

Monte Carlo Calculation of Mean Free Paths of Electrons in Air

I. Introduction

The goal of this project is to simulate (in two dimensions) the motion of an electron as it moves through a collection of 100 molecules. These molecules are given initial random positions and have velocities chosen randomly to match a Boltzmann distribution. The basic quantities computed are the time for the first collision between the electron and a molecule and the distance traveled by the electron during this time. Repeated trials with a number of electrons then gives rise to a mean free path.

II. Computer Program

The calculation may be logically divided into four parts. First, the initial conditions of the system are used to setup the problem. Second, the initial positions and velocities of the molecules are chosen. Third, the molecules' positions are calculated until they cross the line of trajectory of the electron. Finally, a check is made to see if the electron and molecule collide. A search is then made to find the earliest electron-molecule collision and the time of this collision is recorded after correction to convert from a two to three dimensional system.

A. Initial Conditions

The prime consideration of this part of the calculation is to choose the size of the box containing the molecules so as to make the average inter-particle spacing correspond to a real ideal gas at pressure P . The inter-particle spacing may be obtained in the following way. Assume we have an ideal gas at temperature T and pressure P . The volume V occupied can be obtained from the ideal gas law,

$$PV = nkT \quad (1)$$

where n is the number of molecules in the system and k is Boltzmann's constant. Solving for V

$$V = nkT / P \quad (2)$$

We may consider this volume as a cube with side $V^{1/3}$. Then

$$V^{1/3} = (nkT / P)^{1/3} \quad (3)$$

If we consider the n molecules as evenly distributed throughout the cube, then $n^{1/3}$ of the molecules will lie along one edge of the cube. The spacing between these molecules, s , will then be

$$s = \frac{V^{1/3}}{n^{1/3}} = \frac{(nkT / P)^{1/3}}{n^{1/3}} = \frac{kT}{P} \quad (4)$$

If we use N molecules in our two dimensional box, then there will be $N^{1/2}$ molecules on a side. Since the separation between molecules is s , the length of the box is

$$L = N^{1/2} s = N^{1/2} \frac{kT}{P} \quad (5)$$

The square containing the molecules thus has a side of length L and is located in an x-y coordinate system as shown in Figure 1.

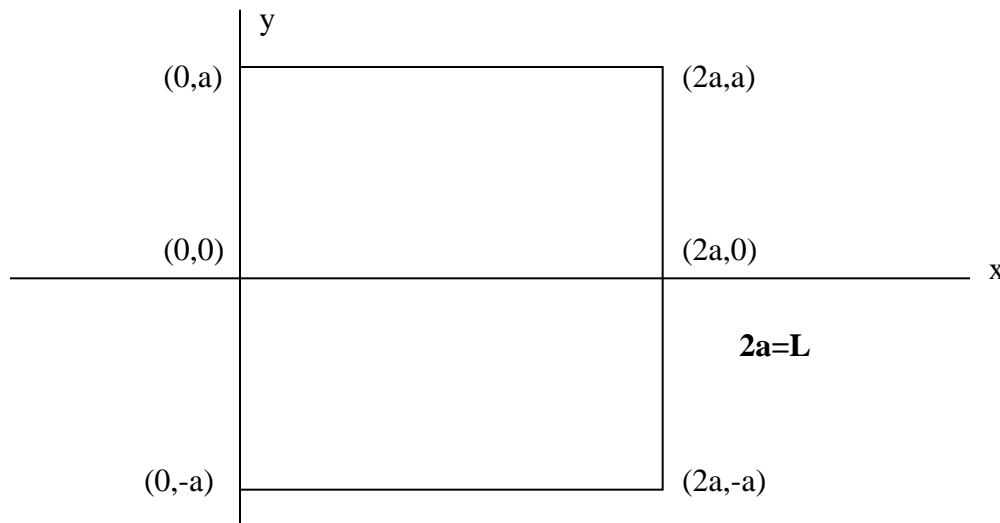


Figure 1.

The electron is introduced at the origin and travels back and forth between $(0,0)$ and $(2a,0)$ along the x-axis.

B. Initial Positions and Velocities of Molecules

The molecules are chosen to have molecular weight 28, thus representing the major component of air, nitrogen. In order to randomly generate initial positions and velocities for the molecules a technique must be found to generate random numbers. Most programming languages offer a random number generator that generates numbers in the range $0 < R < 1$. You should make your own tests to insure randomness as a function of random number order. For example, if you plot 1000 random numbers, they should equally populate ranges from 0-0.1, 0.1-0.2, etc. Secondly, if you compare the distribution of random numbers greater than 0.5 to those less than 0.5 for small sets of random numbers, the two distributions should be equal.

The initial position of a molecule is chosen so that the molecule is equally likely to be anywhere between $x=0$ and $x=2a$. Thus for the i^{th} particle its initial x position is obtained from

$$x_i = 2aR \quad (6)$$

where R is a random number between zero and one. Similarly, the y position is

$$y_i = 2aR' - a \quad (7)$$

where R' is a second random number.

Choosing the velocities for a molecule is a bit more complicated since all velocities are not equally probable. For a large sample of molecules in equilibrium, the fraction of molecules having an x component of velocity between $|v_x|$ and $|v_x| + d|v_x|$ is

$$f(|v_x|)d|v_x| = A \exp\left(-mv_x^2 / 2kT\right)d|v_x| \quad (8)$$

where A is a normalization constant and is determined by requiring that

$$\int_0^\infty f(v)dv = 1 \quad (9)$$

This distribution function must be converted to one that is uniformly distributed between zero and one. We now proceed to discuss this conversion.

Suppose we wish N_0 molecules to have speeds in the range $(0, \infty)$ with distribution $n(v)$. Then

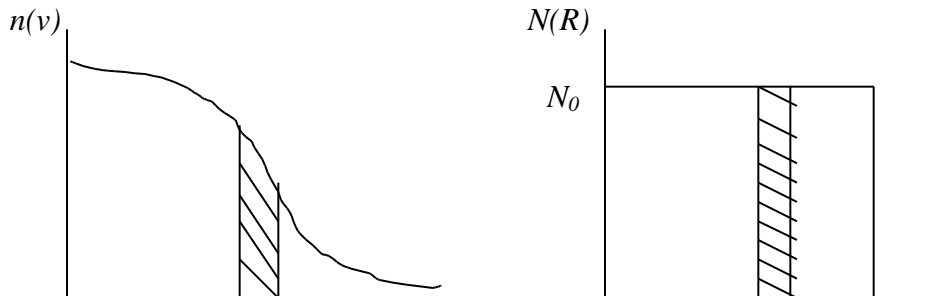
$$N_0 = \int_0^\infty n(v)dv \quad (10)$$

Now consider a random variable R uniformly distributed over the range $(0,1)$ and associate a value of R with each particle. Then denoting the number of molecules associated with an R in the range $(R, R + dR)$ by $N(R)dR$, it follows that (see Figure 3)

$$N_0 = \int_0^1 N(R)dR \quad (11)$$

All the particles lying within the range $(R, R + dR)$ also lie within $(v, v+d v)$. Therefore

$$N(R)dr = n(v)dv \quad (12)$$



$$0 \quad v \quad v+dv \quad v \quad 0 \quad R \quad R+dR \quad 1 \quad R$$

Figure 2
It follows from Equation (12) and Figure 3 that Figure 3

$$n(v)dv = N_0 dR \tag{13}$$

Integrating we find

$$\int_0^v n(v) dv = \int_0^R N_0 dR = N_0 R \tag{14}$$

For a given $n(v)$, this may be solved to give $v=v(R)$ which is the velocity assignment required to produce the velocity distribution $n(v)$.

According to (8), our present concern is with a distribution of the form

$$n(v) = C \exp(-mv^2 / 2kT) \tag{15}$$

where C is determined by

$$N_0 = \int_0^v C \exp(-mv^2 / 2kT) dv \tag{16}$$

This standard definite integral yields

$$C = N_0 \frac{2m}{kT}^{1/2} \tag{17}$$

Now to find $v=v(R)$ we use Equation (14)

$$N_0 R = \int_0^v n(v) dv$$

$$N_0 R = \int_0^v N_0 \frac{2m}{kT}^{1/2} \exp(-mv^2 / 2kT) dv \tag{18}$$

This may be rearranged by a change of variable to yield

$$x = \sqrt{\frac{m}{2kT}} v \tag{19}$$

$$R = \frac{1}{2} \int_0^{\frac{mv^2}{2kT}^{1/2}} \exp(-x^2) dx \tag{20}$$

This can be written as

$$R = \operatorname{erf} \left(\frac{mv^2}{2kT} \right)^{1/2} \quad (21)$$

where

$$\operatorname{erf}(z) = 2 \int_0^z \exp(-t^2) dt \quad (22)$$

We may now solve Equation (20) for v

$$\operatorname{erf}^{-1}(R) = \left(\frac{mv^2}{2kT} \right)^{1/2} \quad (23)$$

or

$$v = \frac{2kT}{m} \operatorname{erf}^{-1}(R) \quad (24)$$

The function $\operatorname{erf}^{-1}(R)$ is the inverse error function and yields the number whose error function is R . This function will not be part of the standard set of functions supplied by computer languages. You will need to find a numerical approximation to calculate this function. Having to do this kind of searching is a normal part of doing research. Contact your instructor for help if you run into trouble.

We may now choose velocity components for our particles in the x and y directions by using Equation (24). The choice of sign is made randomly by choosing another random number and associating a plus sign with the velocity if this number is greater than 0.5 and a minus sign if it is less than 0.5.

C. Collisions of Molecules and Walls

We must solve the equations of motion of the molecules to determine the molecules' trajectories in the box. If we consider an individual molecule, the procedure is as follows. By considering the molecule's position and velocity a determination may be made as to which wall of the box the molecule will strike. A check is made to see if the molecule trajectory will intersect the electron trajectory before striking a wall. If it does, the time of crossing the electron trajectory and the x -position of the crossing point are stored and the next molecule is considered. If the molecule trajectory does not cross the electron trajectory before reaching a wall, the molecule is allowed to bounce off the wall in specular reflection (like light from a mirror) and a determination is made as to which

wall it will strike next. Again we check to see if the electron path is crossed. The process is repeated until the molecule crosses the path of the electron.

After the crossing time is determined for the first molecule, the second molecule is considered, etc. Thus we build up in storage a list which contains the first crossing times and crossing positions for all 100 molecules.

Let us take a sample case and see how the calculation proceeds. Suppose we have a molecule with velocity components v_x and v_y located at position (x,y) and suppose v_x and v_y are positive. If v_x and v_y are positive, the molecule can only strike the top or right walls of the box. To determine which wall it will be, we compute the time required if it were to reach the top wall,

$$t_{top} = (a - y) / v_y \quad (25)$$

and the time required if it were to reach the right wall,

$$t_{right} = (2a - x) / v_x \quad (26)$$

Whichever time is shorter is the wall the molecule will strike. Suppose $t_{top} < t_{right}$. Then the molecule will strike the top wall. Now we can determine the exact position on the top wall where the molecule strikes (x_n, y_n) .

$$x_n = x + v_x t_{top} \quad (27)$$

$$y_n = a \quad (28)$$

Now we must determine if the molecule crossed the electron trajectory. Since the electron always moves on the $y=0$ line, the y -position of the molecule must change sign from its prior position if it is to cross the electron's path. Thus, we must simply test for a sign difference between y_n and y .

The time required to get from (x,y) to the x -axis is

$$t_1 = |y / v_y| \quad (29)$$

and the location of the crossing is

$$x_c = x + t_1 v_x \quad (30)$$

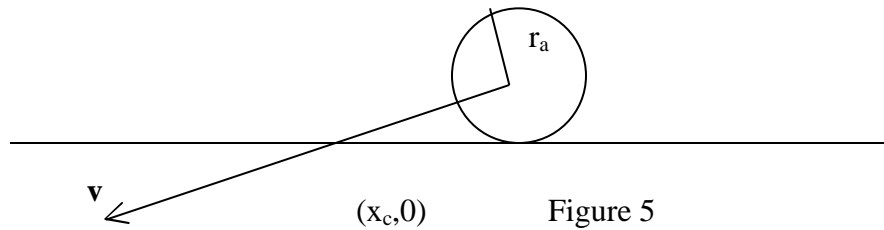
Thus the absolute time of the crossing occurs at

$$t_c = t + t_1 \quad (31)$$

where t is the absolute time at which the molecule was located at (x,y) .

D. Collisions of Molecules and Electrons

Now we must determine if a collision of the electron and a molecule will occur when the molecule crosses the x-axis. The molecule is backed up in time until just a point on the surface of the molecule touches the x-axis. The position of the center of the molecule is obtained.



In the example shown v_y is negative as is v_x . The position of the molecule is

$$x_m = x_c + r_a (v_x / v_y) \quad (32)$$

$$y_m = r_a \quad (33)$$

The absolute time at which the molecule is in this position is

$$t_e = t_c + r_a / v_y \quad (34)$$

Next we need to determine the position of the electron at time t_e . The total distance traveled by the electron is

$$D = v_e t_e \quad (35)$$

where v_e is the velocity of the electron. We define Z as the total number of trips the electron has made.

$$Z = D / 2a \quad (36)$$

Let

$$Z = I + F \quad (37)$$

where I is an integer and F is less than one. If I is even, the electron is running left to right and if I is odd, the electron is running right to left. When I is even the position of the electron at time t_e is obtained from

$$x_e = 2aF \quad (38)$$

and when I is odd from

$$x_e = 2a - 2aF \tag{39}$$

In the latter case v_e is set equal to $-v_e$.
 Now to determine if a collision will take place, a coordinate transformation is performed. The transformed coordinates are such that the molecule is at rest and all motion is centered in the electron. This situation is depicted in Figure 6.

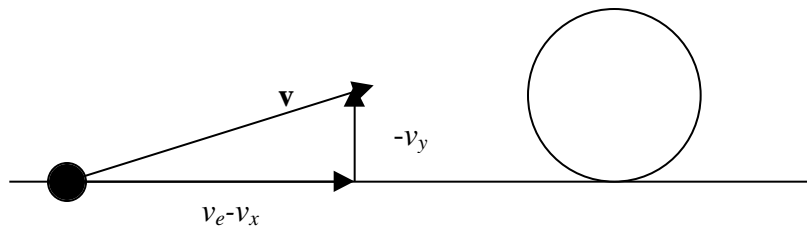


Figure 6

The velocity of the electron is now $v_e - v_x$ in the x-direction and $-v_y$ in the y-direction.

The question of whether or not the electron will collide with the molecule is now reduced to one of geometry. As can be seen from Figure 6, the angle is determined by the transformed velocity of the electron

$$\tan \theta = \frac{-v_y}{v_e - v_x} \tag{40}$$

If this angle is less than the angle θ_c in Figure 7 a collision will occur.

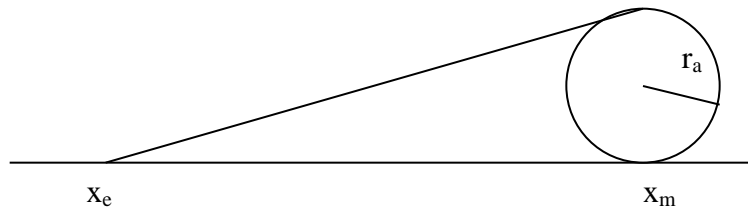


Figure 7

In Figure 7,

$$\tan = \frac{2r_a}{x_m - x_e} \quad (41)$$

If a collision occurs, the exact time of the collision is determined and the total distance traveled by the electron is calculated and stored. All 100 molecules are checked for collisions. The time of the earliest collision is saved and the calculations continue until the crossing times for all molecules have exceeded the time of the earliest collision. The distance traveled by the electron during the time until the earliest collision represents the free path of the electron.

Finally, to compare this two-dimensional calculation to experimental data that is obtained in the real three-dimensional world it is necessary to derive a correction factor. This correction factor will then multiply the above-calculated free path to make it correspond to the three-dimensional case.

We may consider the two-dimensional case we have calculated to be a slice from a three-dimensional box of dimension $2a \times 2a \times 2a/10$. Here the added dimension $2a/10$ represents the average spacing between molecules. In reality, our 100 molecules should be distributed throughout the volume of this box, not confined to a plane. This means we are overestimating the probability of a collision by a factor of the added dimension of the box divided by the diameter of the molecules. The required correction factor is thus

$$\frac{2a}{10} / 2r_a = \frac{a}{10r_a} \quad (42)$$

The free paths obtained earlier are thus multiplied by this factor.

The calculation is now repeated from the beginning for another electron and a new electron free path is obtained. The electron mean free path is then obtained by taking the average of many such free paths.

III. Calculations

You should run calculations to assess the influence of pressure and electron energy on the mean free path. Each calculation should run several hundred electrons.

Begin with a pressure of 10 μ Hg and a temperature of 350°K. Take the radius of nitrogen to be 3 Angstroms and use an electron energy of 100 eV. You should get a mean free path of 8 or 9 cm. The individual free paths will vary over a wide range.

You should consider what happens if a molecule's velocity in the y-direction is very small. The program may run for an inordinate amount of time before the molecule manages to cross the x-axis and if a collision doesn't occur the program will again run for a very long time before another crossing occurs. Consider discarding y-velocities below some arbitrary value or alternatively if the electron has already run many meters without a collision stop the calculation and re-do that molecule.

Do calculations for a range of electron energies. How does the mean free path depend on energy?

What is the distribution of free paths? What do we expect? Suppose we have a beam of electrons. We further suppose that in traversing a distance x , the beam suffers a decrease in number of electrons n . We expect the fraction of electrons lost, dn/n , to be proportional to x . If $1/\lambda$ is the proportionality constant then

$$\frac{dn}{n} = -\frac{1}{\lambda} dx \quad (43)$$

The minus sign signifies that the number of particles in the beam decreases for an increase in distance traveled. This expression can be converted to the differential form

$$\frac{dn}{n} = -\frac{1}{\lambda} dx \quad (44)$$

which upon integration yields

$$n(x) = A \exp(-x/\lambda) \quad (45)$$

where λ is the mean free path. The number of electrons colliding in dx is

$$dn = -\frac{A}{\lambda} \exp(-x/\lambda) dx \quad (46)$$

Thus, a plot of the \ln of the number of electrons colliding versus x should yield a straight line with slope of $-1/\lambda$.

Separate your free path data into intervals and plot \ln of the number in each interval as a function of x . Do you get a straight line? What is its slope? How does this value compare to the mean free path you calculated earlier? What can you conclude about the distribution of free paths as a function of distance?

Repeat the calculations at a single electron energy for a range of pressures. How does the mean free path depend on pressure? How should it depend on pressure?