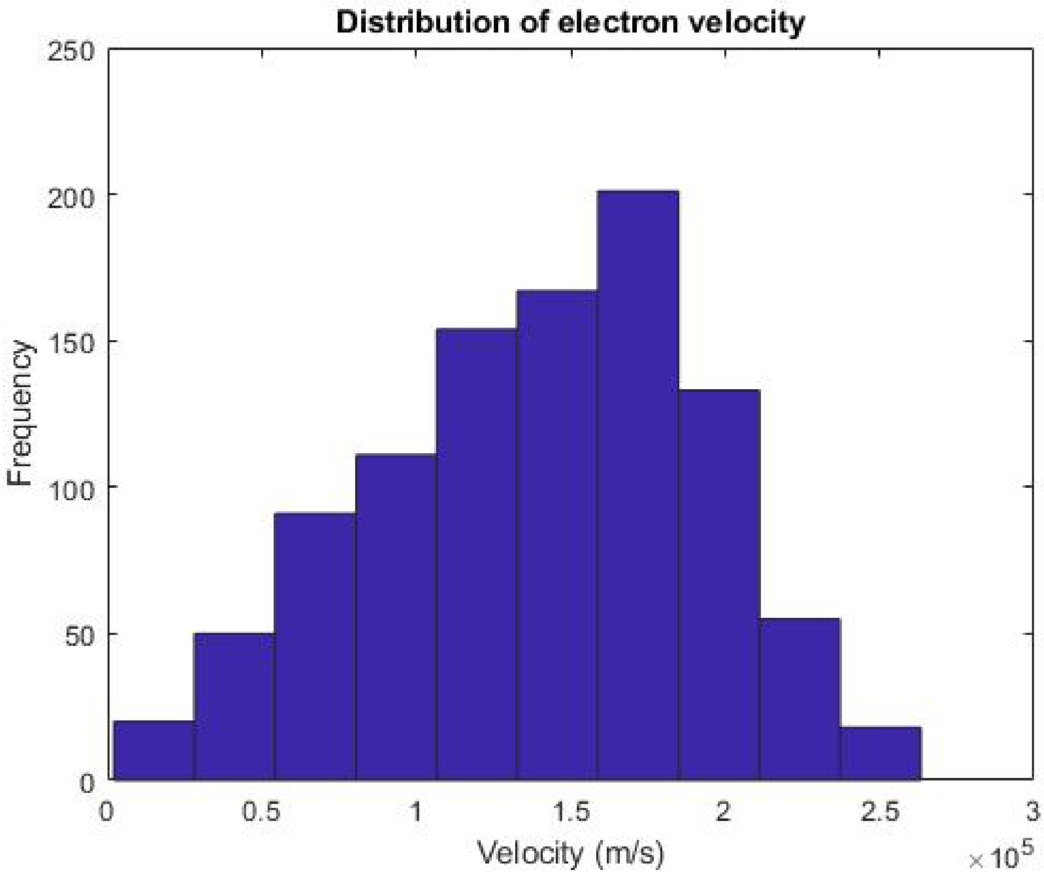

Figure 3: Histogram of the initial velocity

A 2-D plot of the particles trajectories is shown below;

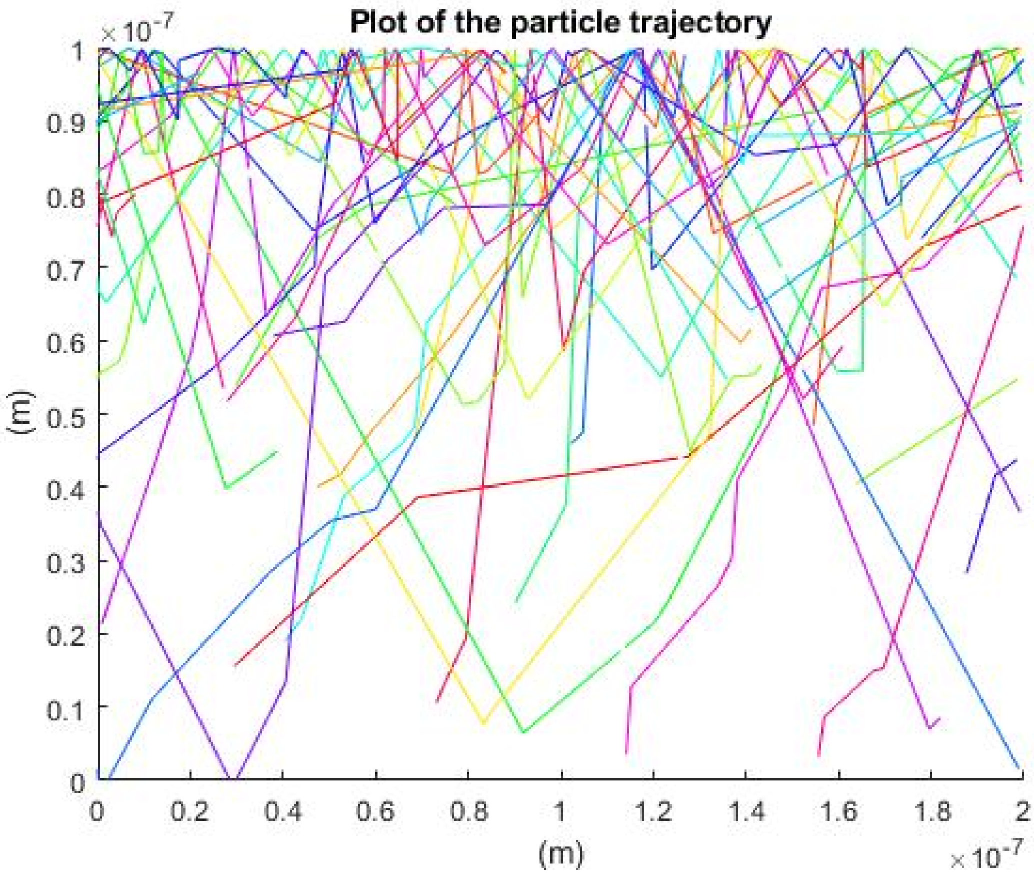

Figure 4: Trajectory plot of the particles

A plot of the temperature is shown;

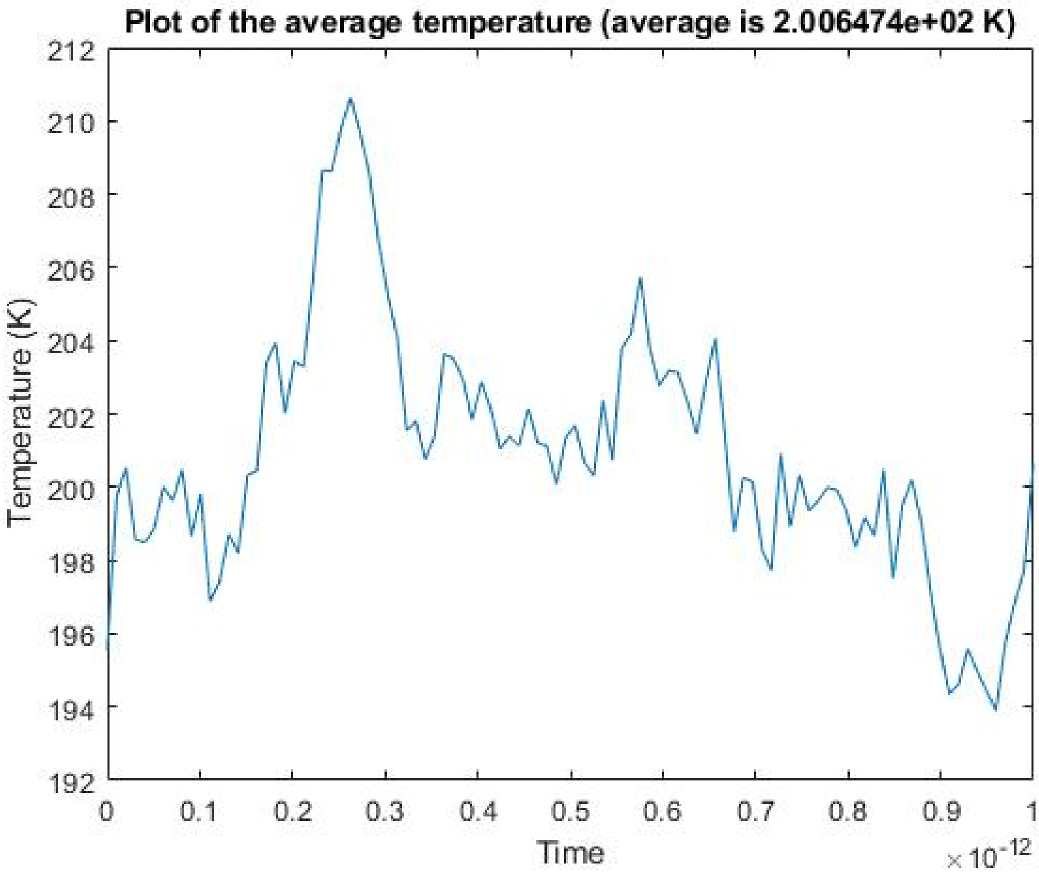

Figure 5: Temperature plot of the particles

The average temperature for this run was 200 K. The mean free path was calculated as follows;

$$MFP = \frac{d}{n_{collisions}} \tag{4}$$

where d is the distance travelled and $n_{collisions}$ is the number of collisions. It was evaluated to be

$$\boxed{MFP = 4.01441e-08m}$$

The average time between collisions was calculated as;

$$\tau = \frac{time}{n_{collisions}} \tag{5}$$

it was evaluated to be;

$$\boxed{\tau = \text{2.09e-16 sec}}$$

3 Part 3: Enhancements

A bottleneck was added with specular and diffusive boundary conditions. Using specular boundaries, the following plots were obtained;

The simulation was run for 100 time steps and for 500 particles (20 particles were plotted). A 2-D plot of the particles trajectories is shown below;

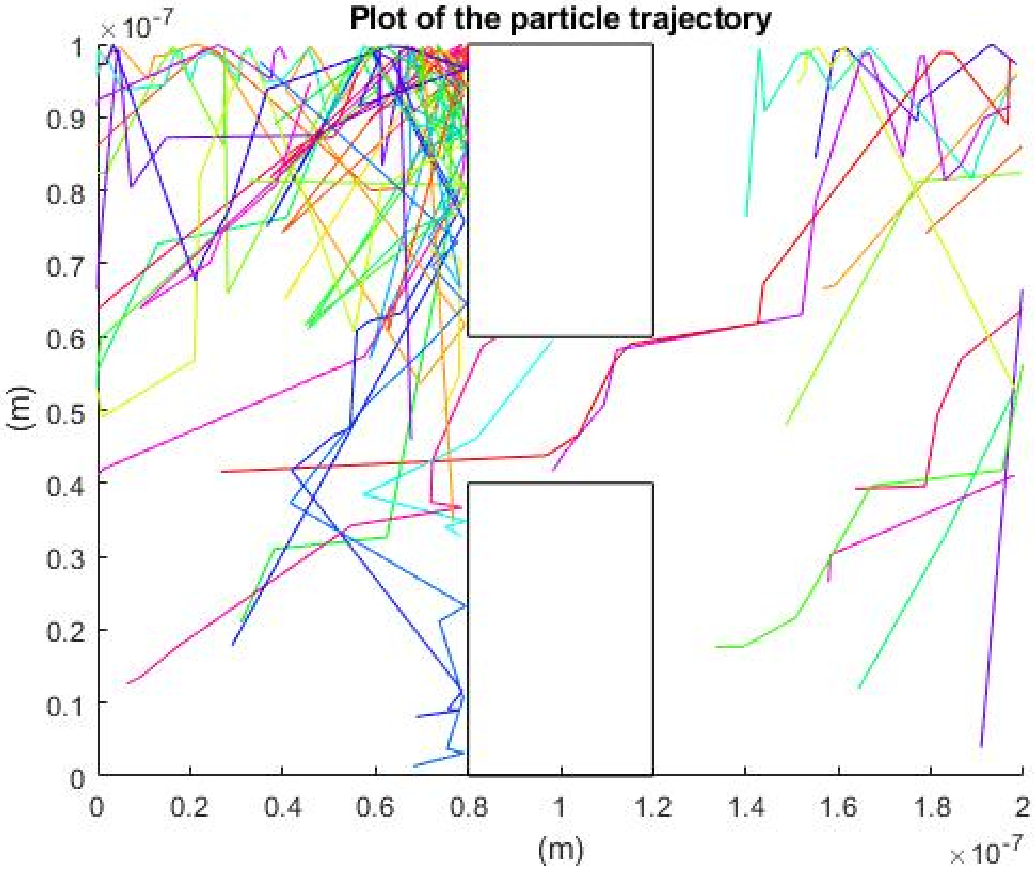

Figure 6: Trajectory plot of the particles

An electron density map is shown below;

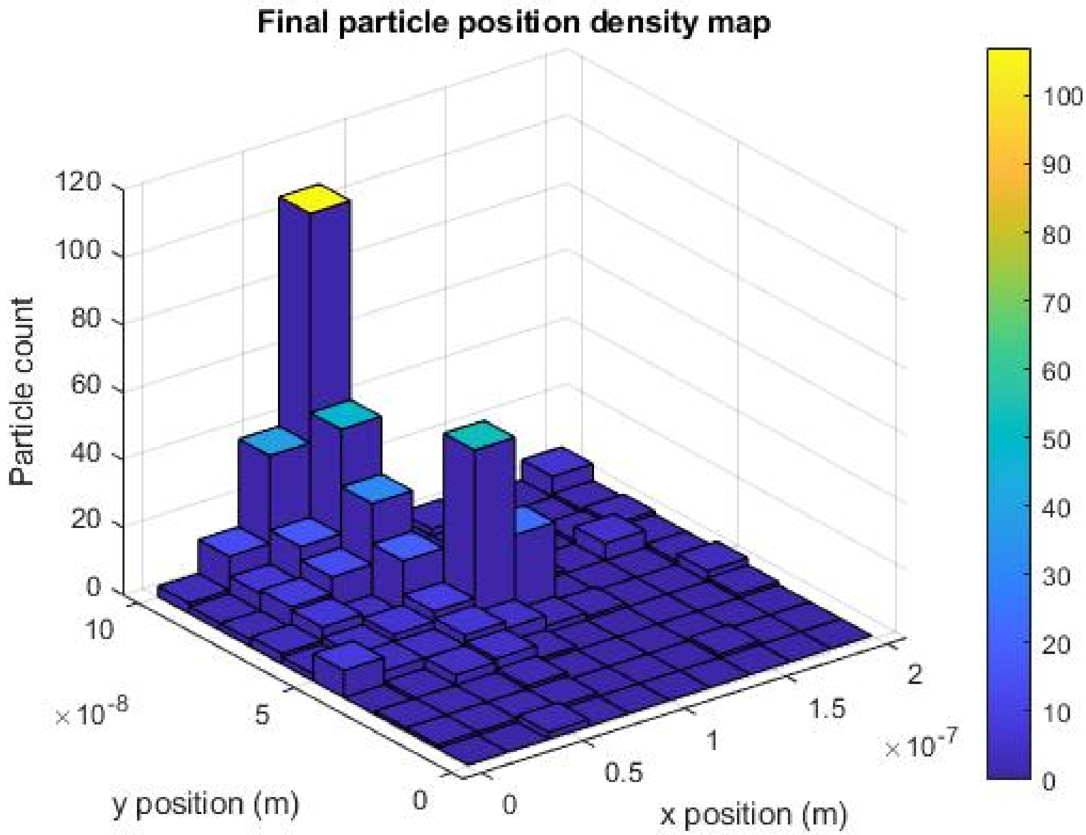

Figure 7: Density map of the particles

A plot of the temperature is shown;

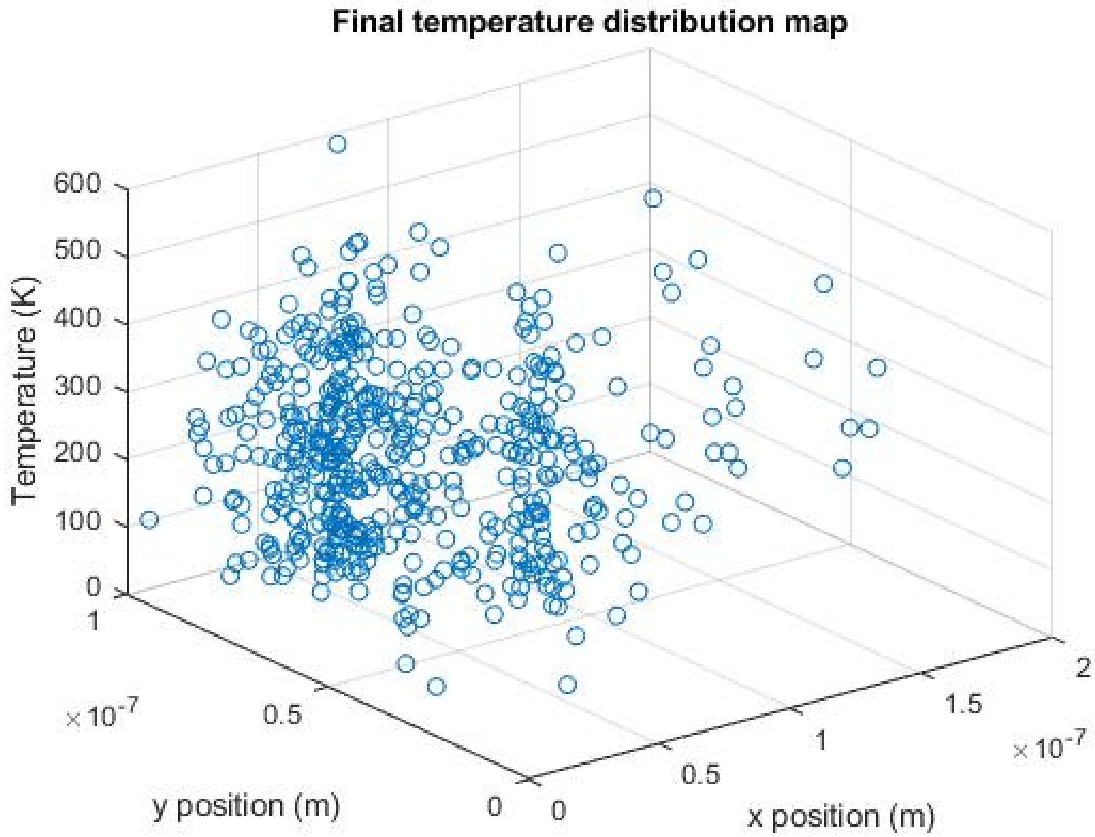

Figure 8: Temperature plot of the particles