The 3rd International Conference on Materials Chemistry and Environmental Engineering
DOI: 10.54254/2755-2721/3/20230399

The Relationships in the Law of Conservation of Mechanical Energy and the Ideal Gas Equation in Argon Molecules – based on Moldy and Gnuplot

Qinyu Zhang

Suzhou High School of Jiangsu Province, Suzhou, Jiangsu Province, China, 215000

selinazhang12@163.com

Abstract. Science and technology have been progressing by leaps and bounds over the past few decades all over the world, resulting in the rapid development of advanced computer programs. Under such circumstances, we are able to prove plenty of theories in a new way with the help of different kinds of modern computer programs. For example, we are capable of investigating the relationship between kinetic energy and potential energy, as well as the connection between temperature and pressure, by applying computer programs to draw graphs. In this paper, moldy and gnuplot which are progressive computer programs are used to paint the graphs about the two relationships in the conservation law of mechanical energy and ideal gas equation respectively in argon gas with the help of the information obtained from the Internet. These two computer programs not only remove the burden of calculation, but also make the relationship clearer. In the end, this paper proves that the sum of kinetic energy and potential energy in argon molecules is invariable in a closed system under different temperatures. Pressure is also tested to have a positive linear association with temperature although the density changes when the argon gas is an ideal gas.

Keyword: kinetic energy and potential energy, law of conservation of mechanical energy, temperature and pressure, ideal gas equation, moldy, gnuplot.

1. Introduction

The law of conservation of mechanical energy is the law of conservation in mechanics. It claims that the total mechanical energy of a closed system remains constant when only conservative forces interact in it [1]. As a result, the sum of kinetic energy and potential energy, which is mechanical energy, are supposed to be constant in the system. In addition, the ideal gas equation tells us that when the gas is a theoretical gas composed of a set of randomly – moving point particles that collide elastically, there is a positive linear association between temperature and pressure [2].

Nowadays, with progressive science and technology, a lot of computer programs are invented. These computer programs are widely used today, and they will definitely play irreplaceable roles in the future since they have several advantages over traditional methods of addressing things. Among them, there are programs that are able to simulate the motion of molecules or draw graphs to display the relationship between physical quantities.

© 2023 The Authors. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (https://creativecommons.org/licenses/by/4.0/).

DOI: 10.54254/2755-2721/3/20230399

In this paper, moldy and gnuplot are used to gain the two relationships in the conservation law of mechanical energy and in the ideal gas equation. Moldy is a C program that can be used for molecular-dynamics simulations of solids and liquids by using periodic boundary conditions [3]. Gnuplot is a command-driven interactive function-plotting program [4]. It is utilized to show data in graphical format, which is necessary in any branch of science [5]. People are capable of plotting graphs by typing commands. These two programs work together to make the explorations in this paper possible.

The success of the explorations in this paper also offers references for high school students to use computer programs in order to probe into knowledge from books.

2. Methodology

Firstly, in order to do the stimulations of argon on the moldy, the parameters of argon provided by A. Rahman are found on the Internet [6]. Then the parameters of the argon molecules are adjusted. The scale-end(when to stop scaling) is changed from 2500 to 10000 and the nsteps(number of timesteps to be done in a run) is regulated from 5000 to 60000 [7,8]. Besides, print-interval(how frequently to print normal output) and roll-interval (period over which to calculate rolling averages) are varied from 500 to 100, begin-average(when to start accumulating the thermodynamic averages) and begin-rdf(when to start accumulating radial distribution function information) are altered from 2501 to 10001 and average-interval(how frequently to calculate and print averages), as well as rdf-out (how frequently to calculate and print RDFs), is adjusted from 2500 to 5000 [7]. In this way, the results will be more precise. Moreover, the temperature is set to be 76K and the density of argon gas is stipulated to be 1.428 kg/m^3.

Secondly, moldy is made use of to simulate and obtain information about the motion of argon molecules under different temperatures and densities.

So as to study the relationship between the kinetic energy and potential energy of argon molecules at 76K, the program runs itself and saves the results into output1_76. Then, the results that I need, which are kinetic energy, potential energy, and temperature, are moved to output2_76. In this way, the data becomes clearer and easier to be used. Nevertheless, the first 100 lines are supposed to be deleted, because during the first 100 lines, the computer is still preparing itself to get accurate data, which means that the data from the beginning of the simulation is not precise. This study repeats all of the previous steps after obtaining the information at 76 to get the information at 80K, 84K, 88K, 92K and 96K.

After that, the research turns the focus to the connection between temperature and pressure. Before simulation, the temperature has to be increased in order to make the results more accurate. Consequently, the temperature is augmented from 96K to 110K (the density maintains at 1.428 kg/m^3). After running the program, average pressure at 110K is recorded. Then, the results at 115K, 120K, 125K, 130K, 135K 140K and 145K are recorded one-by-one and are put into a new file called output3_1.428. after that, the density is altered to be 1.478 kg/m^3, 1.528 kg/m^3, 1.578 kg/m^3, 1.628 kg/m^3, 1.678 kg/m^3 and the average pressures at 110K, 115K, 120K, 125K, 130K, 135K 140K and 145K for each density are received. Each time the information about groups of average pressures and temperatures at a certain density is gotten, a new file is opened.

Thirdly, gnuplot is utilized to paint the graphs of the connection between kinetic energy and potential energy under different temperatures and the relationship between temperature and pressure of different argon gas densities based on the information offered by moldy.

The data from the second column and the third column of output2 files, which represent kinetic energy and potential energy respectively, is selected to draw the graph of the relationship between kinetic energy and potential energy. After that, the data from the first column and the second column of output3 files, which represent temperature and pressure respectively, is chosen to paint the graph about the connection between temperature and pressure.

DOI: 10.54254/2755-2721/3/20230399

3. Results and Analysis

Here are the graphs presenting the relationship between kinetic energy and potential energy. The x-axis represents kinetic energy and the y-axis represents potential energy.

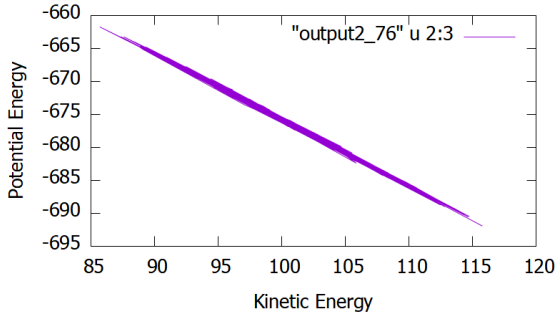

Figure 1. The relationship between kinetic energy and potential energy at 76K (credit: Original).

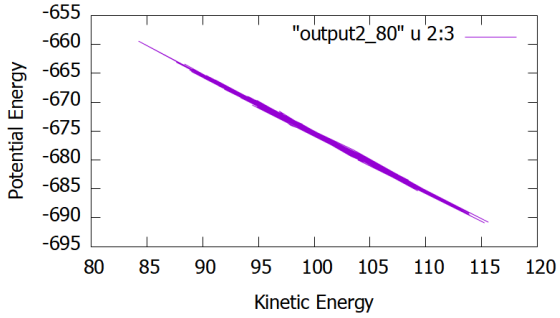

Figure 2. The relationship between kinetic energy and potential energy at 80K (credit: Original).

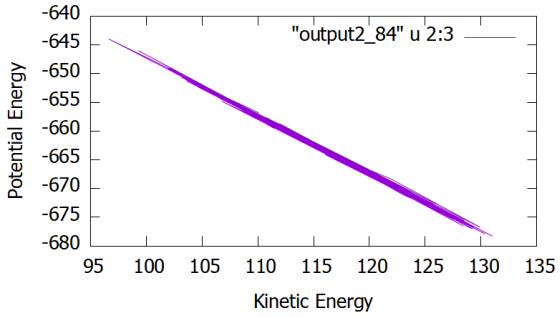

Figure 3. The relationship between kinetic energy and potential energy at 84K (credit: Original)

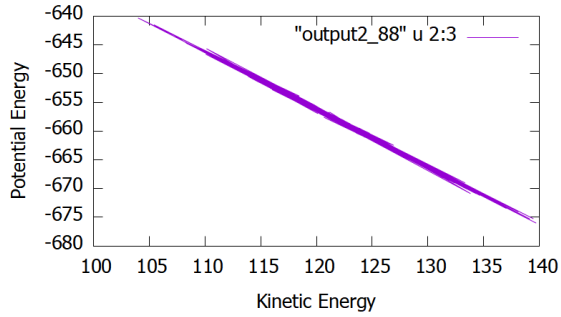

Figure 4. The relationship between kinetic energy and potential energy at 88K (credit: Original).

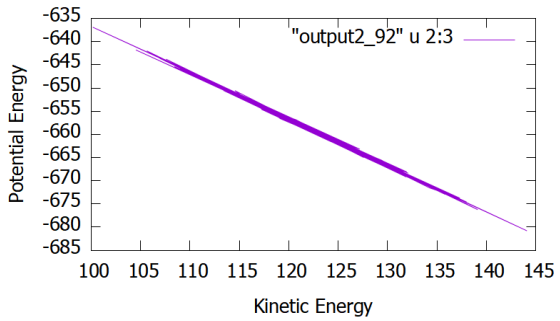

Figure 5. The relationship between kinetic energy and potential energy at 92K (credit: Original).

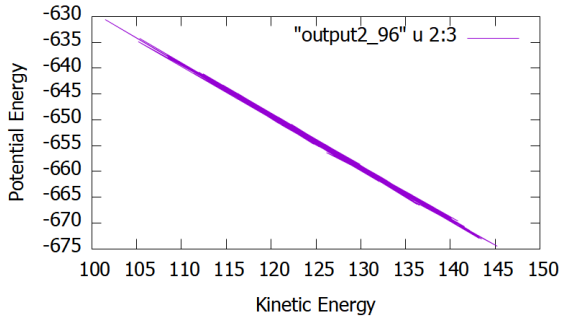

Figure 6. The relationship between kinetic energy and potential energy at 96K (credit: Original).

As shown in Figure 1, Figure 2, Figure 3, Figure 4, Figure 5 and Figure 6, it is clear that there is a linear relationship between kinetic energy and potential energy under different temperatures. In addition, based on the graphs, it can be concluded that the potential energy is equal to constant quantity of energy minus kinetic energy. As a conclusion, the constant sum of potential energy and kinetic energy can be concluded when the system is a closed system.

The graphs below are about the connection between temperature and pressure. The x-axis represents temperature and the y-axis represents pressure.

DOI: 10.54254/2755-2721/3/20230399

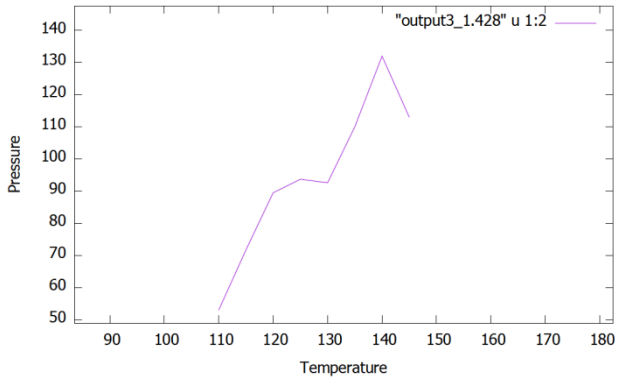

Figure 7. The relationship between temperature and pressure at 1.428 kg/m^3 (credit: Original).

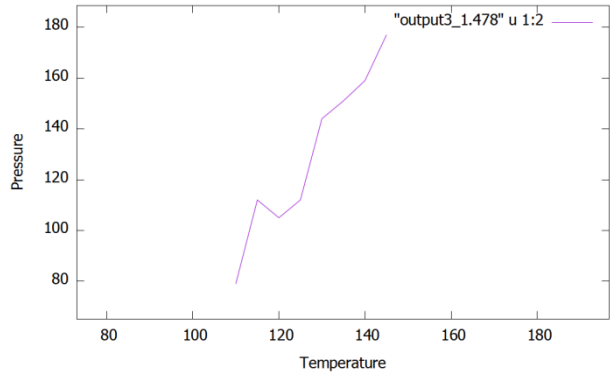

Figure 8. The relationship between temperature and pressure at 1.478 kg/m^3 (credit: Original).

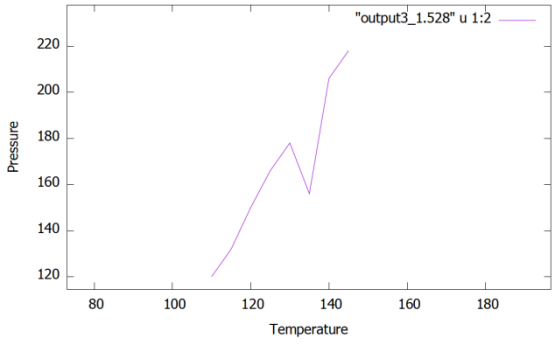

Figure 9. The relationship between temperature and pressure at 1.528 kg/m^3 (credit: Original).

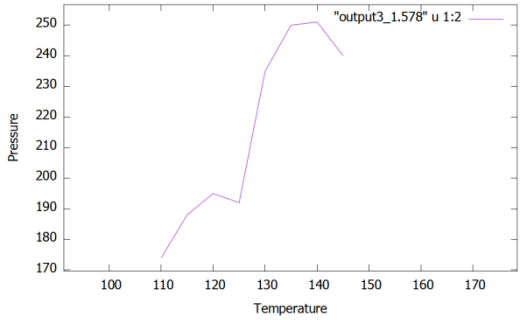

Figure 10. The relationship between temperature and pressure at 1.578 kg/m^3 (credit: Original).

DOI: 10.54254/2755-2721/3/20230399

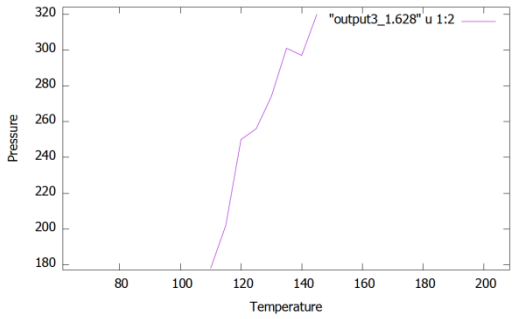

Figure 11. The relationship between temperature and pressure at 1.628 kg/m^3 (credit: Original).

According to Figure 7, Figure 8, Figure 9, Figure 10 and Figure 11, which are graphs about the relationship between temperature and pressure, a positive association between temperature and pressure is able to be concluded approximately. In addition, these graphs indicate that as density increases, pressure at each temperature augments. These two discoveries fit the ideal gas equation which is $pM = \rho RT$ (the transfiguration of $pV = nRT$) a lot.

4. Conclusion

By using progressive computer programs - moldy and gnuplot, the relationship between kinetic energy and potential energy of argon molecules in a closed system and the connection between temperature and pressure for ideal argon gas, which are the goal of this research, are found in this paper. The results are shown apparently by the graphs that the sum of kinetic energy and potential energy in argon molecules is invariable and there is a positive linear association between temperature and pressure in argon gas.

However, there are still some defects. For each graph of the relationship between temperature and pressure, there are apparent fluctuations because there are always some changes in volume, and these changes can't be avoided in moldy. In conclusion, the positive linear association is not quite persuasive.

Although some defects still exist, the testification is a great success. Due to the contribution of moldy and gnuplot, pale knowledge learned at high school is able to be explored with real life instances. Consequently, we can find out that as computer programs are tied closer to school studies, students are capable of studying in a more vivid way.

Acknowledgment

Here, I want to thank to the help of Prof. Erik Luijten. At the beginning, I knew nothing about moldy and gnuplot. It was Prof. Erik Luijten who taught me what they were and how to make use of them. What's more, every time I found out that the results I received were strange and I had no idea about the reasons, he helped me find the problem and inspired me about the solution. I cannot complete this paper without his help.

References

[1] Olexander N. Romanyuk, Olena E. Avramchuk, Volodymyr V. Martynyuk, Nurbapa Mekebayev, and Cezary Kaczmarek "Experimental testing of the law of conservation and transformation of energy", Proc. SPIE 10808, Photonics Applications in Astronomy, Communications, Industry, and High-Energy Physics Experiments 2018, 108085V (1 October 2018);

[2] https://byjus.com/chemistry/derivation-of-ideal-gas-equation/

[3] Keith Refson. Moldy: a portable molecular dynamics simulation program for serial and parallel computers, Computer Physics Communication,1999, 126(2000): 1

[4] Tan Kiat Shi, Willi-Hans Steeb, Yorick Hardy. Gnuplot and PostScript, Springer, London, 2000:

DOI: 10.54254/2755-2721/3/20230399

659
[5] Dr. Dwaipayan Deb. Gnuplot Helper – a new Utility for gnuplot Graph Plotting Software, May 24th, 2021
[6] A. Rahman. Correlations in the Motion of Atoms in Liquid Argon[J], the American Physical Society, 1964, 136(2A)
[7] Keith Refson. Moldy User's Manual, Department of Earth Sciences, Parks Road Oxford OX1 3PR, January 29, 1998
[8] G. J. Acklanda,*, K. D'Mellowa, S. L. Daraszewicza, D. J. Hepburna, M. Uhrina, K. Stratforda. The MOLDY short – range molecular dynamics package, aSchool of Physics and Astronomy, The University of Edinburgh, King's Buildings, Edinburgh, EH9 3JZ: 15