An Ideal Gas Law Simulator for Atmospheric Gas Molecules

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Abstract

The ideal gas law which is the equation of state of a hypothetical ideal gas that allows us to gain useful insights into the behavior of most real gases at low densities was utilized in this work to conceptualize, design and develop the ideal gas law simulator in a 3 dimensional space using Microsoft Visual Studio, Microsoft Paint and 3D Game studio for pedagogic purposes. The gas law variables due to changes in atmospheric conditions were simulated and the parameters considered in the developed software which visually depicts the motion of gas molecules could be modified by the user in order to see a visual representation of this effect on the other parameters. The developed software depicts adequately the visual representation of the motion of gas molecules based on changes in atmospheric conditions and the understanding of the thermodynamics of some of the trace gases in the atmosphere.

Keywords: ideal, hypothetical, simulator, pedagogic, visual

1.0   Introduction

The atmosphere is the layer of gases surrounding a planet or celestial body that is retained by the gravitational pull of that celestial body. The atmosphere of the Earth is called air. Air is characterized by the percentage composition of its constituent gases, which is different from the percentage composition of the constituent gases of the atmospheres of other celestials' bodies. Air is mainly composed of nitrogen (78%), oxygen (21%), and argon (1%), which are known as the major gases of the atmosphere [1]. All other gases appear in trace quantities. The concentration of water vapor varies greatly between the colder regions of the earth and the hotter, humid regions and so the concentrations of gases in the atmosphere are usually stated for dry air, which is air without any water vapor [2]. The motion of air called wind is one of the factors that determine the weather, which is the state of the atmosphere at any particular place and time. The average weather of any particular location or region over a long time interval determines the climate. Since the ideal gas describes the macroscopic properties of a gas, hence the ideal gas law properties of gas can be used to deduce the properties of gases in a simple way. Although there is no such thing in nature as a truly ideal gas, but all gases approach the ideal state at low enough densities. Thus, an ideal gas equation which was first stated by Emile Clapeyron as a combination of Boyles' law and Charles' law allows us to gain useful insights into the behavior of most real gases since it is the equation of state of a hypothetical ideal gas [3, 4, 5].

2.0   Materials and Methods

This work involves the development of a software that can be used to demonstrate to students the effect of changes in the atmospheric conditions on the motion of gas molecules with the aid of a three dimensional video representation of the molecules of the gas using the fundamental laws of thermodynamics [6]. The user will be able to vary the value of the variables that affect the motion of molecules and see immediately the changes that will be produced in the general motion of these molecules. The developed software applies the laws of physics to the motion of the molecules without making lengthy calculations and the user will be able to change the value of a variable in order not only to see how it affects the value of another variable, but also how it affects the motion of the molecules. The software will aid in learning and understanding the motion of gas molecules under various atmospheric conditions.

This Ideal Gas Law Simulator software was developed using 3D Gamestudio /A8, a programming tool [7] for the creation of 3D applications and video games. This tool was chosen because we wanted to create a completely 3 Dimensional

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representation of the motion of gas molecules and leave nothing to the imagination of the user. 3D Gamestudio A8 uses a programming language called Lite-C, which is a proprietary variant of the C and C++ programming languages. Lite-C is a language that only exists within 3D Gamestudio and makes programming of certain 3D features, such as a camera that can be controlled by the user, easier than it would have been to program such a feature in the more traditional programming languages.

The Graphical User Interface (GUI) of the Ideal Gas Law Simulator was created in Microsoft Visual Studio and then transferred to 3D Gamestudio using Microsoft Paint. We used Microsoft Visual Studio to create the user interface because Visual Studio is normally used for creating professional enterprise applications, and it comes with standard tools for creating neat user interfaces (Fig. 1). The 3D Gamestudio is more suited in creating both 2D and 3D graphic-oriented applications, and so the interface creation tools are very image-focused. Hence, there is the need to use an image-editing tool and Microsoft Paint, to transfer the interface between the two programs. The images for the thermometer, barometer and spring scale used to visually depict the value of certain variables while the simulation is running were created in Microsoft Paint.
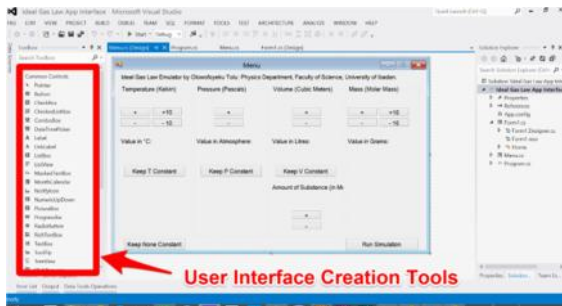

Fig. 1: - Creation of Graphical User Interface in Microsoft Visual Studio2

The methods of converting the Ideal Gas Law into instructions for the 3D Gamestudio engine to simulate the motion of the gas molecules include the following processes:

1. All the quantities considered by the common form of the Ideal Gas Law were created and given their STP values as the starting values before the user makes any changes.
2. Quantities whose values depend on other quantities were given values based on the formulae of the Ideal Gas Law, and their values will automatically change whenever the   values of the quantities they depend on are changed.
3. The motion of each molecule was randomized by randomizing the speed and the direction in 3D space every time there is a collision.

3.0   Results and Discussions
3.1   The Graphical User Interface (GUI)
The Ideal Gas Law Simulator application has two major user interfaces: the Standard Mode and the Simulation Mode [8, 9].
3.1.1   Standard Mode of the Ideal Gas Law Application
On start up, the application is in Standard Mode. This mode displays all the major variables and allows the user to edit them. The most commonly used form of the ideal gas law [10, 11] is:

$$PV = nRT \qquad \text{--------------} \tag{1}$$

Where:

P is the pressure; V is the volume; n is the number of moles; R is the ideal or universal gas constant and T is the temperature. Various expressions of equation (1) through which the above parameters could be obtained are:

$$T = {}^{PV}/_{nR} \qquad \text{-------------} \tag{2}$$

$$P = {}^{nRT}/_{V} \qquad \text{-------------} \tag{3}$$

$$V = {}^{nRT}/_{P} \qquad \text{-------------} \tag{4}$$

$$n = {}^{PV}/_{RT} \qquad \text{-------------} \tag{5}$$

Since the value of R is fixed, the user can only alter the other four variables. We created four columns of controls, each representing one of the four variables that we are considering. From left to right, the columns are for viewing and editing the values of temperature, pressure, volume and mass (Figs. 2 and 3).
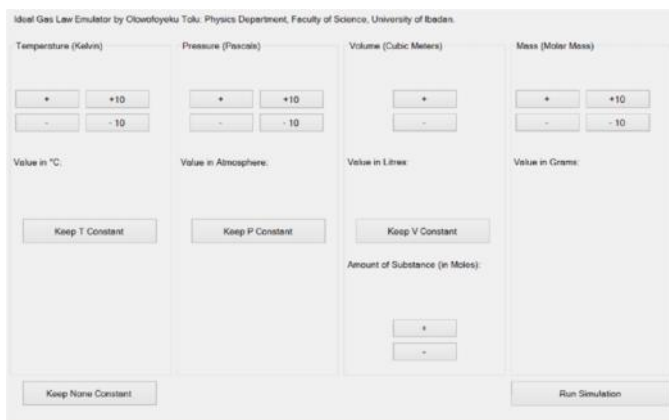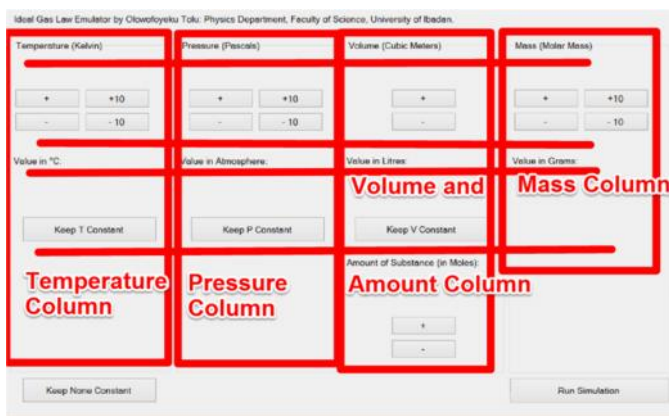
Fig. 2 - The Standard Mode Interface

Fig. 3 - The rows and columns of the controls in standard mode

3.1.2   Simulation Mode of the Ideal Gas Law Application

When the user clicks the "Run Simulation" button or presses the "Enter" key on his keyboard while in Standard Mode, the software will move into Simulation Mode, using the values of the variables the user has set, or using the Standard Temperature and Pressure (STP) values if the user didn't vary anything at all. In Simulation Mode, all the information is presented in a visually captivating way that is easy to understand (Fig. 4). The information is merely represented visually, and not depicted accurately to scale. The aim is for the user to monitor the change in behavior of one or more variables brought about when he (the user) changes the value of a variable during simulation.

A gray, hollow cube represents the container of the gas and the size of this cube is determined by the volume set by the user. Small, randomly colored balls represent the molecules of the gas. The balls are generated with different colors at random to make it easier to visually distinguish each ball from another. The number of balls displayed is not equal to the number of molecules, but a representative of it for simulation purposes. Whereas, the number of molecules is determined by

Number of Molecules = Avogadro's number X Number of Moles   (6)

We used our own formula to determine how many balls to display on screen:

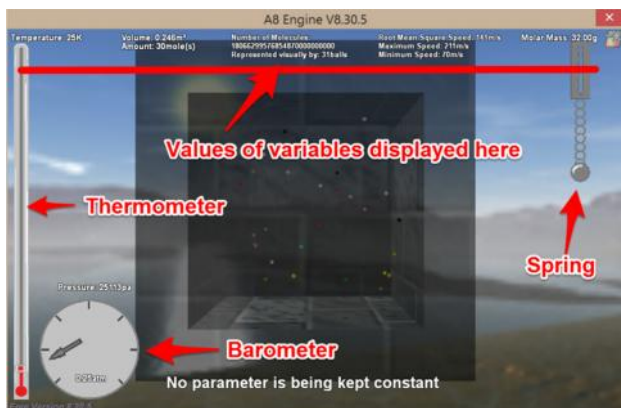Number of Balls = Number of Moles + 1   (7)

Fig. 4: - The Simulation Mode of the Ideal Gas Law Simulator

At the top most part of the screen, the value of all the variables is displayed apart from the value of pressure, which is displayed at the bottom left of the screen above the barometer graphic. The values of the temperature and mass are displayed above the thermometer graphic and the spring graphic respectively, but the barometer graphic is located at the bottom of the screen for neatness purpose and so we chose to display the value of the pressure there. At the top of the screen, the user can see the volume of the container, the amount of substance, the exact number of molecules being represented and the number of balls representing them, the root mean square speed at which the molecules are moving and the molar mass of the molecules. To enhance visualization, we also added images of a thermometer, barometer and spring to represent the values of the temperature, pressure and molar mass respectively.

To aid simplicity and ease of use, we gave allowance for the user to be able to adjust the variables directly from the graphics representing those variables. The value of the temperature can be changed simply by clicking and dragging the slider on the thermometer. The value of the pressure can be changed by clicking and dragging the needle on the barometer and the value of the molar mass can be changed by clicking and dragging the bob at the end of the spring scale. The graphics are not graduated, but the value of the respective variables is always displayed directly above the graphic. The value of these variables can also be changed by using keyboard shortcuts. Pressing the "Help" button at the bottom right of the screen, or pressing the 'F1' key will bring up the Keyboard Shortcuts Screen (Fig. 5), which tells the user all the keyboard shortcuts that are available to him. In addition to changing the values of the variables, the user can adjust the camera or keep a particular variable constant using the keyboard shortcuts.
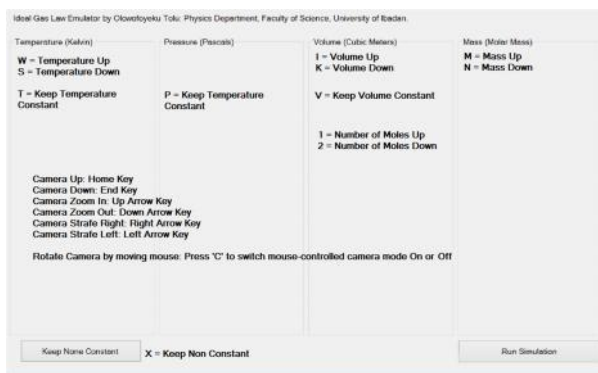
Fig. 5 - The Keyboard Shortcuts Screen

3.1.3 The Code behind the simulation and its representation of the Ideal Gas Law theory

The code behind any software refers to the set of instructions by which the software is been run as written in one or more programming and/or scripting languages. As stated earlier, 3D Gamestudio uses a language called Lite-C, and all our code was written in this language. A lot of the code deals only with how things are visually displayed on screen and the code that deals with the motion of the gas molecules in obedience to the Ideal Gas Law is only discussed. The first step taken towards simulating the Ideal Gas Law was to create all the variables considered by the common form of the law, and to assign them the values they have at Standard Temperature and Pressure (STP) in order for the variables to be able to match real life quantities and values (Fig. 6).

Fig. 6: - Variables created to match the real life quantities and values

The value of some of these variables is dependent on the values of some of the other variables. For example, the value of the Root Mean Square Speed is determined by the values of the temperature, molar mass and the universal gas constant. Looking at Fig. 6, one can see that we did not allocate any value to the variables representing speed, shown at the bottom of the image. Those quantities whose values depend on the value of other variables were assigned values later on as shown in Fig. 7, and their values will automatically change whenever the user changed the value of any variable on which they depend.

Fig.7: - Varying the values of some quantities based on the values of some other quantities

The motion of each individual molecule was made random with the collisions perfectly elastic. To make the motion random, we allocated each molecule a random speed whose value fluctuates around the root mean square velocity as indicated in our code governing the behavior of each gas molecule (lines 75 to 78 of Fig.8) and the speed of each molecule is changed to another random value after each collision. The orientation of the molecule in 3D space, determined by its Euler angles in the X, Y and Z axes is also randomly changed at each collision.

Fig.8: - Code governing the behavior of each gas molecule

It must be noted that at Standard Temperature and Pressure (273K, 100kPa), one mole of an ideal gas occupies 0.0224m³. Hence, the software was initialized to use these values. However, the computed value obtained from an Ideal Gas Law simulator differs slightly from the ideal gas value. For example, based on ideal gas equation, one mole of an ideal gas at 273K, occupying 0.0224m³ will have a pressure of 105,804Pa, and not 100,000Pa which is the value an ideal gas suppose to have at STP. Similarly, the Ideal Gas Law simulator depicts adequately the visual representation of the motion of gas molecules.

4.0   Conclusion

The Ideal Gas Law simulator designed for pedagogic uses depicts the motion of gas molecules which could be modified by the user in order to see a visual representation of this effect on gas molecules based on changes in atmospheric conditions. The developed software depicts adequately the visual representation of the motion of gas molecules based on changes in atmospheric conditions and the understanding of the thermodynamics of some of the trace gases in the atmosphere.

5.0   Acknowledgement

6.0   References

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