SOUL - Physics Simulations Project using Apps on Physics

Motion of Particles in an Ideal Gas

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ABSTRACT

The experiment determines the **probability distribution of particles in an ideal gas.** Ideal gas is a hypothetical gas, theorised by the assumptions of the Kinetic Theory of Gases; it is composed of randomly moving particles without interparticle interactions.

Ideal gas obeys the Ideal Gas Law (given below), from which other gas laws can be derived.

$$pV = nRT$$

where, P = pressure, V = volume

n = number of moles, R = universal gas constant

T = temperature

Maxwell-Boltzmann distribution provides a statistical framework to understand the microscopic behaviour of particles in a gas. It describes the distribution of speed of particles in a gas at thermal equilibrium. From this probabilistic distribution, we find the values of
(i) most probable speed (ii) mean speed (iii) root mean square speed.

The required experiment, **Motion of Particles in an Ideal Gas**, is provided in **Apps on Physics**, under **Thermodynamics**. The app shows a virtual interface of particles moving in a box. Variable values within certain limits can be entered such as the amount of substance, temperature and, pressure, which yields the volume.

The app provides the (i) component of velocity of the particles in an ideal gas and (ii)magnitude of velocity. The latter provides the varied speeds of particles in the ideal gas in accordance with Maxwell-Boltzmann distribution. On selecting any of the four gases provided in the app, and varying the values of pressure, temperature and, amount of substance, we deduce the behaviour of component of velocity, most probable speed, mean speed and, root mean square speed.

While the ideal gas model simplifies the complexity of real gases, it is in fact a fundamental tool for analysing the macroscopic and microscopic dynamics of gases.

AIM OF THE EXPERIMENT

To determine the probabilistic distribution (component and magnitude of velocity) of gases and verify simple gas laws.

INTRODUCTION

In a gas, unlike solids or liquids, the particles (atoms or molecules) are spaced relatively far apart that fill its container volume and exert pressure on its walls at a certain temperature. To illustrate the random motion of gas particles, a simulation is presented, using the ideal gas model as a foundation. The behaviour of gases is described by the Kinetic Molecular Theory of Gases (KMT) and is used to explain macroscopic properties of a gas, such as pressure, temperature, and volume, in terms of its microscopic components, such as atoms. This theory was developed in reference to ideal gases, although it can be applied to real gases as well. The assumptions of KMT are-

- Gases are made up of particles with no defined volume but with a defined mass.
- Gas particles undergo no intermolecular attractions or repulsions which implies that the particles possess no potential energy and their total energy is simply equal to their kinetic energies.
- These particles are in continuous, random motion in straight lines
- Collisions between them are completely elastic.
- The average kinetic energy is the same for all gases at a given temperature, regardless of the identity of the gas.

An ideal gas is a hypothesized gas for which the pressure P, volume V, and temperature T are related by the Ideal Gas Law. It states;

$$pV = nRT \tag{1}$$

where n is the number of moles of gas and R is called gas constant with a universal value of R=8.31 J/mol K.

This equation is straightforward and therefore highly idealized. While an ideal gas does not exist in reality, all real gases approximate ideal behaviour at low densities, where their molecules are sufficiently far apart to minimize interactions. Thus, the ideal gas concept allows us to gain useful insights into the limiting behaviour of real gases.

From the Ideal Gas Law, we observe that:

i. Pressure is directly proportional to number of molecule and temperature.
ii. Pressure, however, is indirectly proportional to volume.

The simple gas laws (Boyle's Law, Charles' Law, and Avogadro's Law) form the basis of the Ideal Gas Law.

Boyle's Law states that at constant temperature, the pressure of a gas (P) is inversely proportional to its volume (V).

$$P \propto \frac{1}{V} \quad \text{or} \quad PV = \text{constant} \tag{2}$$

Charles's Law states that the volume of a fixed amount (V) of gas is directly proportional to its temperature (T, measured in Kelvin) when the pressure remains constant.

$$V \propto T \quad \text{or} \quad \frac{V}{T} = \text{constant} \tag{3}$$

Avogadro's Law states that at constant temperature and pressure, the volume of a gas (V) is directly proportional to the number of moles (n).

$$V \propto n \quad \text{or} \quad \frac{V}{n} = \text{constant} \tag{4}$$

The gas particles move with various speeds. In 1852, Scottish physicist James's clerk maxwell solved the problem of finding the speed distribution of gas molecules. His result known as **maxwell's speed distribution law**, is

$$\boldsymbol{P(v) = 4\pi \left(\frac{M}{2\pi RT}\right)^{3/2} v^2 e^{-\frac{Mv^2}{2RT}}} \tag{5}$$

where M is the molar mass of the gas, R is the gas constant, T is the gas temperature, and v is the molecular speed. It provides the fraction of particles in a system moving at specific speeds or possessing certain kinetic energies. The quantity P(v) (in Eq. 5 and Fig. 1) is a probability distribution function: for any speed v, the product **P(v) dv** is the fraction of molecules with speeds in the interval dv around v. This fraction is equal to the area of a strip with height P(v) and width dv. The total area under the distribution curve corresponds to the fraction of the molecules whose speeds lie between zero and infinity.

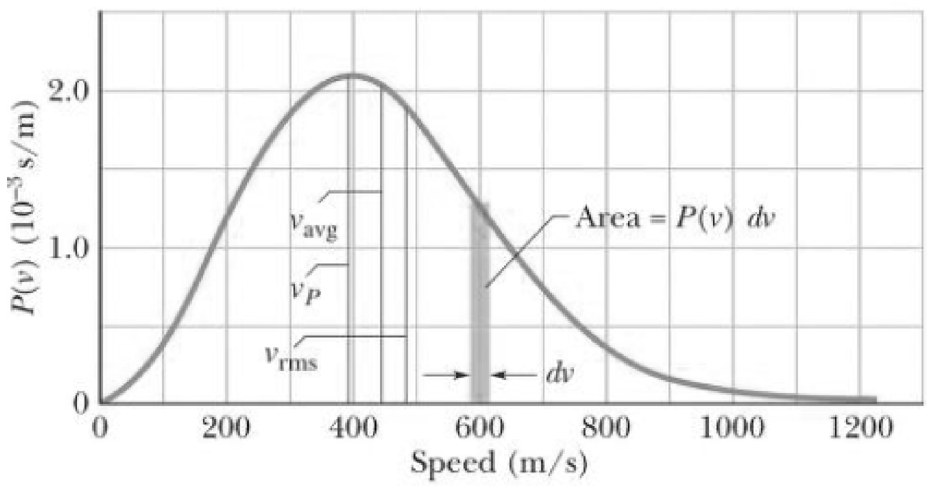

Figure 1- The Maxwell speed distribution with the three characteristic speeds marked. Speed (m/s) is in x-axis and probability in y-axis.

From this distribution, we get;

Most Probable Speed, v_p, is the speed at which most particles are moving.

$$\boldsymbol{v_p = \sqrt{\frac{2RT}{M}}} \tag{6}$$

Mean Speed, ⟨v⟩, is the average speed of the particles.

$$\boldsymbol{\langle v \rangle = \sqrt{\frac{8RT}{\pi M}}} \tag{7}$$

Root Mean Square Speed, v_{rms}, is the square root of the average of the squares of speeds.

$$\boldsymbol{v_{rms} = \sqrt{\frac{3RT}{M}}} \tag{8}$$

Now, let's familiarise ourselves with the app. The control panel of this app features two buttons. The first, "Reset" initializes the system to its starting state, while the second, "Start/Pause/Resume" allows you to start, stop, or continue the animation. The "Slow motion" option reduces the animation speed. Users can select the gas type from four options: nitrogen (N_2), oxygen (O_2), argon (Ar), and hydrogen (H_2). The behaviour of gases varies due to differences in their molecular properties.

Numerical inputs are available—within specified limits—for the amount of substance (measured in moles), absolute temperature (in Kelvin), and pressure (in kilopascals). These inputs must be confirmed by pressing the Enter key. Below the input fields, the calculated volume is displayed in cubic centimetres. In certain cases, the pressure is adjusted to ensure the volume remains between 100 cm^3 and 1000 cm^3. Users can control the speed of the simulation, pausing or slowing down the movement of particles to better understand the interactions and how they evolve over time.

The radio buttons in the lower part of the control panel determine what will be displayed in the drawing area:

- Animated illustration of the particle motion in a cube-shaped container with edge length 10 cm; of course, the number of represented particles is much smaller than the real number (1 mole corresponds to about 6×10^{23} particles). The blue arrow in the center of the lid illustrates the force required to hold the lid at a constant height.
- Diagram for the probability distribution of a velocity component (v_x, v_y, or v_z). The component of velocity refers to the projection of the velocity vector of a particle along one of the three Cartesian coordinate axes (x, y, or z).
- Diagram for the probability distribution of the velocity magnitude v (Maxwell-Boltzmann distribution)

We will now solve the problem from *Fundamentals of Physics* and explore the app to get accustomed to its functionality.

1) *The molar mass M of oxygen is 0.0320 kg/mol. Suppose you have 0.100 mol of oxygen gas.*
   (a) *What is the average speed $\langle v \rangle$ of oxygen gas molecules at T=300 K?*
   (b) *What is the root-mean-square speed v_{rms} at 300 K?*
   (c) *What is the most probable speed v_p at 300 K?*

2) *Then consider any gas from the App and adjust the variables-amount of substance, temperature, and pressure, to note down the values of volume. We verify the simple gas laws.*

CALCULATIONS

Solving for the speeds of oxygen, we refer equations (6), (7), (8).

The given values are;

Molar mass of oxygen, M=0.0320 kg/mol

Number of moles, n=0.100 mol

Temperature, T=300 K

Universal gas constant, R=8.314 J/mol K

(a) To find the average speed $\langle v \rangle$,

Substitute the values in eq. (7) and take the square root,

$$\langle v \rangle = \sqrt{\frac{8 \times 8.314 \times 300}{3.14 \times 0.0320}} \approx \sqrt{198458.4} = 445.4 \text{ m/s}$$

(b) To find the root-mean-square speed v_{rms},

Substitute the values in eq. (8) and take the square root,

$$v_{rms} = \sqrt{\frac{3 \times 8.314 \times 300}{0.0320}} \approx \sqrt{233831.25} = 483.5 \text{ m/s}$$

(c) To find the most probable speed v_p,

Substitute the values in eq. (6) and take the square root,

$$v_p = \sqrt{\frac{2 \times 8.314 \times 300}{0.0320}} \approx \sqrt{155887.5} = 394.8 \text{ m/s}$$

Therefore, $\langle v \rangle = 445.4 \text{ m/s} \approx 446 \text{ m/s}$; $v_{rms} = 483.5\, m/s \approx 484\, m/s$;

$v_p = 394.8\, m/s \approx 395\, m/s$

PROCEDURE

1. Open Apps on Physics. Select Motion of Particles in an Ideal Gas, under Thermodynamics. We see a panel with reset button, start/pause button. There are boxes to enter values of amount of substance, temperature, pressure, and a display showing the calculated volume. *The app provides a simulation of particles moving inside a box subjected to the entered variables.* The component of velocity, and magnitude of velocity

is also observed under ‘Probability Distribution’ in the green panel, as shown in figure 2.

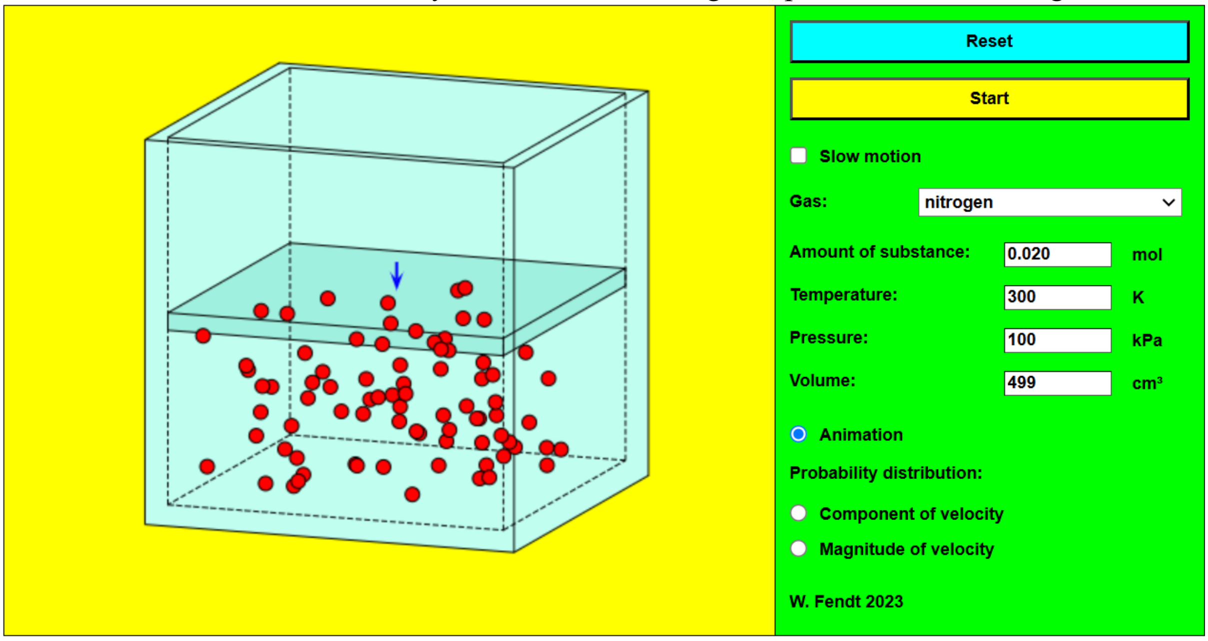

Figure 2

2. Select the gas as Oxygen from the drop-down menu ‘Gas’ as shown in figure 3.

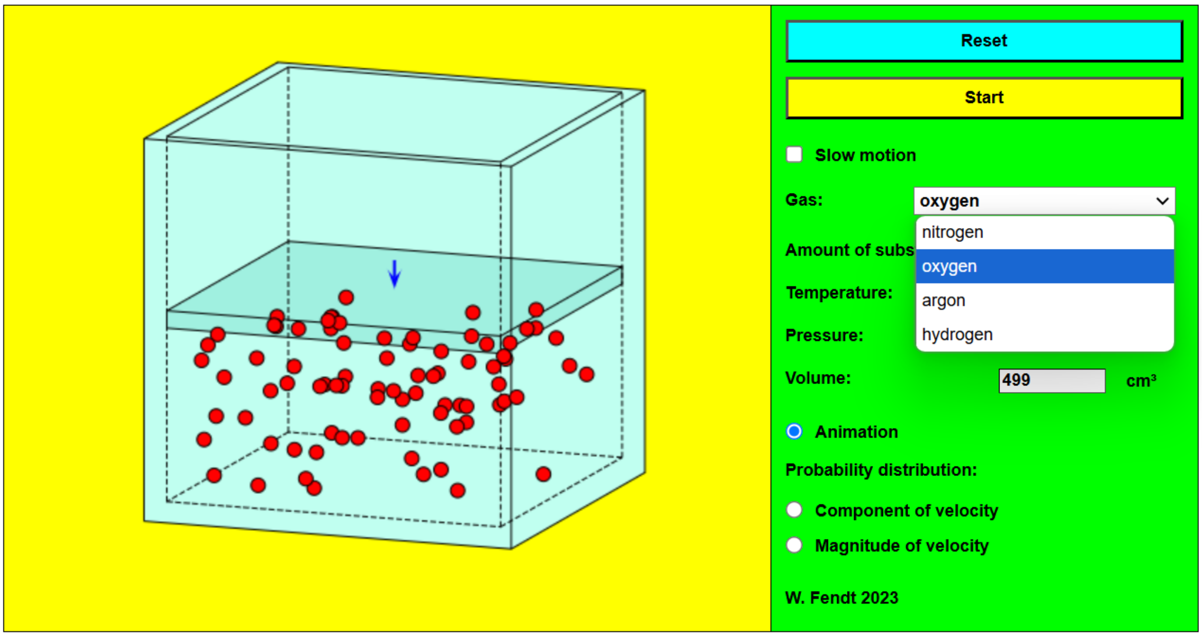

Figure 3- Oxygen is highlighted in blue in the drop down menu

3. As per the question, enter the values of amount of substance (=0.100 mol), temperature (=300 K), and pressure is set to default, i.e., 100 kPa, as shown in figure 4.

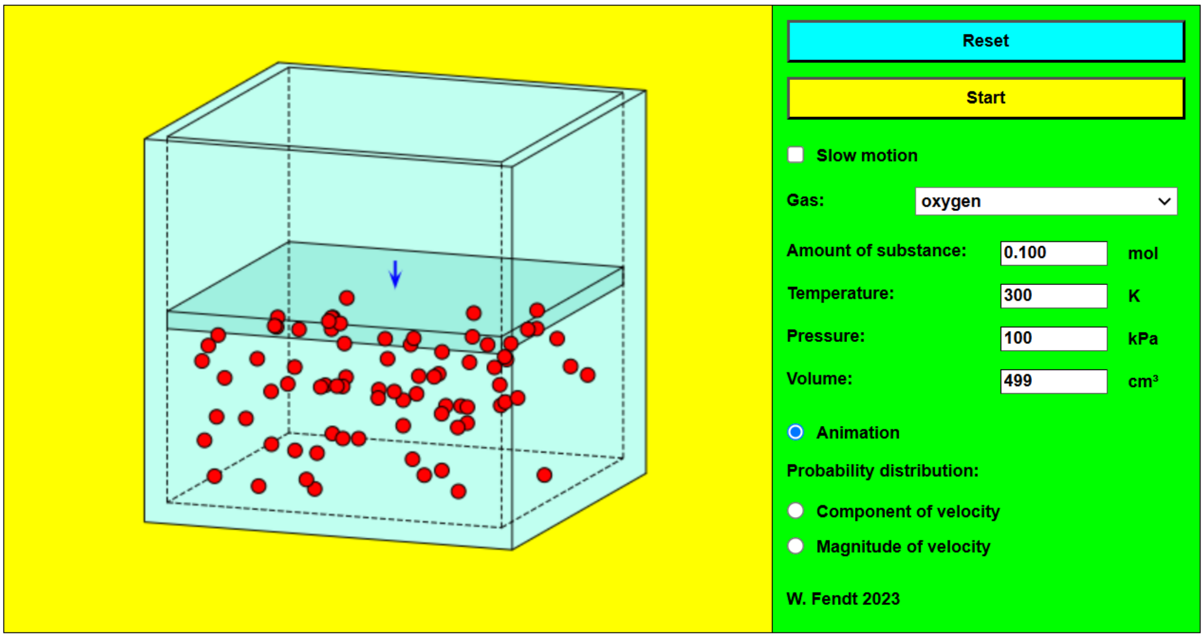

Figure 4

4. Now, click start. The message- 'Pressure modified because volume too large!' appears and the pressure is modified to 249 kPa to accommodate for the larger volume. The volume is 1000 cm^3. Click start again to observe the particles move within the container. Refer figure 5.

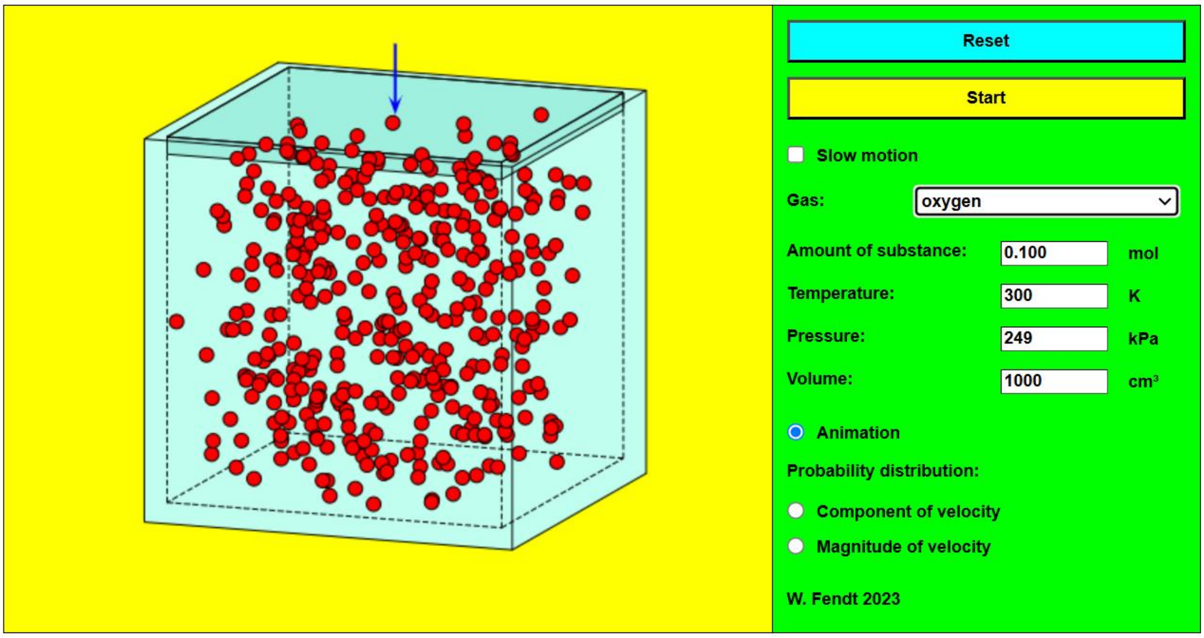

Figure 5- The pressure and volume have changed, and the number of particles in the container has increased.

Note- the animation radio button is selected by default.

5. Change the radio button to 'Component of Velocity' under 'Probability Distribution' to observe the distribution of one velocity component in the yellow panel as shown

in figure 6.

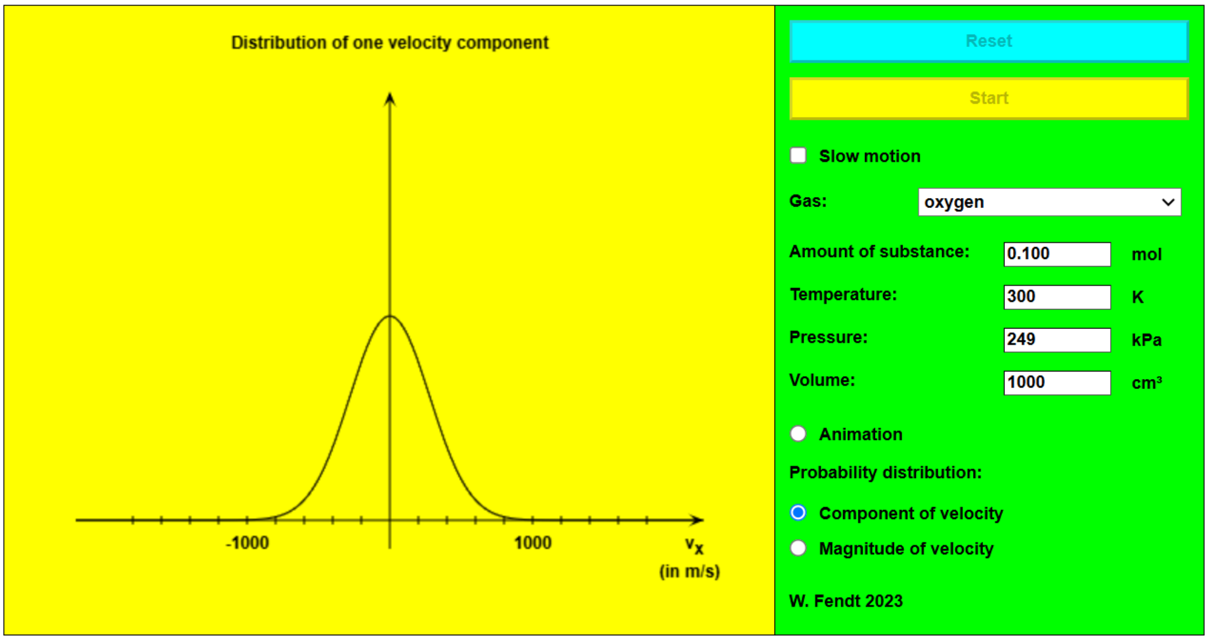

Figure 6- The 'Distribution of one velocity component' represents how the velocities are distributed along a specific axis for the gas particles; here, along the x-axis, v_x.

6. Change the radio button to 'Magnitude of Velocity' under 'Probability Distribution' to observe the Maxwell-Boltzmann speed distribution curve of oxygen molecules as shown in figure. In the yellow panel, we also find the distribution of velocity magnitudes, i.e., most probable speed, mean speed, root mean square speed. On the distribution curve, these speeds are identified by colour coded lines. Hence, the speeds are found from the Maxwell-Boltzmann speed distribution curve.

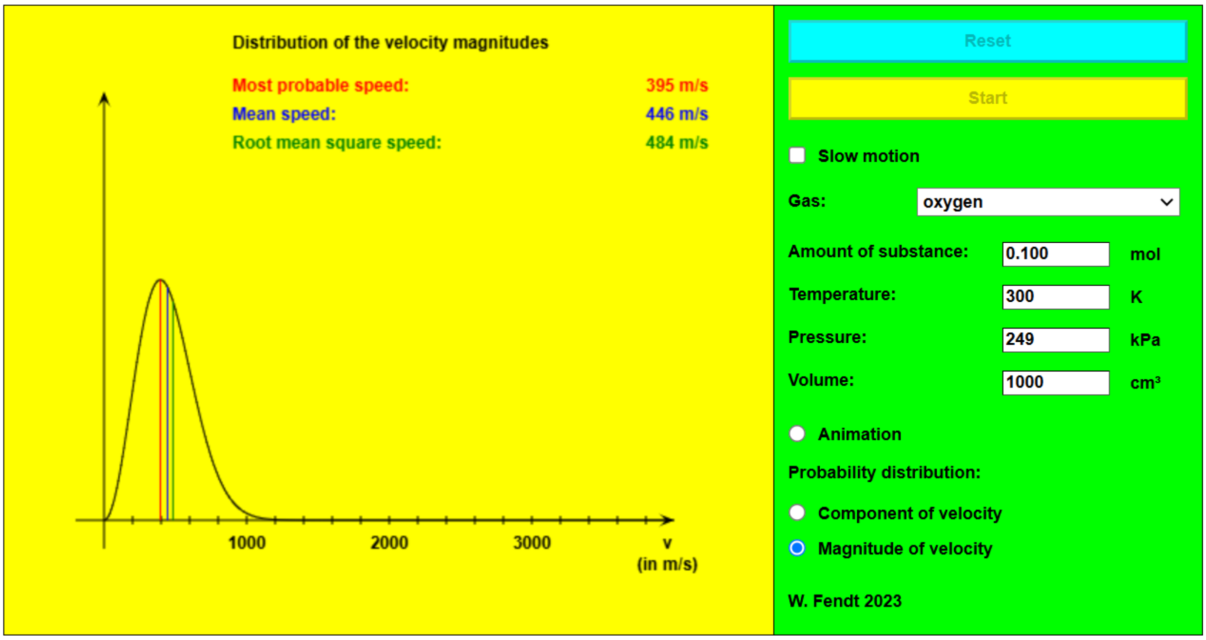

Figure 7- the 'Distribution of the Velocity Magnitudes' represent the Maxwell-Boltzmann distribution. The different speeds are given in the yellow panel.

Now, let's verify the gas laws- Boyle's Law, Charles Law, and Avogadro's Law.
The values of amount of substance can be adjusted within a range of 0.100 mol to 0.010 mol, temperature within a range of 1000 K to 100 K, and pressure within a range of 499 kPa to 50 kPa.

7. Reset the App to the default values; amount of substance (=0.020 mol), temperature (=300 K), and pressure (=100 kPa). The volume is 499 cm^3. Choose any gas of choice from the drop-down menu 'Gas'. We choose 'Argon'. Refer figure 8.

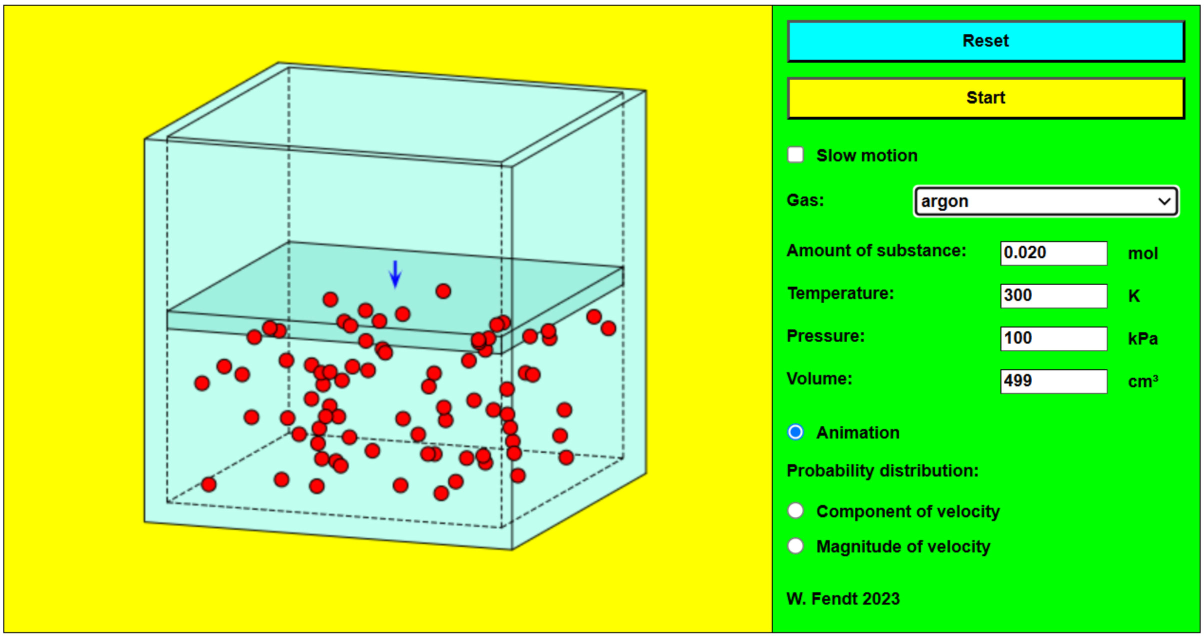

Figure 8

Select start after each entry and observe the following-
   i. Motion of particles inside the container
   ii. Value of volume
8. Vary the value of pressure and observe the change in volume. The amount of substance and temperature is set to default
9. Vary the value of temperature and observe the change in volume. The amount of substance and pressure is set to default.
10. Vary the value of the amount of substance and observe the change in volume. The temperature and pressure is set to default.

The shift in volume and changing parameters are used to validate the simple gas laws.

RESULTS

From the App, we find the values of speeds to be:

Most probable speed: 395 m/s

Mean speed: 446 m/s

Root mean square speed: 484 m/s

These values agree with the theoretical calculations (refer calculations).

'Component of Velocity' graph *(refer figure 6)*- The velocity of a gas particle is expressed as a vector with three components: v_x, v_y, and v_z, which correspond to the particle's velocity in the x, y, and z directions. The curve describes the probability distribution of these velocity components in a gas at a given temperature. For a single velocity component (v_x, v_y, and v_z), the distribution is Gaussian (bell-shaped) and symmetric around zero.

The graph of a single velocity component forms a Gaussian curve centered at zero, showing that particles are equally likely to move in either the positive or negative direction along that axis. The majority of particles exhibit relatively low velocities, with extreme velocities being less common. The width of the Gaussian curve is influenced by the gas temperature and particle mass—higher temperatures lead to broader curves and a wider range of velocities. The area under the curve represents the probability of a particle having a velocity within a specific range along that component.

'Magnitude of Velocity' graph *(refer figure 7)*- The graph represents the Maxwell-Boltzmann distribution of speeds. The x-axis represents the magnitude of velocity. The y-axis represents the relative probability of particles having a specific speed v. The graph is a skewed bell curve. Unlike the symmetric Gaussian curve for velocity components (v_x, v_y, and v_z), this curve is asymmetric because speed is always positive. The curve starts at zero speed, rises to a peak (most probable speed), and then decreases as speed increases. The average speed is slightly higher than the most probable speed, reflecting contributions from faster-moving particles.

At higher temperatures, the curve becomes wider and flatter, indicating a broader range of speeds and a higher number of fast-moving particles. In contrast, at lower temperatures, the curve is narrower and taller, signifying a more restricted range of speeds. For lighter particles, the curve has a higher peak and is more spread out, as they generally move faster.

When varying value of pressure at constant temperature of 300 K and amount of substance is 0.020 mol-

Pressure (kPa)	*Volume (cm^3)*
100	499
150	333
200	249
250	200
300	166

Table 1

In Table 1, as the pressure increases in steps of 50 kPa, the volume decreases, consistent with **Boyle's Law**. Thus, pressure and volume are inversely related. Observe that in the yellow panel, increasing the pressure reduces the space available for particles to move within the container.

When varying value of temperature at constant pressure of 100 kPa and amount of substance is 0.020 mol-

Temperature (K)	*Volume (cm^3)*
300	499
350	582
400	665
450	748
500	831

Table 2

In Table 2, as the temperature increases in steps of 50 K, the volume increases, consistent with **Charles's Law**. Thus, temperature and volume are directly proportional. Observe that in the yellow panel, increasing the temperature increases the space available for particles to move within the container, and their speed increases.

When varying value of amount of mol at constant pressure of 100 kPa and temperature is 300 K-

Amount of substance (mol)	*Volume (cm^3)*
0.020	499
0.025	624
0.030	748
0.030	873
0.040	998

Table 3

In Table 3, an increase in the amount of substance leads to a corresponding increase in volume, consistent with **Avogadro's Law**. Thus, amount of substance and volume are directly related.

CONCLUSION

In conclusion, the study of the motion of particles in an ideal gas offers a hypothetical scenario, as ideal gases assume no intermolecular forces and perfectly elastic collisions, which do not occur in real gases. Although real gases deviate from ideal behaviour in most cases, ideal gases helps us understand key thermodynamic principles, providing a foundation for analysing real gases.

With the app, we explored particle motion, speed distribution, and the effects of temperature, particle mass, and volume, verifying gas laws and the Maxwell-Boltzmann distribution. The App provides a simple interface and aids students in grasping the microscopic foundations of the laws of thermodynamics.

REFERENCES

1. **Apps on Physics - https://www.walter-fendt.de/html5/phen/gas3d_en.htm**
2. **D. Halliday, R. Resnick, and J. Walker, *Fundamentals of Physics*, 10th ed. Hoboken, NJ: Wiley, 2013**
3. **R. H. Petrucci, W. S. Harwood, F. G. Herring, and J. D. Madura, *General Chemistry: Principles and Modern Applications*, 9th ed. Upper Saddle River, NJ: Pearson Education, Inc., 2007**
4. **Figure 1- D. Halliday, R. Resnick, and J. Walker, *Fundamentals of Physics*, 10th ed. Hoboken, NJ: Wiley, 2013, p. 561.**