Problem 1: Derivation of a 2-dimensional gas that can't escape a surface

a) Derive the maxwell-Boltzmann speed distribution for a 2-dimensional gas

$$in\ a\ one - dimensional\ plane\ we\ know\ that$$

$$P(v_x)\ dx = \left(\frac{m}{2\pi kT}\right)^{\frac{1}{2}} * \exp\left(-\frac{1}{2} * m * \frac{v_x^2}{kT}\right)\ dv_x$$

$$From\ a\ cartesian\ coordinate, we\ have$$

$$v^2 = v_x^2 + v_y^2$$

$$P\left(v_x, v_y\right)\ dv_x dv_y = P(v_x)P\left(v_y\right)\ dv_x dv_y = \frac{m}{2\pi kT} * exp\left(-m * \frac{v_x^2 + v_y^2}{2KT}\right)\ dv_x\ dv_y$$

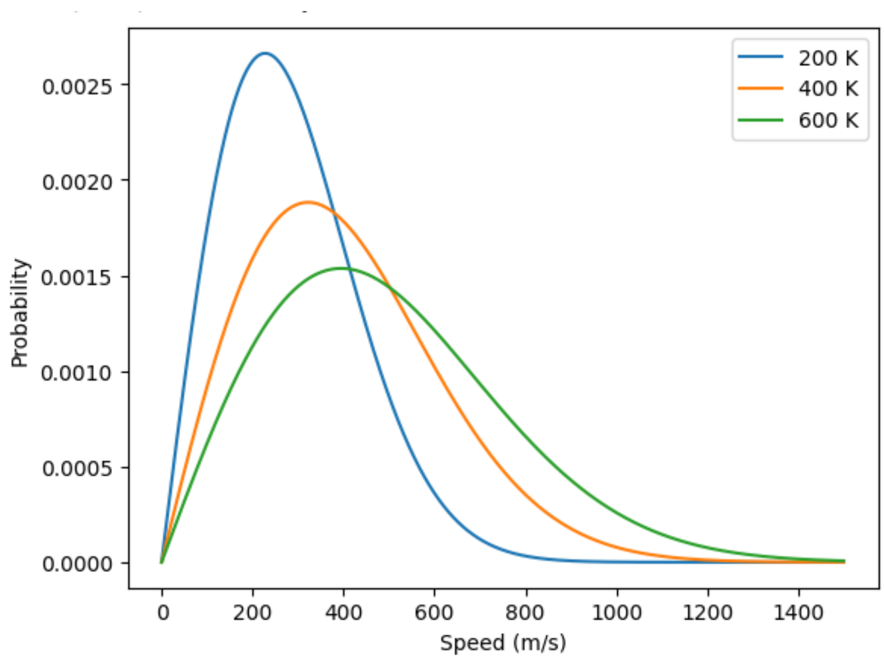
$$We\ convert\ to\ a\ polar\ coordinate, recall\ dv_x dv_y = v\ dv\ d\theta$$

$$P(\mathrm{v}) = \int_0^{2\pi} \frac{mv}{2 * \pi * k * T} * exp\left(-\frac{mv^2}{2KT}\right)\ \ d\theta$$

$$= 2\pi * v * \frac{m}{2 * \pi kT} * exp\ (-\frac{mv^2}{2KT})$$

$$= \frac{mv}{kT} * exp\ (-\frac{mv^2}{2KT})$$

b) Plot this 2-dimensional speed distribution for O2 molecule at 200, 400, and 600 K
See code in ipynb




```
m = 32*1.6605e-27 # kg k = 1.38e-23 # j/K
k = 1.38e-23 # j/K


## Making a function as defined p(v)
def Probability(v,T):
    return v*m/(T*k)*np.exp(-m*v*v/(2*k*T))

plt.figure()

v = np.linspace(0,1500,1000)
for T in [200,400,600]:
  Prol = Probability(v,T)
  plt.plot(v,Prol,label = '{} K'.format(T))

legend = plt.legend()
plt.xlabel('Speed (m/s)')
plt.ylabel('Probability')
```

c) Calculate the mean speed of a 2-dimensional gas of molecules. How does your answer compare to a one and 3-dimensional gas?

$$From\ class, we\ have < v > = \int_0^{\infty} P(v) * v\, dv$$

$$we\ plug\ into\ the\ equation\ to\ get < v_z >, which\ is\ the\ mean\ velocity$$

$$< v > = \int_0^{\infty} \frac{v^2 * m}{kT} \exp\left(-\frac{mv^2}{2kT}\right) dv$$

$$using\ a\ u\ sub$$

$$u^2 = \frac{mv^2}{2kT}$$

$$2\ u\ du = \frac{mv}{kT}\ dv$$

$$dv = \frac{kT}{mv} * 2\ u * du$$

$$< v > = \int_0^{\infty} \frac{v^2 m}{kT} \exp(-u^2)\ \frac{kT}{mv}\ 2\ u\ du$$

$$simplifying, it\ becomes$$

$$< v > = \int_0^{\infty} 2 * v * u * \exp(-u^2)\, du$$

$$v = \ u * \left(\frac{2 * k * T}{m}\right)^{\frac{1}{2}}$$

$$< v > = \left(\frac{2 * k * T}{m}\right)^{1/2} \int_0^{\infty} 2\ u^2 * \exp(-u^2)\, du$$

$$\int_0^{\infty} 2\ u^2 * \exp(-u^2)\ du = \frac{\sqrt{\pi}}{2}$$

$$< v > = \left(\frac{\pi\ k\ T}{2\ m}\right)^{\frac{1}{2}}$$

Compared to the square root of the 3-dimensional gas, they are all dependent on the square root of T/m. It's expected to be bigger in 3-dimensions

d) Calculate the mean kinetic energy of the particle

$$< v^2 >= \int_0^{\infty} \frac{v^2 * m}{kT} \exp\left(-\frac{mv^2}{2kT}\right) * v\, dv$$

$$< \epsilon > =< \frac{1}{2} mv^2 > = \frac{1}{2}\, m < v^2 > = \frac{1}{2}\, m \int_0^{\infty} \frac{v^3 * m}{kT} \exp\left(-\frac{mv^2}{2kT}\right) dv$$

$$< \epsilon > = \frac{1}{2} \int_0^{\infty} \frac{v^3 * m^2}{kT} \exp\left(-\frac{mv^2}{2kT}\right) dv$$

$$u^2 = \frac{mv^2}{2kT}$$

$$2u\, du = \frac{mv}{kT}$$

$$dv = \frac{kT}{mv} * 2\, u * du$$

$$< \epsilon > \; = \frac{1}{2} \int_0^{\infty} \frac{v^3 * m^2}{kT} \exp(-\, u^2)\ \frac{kT}{mv} * 2u * du$$

$$< \epsilon > \; = \; m \int_0^{\infty} v^2\ \exp(-u^2) * u * du$$

$$< \epsilon > \; = m \int_0^{\infty} \frac{u^2 2kT}{m}\ \exp(-u^2) * u * du$$

$$< \epsilon > = 2\ kT \int_0^{\infty} u^2\ \exp(-u^2) * u * du$$

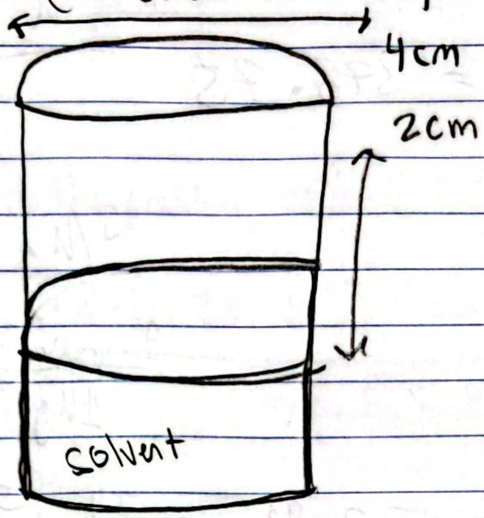
$$\int_0^{\infty} u^2\ \exp(-u^2) * u * du = 1/2$$

$$< \epsilon > = 1.0\ k\ T$$

1 dimensional gas, the mean kinetic energy is 0.5 kT, 3D is 1.5 kT; 2 dimensional is 1.0 kT. The mean kinetic energy degree of freedom cost is 0.5 kT

HW#2

Problem 2. (Kinetics and Transport)



5. What does gas Kinetic theory predict for the gas self-diffusion constant D_{11} of CO_2 gas in the cell, in $cm^2 s^{-1}$?

Solution:

Lets gather the data we need first:

CO_2 :

Carbon: 12.01 amu
Oxygen: 15.99 amu

CO_2 : 44 amu

$$44 \cancel{amu} \times \frac{1.66 \times 10^{-27} Kg}{1 \cancel{amu}} = 7.30 \times 10^{-26} Kg$$

$K_B = 1.38 \times 10^{-23}$ J/K

$T = 298$ K

$d_{collision} = 0.40$ nm , 1 nanometer $= 1 \times 10^{-9}$ m

Next, going back to what was seen in class we know that:

$$\langle v \rangle = \left(\frac{8K_BT}{\pi m} \right)^{1/2}$$ mean speed is the expected value of the speed distribution

According to the problem, we have CO_2 at 298K

After calculating the mean speed, we can calculate the collision cross section:

$A = \pi d^2$; In lecture notes A was called sigma σ. d is the collision diameter.

The following step is to calculate the mean free path: distance between collisions

$$l = \frac{K_BT}{P} \cdot \frac{1}{\sqrt{2} A}$$; Pressure is 1 bar or 1×10^5 Pascal.

Lastly, calculating the self-diffusion constant:

$$D_{11} = \underbrace{\frac{1}{3}}_{\text{dimensionality of the space in which diffusion occurs}} \cdot l \cdot \langle v \rangle$$ In 3-D

Calculations are in jupyter notebook. The gas self-diffusion constant is 0.07 cm^2/s approximately.

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6. Use the Stokes-Einstein relationship to estimate the diffusion constant of CO_2 in the Stoddard solvent. How does this compare with the diffusion constant in the gas phase? Why?

Solution:

For stick boundary, as seen in class we have

$$D = \frac{K_B T}{4\pi \eta r}$$

; appropiate to things of size comparable to liquid

; η represents the viscosity of the fluid in Stokes-Einstein relationship in which the particles are diffusing

1 nanometer $= 1 \times 10^{-9}$ m

Collision radius $= 0.2 \times 10^{-9}$ m

η viscosity = this can be in a range of .74 to 1.65 mPa·s

$\eta = 1e^{-3} \frac{Kg}{m \cdot s}$; $1 Pa = 1 \frac{Kg}{ms^2}$

and 0.001 Pa·s $= 1$ mPa·s

Calculations are in jupyter notebook. The diffusion constant of CO_2 in the Stoddard solvent is approximately 1.63×10^{-5} cm^2/s.

The diffusion constant of CO_2 in the Stoddard solvent is lower compared to the diffusion constant in the gas phase. The solvent introduces additional interactions that impedes the moverent of solute particles.

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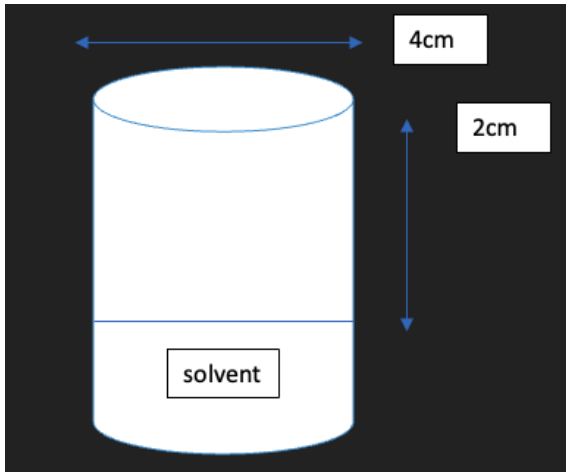
PChem: HW#2

Problem 2. (Kinetics and Transport)



5. What does gas kinetic theory predict for the gas self-diffusion constant D11 of CO2 gas in the cell, in cm^2 s^-1 ?

Solution:

In [72]:
```
import numpy as np
```

Let's gather the data we need first:

In [85]:
```
m = 44*1.66e-27 #kg/atomic mass unit; 1 atomic mass unit = 1.66e-27 kg
kB = 1.38e-23 #J/K
T = 298 #K
d = 0.4e-9 #collision diameter (m)
P = 1e5 #Pa
```

Next, calculating the mean speed and plugging in the data we obtain:

In [86]:
```
v = (8*kB*T/(np.pi*m))**0.5 # mean speed (m/s)
print("The mean speed is {:.2f} m/s".format(v))
```

```
The mean speed is 378.65 m/s
```

Third, calculate collision cross section:

In [87]:
```
A = np.pi*d**2 # collision cross section (m^2)
print(A)
```

```
5.026548245743669e-19
```

The following step is to calculate the mean free path:

In [88]:
```
l = kB*T/p*(1/(2**0.5*A)) # mean free path (m)
print(l)
```

```
5.785095029007004e-08
```

Lastly, calculating the self-diffusion constant:

In [89]:
```
D11 = 1/3*l*v*10000 # self-diffusion constant (cm^2/s); Extra factor 10000 to convert to cm^2/s
print("The gas self-diffusion constant is {:.2f} cm^2/s".format(D11))
```

```
The gas self-diffusion constant is 0.07 cm^2/s
```

6. Use the Stokes-Einstein relationship to estimate the diffusion constant of CO2 in the Stoddard solvent. How does this compare with the diffusion constant in the gas phase? Why?

Solution:

Defining constants

In [90]:
```
r = 0.2e-9 # defining collision  radius (meters)
eta = 1e-3 #units:kg/(meters * seconds);
#eta represents the viscosity of the fluid in Stokes-Einstein relationship in which the particles are di

kB = 1.38e-23 #J/K
T = 298 #K
```

Then calculating the diffusion constant:

In [91]:
```
D_stoddard = kB*T/(4*np.pi*eta*r)*10000 # slip boundary (cm^2/s); Extra factor 10000 to convert to cm^2/s
print ('The diffusion constant of CO2 in the Stoddard solvent is {:.5E} cm^2/s.'.format(D_stoddard))
```

```
The diffusion constant of CO2 in the Stoddard solvent is 1.63627E-05 cm^2/s.
```

The diffusion constant of CO2 in the Stoddard solvent is lower compared to the diffusion constant in the gas phase. There is a solvent in this case compared to the one before. The solvent introduces additional interactions that impedes the movement of solute particles.