

Introducing the first Law of thermodynamics using states of matter PhET simulation

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Abstract

Thermodynamics is a crucial topic in science education, yet it poses significant challenges for students at all educational levels. This study explores an alternative instructional approach for teaching the First Law of Thermodynamics using the PhET gas and properties simulation, guided by the Johnstone triangle framework. In contexts like South Africa, traditional teacher-centered and lecture-focused methodologies often leave students with misconceptions about thermodynamic concepts. The study utilizes the PhET simulation to visually illustrate key principles, such as temperature, heat, and thermal energy, while intentionally minimizing mathematical complexity to enhance understanding. Results indicate that this simulation effectively clarifies thermodynamic dynamics at a sub-microscopic level, fostering a more intuitive grasp of the subject. The implications of this teaching practice suggest that it can significantly improve students' conceptual understanding. Future research should consider employing the simulation to explain P-V diagrams, further enriching students' comprehension of thermodynamic principles.

Keywords: First law; heat; internal energy; PhET simulation; system; temperature.

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1. INTRODUCTION

Temperature and heat are essential elements in our everyday lives, and they serve as foundational concepts in STEM subjects, particularly in thermodynamics, which is a critical area of study from primary through higher education. Nevertheless, understanding the physics of heat is recognized as a significant challenge for students. Both students and educators frequently struggle to grasp the energy flow involved in chemical and physical changes (Finkenstaedt-Quinn et al., 2020). The First Law of thermodynamics builds upon the conservation of energy principle, focusing on the internal energy of a closed system, as well as the heat and work performed by the system on its environment. Various energy-related concepts, such as work, heat, free energy, and entropy, are abstract in nature, contributing to their complexity in both physics and chemistry (Landa et al., 2020). Numerous innovative teaching tools have been proposed in academic literature to address these challenges and aid in the comprehension of these intricate topics (Becker & Towns, 2012; Bain et al., 2018; Finkenstaedt-Quinn et al., 2020).

Research has demonstrated that both kinetics and thermodynamics significantly influence student learning at the secondary and postsecondary levels (Bain & Towns, 2016). At the high school level, students often find it challenging to bridge the gap between particulate representations of kinetics and observable macroscopic behaviors. Similarly, students in Higher Education Institutions (HEIs) face difficulties in developing a mathematical grasp of kinetics and in transitioning between mathematical and conceptual models (Moon et al., 2016; Hamnell-Pamment, 2024). Consequently, comprehending thermodynamic concepts necessitates an understanding of how mathematical representations correlate with their physical interpretations (Liu, 2022). According to Xiang et al. (2023), two effective methods for introducing the First Law of thermodynamics are physical experiments and virtual tools, including simulations. They contend that each of these approaches offers distinct advantages that can enhance the learning of thermodynamics.

This study's approach focuses on simplifying the introduction of the First Law of Thermodynamics by utilizing the States of Matter PhET Simulation. For physics instruction to be effective, it is essential to actively engage students and promote a deep conceptual understanding of the subject matter. Khumalo and Maphalala (2018) suggest that students' understanding can only be achieved through active engagement in the learning activities. Physics Education Technology (PhET) simulation activities have been reported to lead to a deeper understanding of physics concepts and visualization (Sylvere & Minani, 2023). Visualization is especially important because it helps students view the dynamic processes that are not observed in books (Scholte et al., 2024; Ndukwe & Daniel 2020).

Physics is an abstract subject that requires students to operate at three levels of thought. This study is grounded by the Johnstone triangle (Johnstone, 2010; Taber, 2013) developed by Alex Johnstone. This theory acknowledges that physics knowledge can be understood on three fundamental 'levels' or 'representations' or 'domains'. As suggested by Johnstone (2010), the three domains are macroscopic, symbolic, and the sub-microscopic. The macroscopic level includes all that students can see, smell, and feel with their sensory organs. The sub-microscopic levels are the atoms and molecules that are dynamic in an ideal gas. It is also unseen and consists of explanatory models such as the particle nature of matter. The representational level includes symbols, equations, mathematical formulae, graphs, and diagrams. The use of physics visualizations by physicists in communicating phenomena is one of the reasons why physics can be challenging for students.

1.1. Conceptual background

The South African National Curriculum Statement (NCS) and Curriculum Assessment Policy Statement (CAPS) of the Further Education and Training (FET) phase, in the Physical Sciences curriculum, is divided into two sections namely Physics and Chemistry. The physics section has three topics: mechanics, waves sound, and light, and electricity and magnetism. Khumalo and Maphalala (2018) bemoan that in Sub-Saharan Africa, in most public schools in South Africa, the prevalent teaching instruction is chalk and talk. The traditional or teacher-centered approach is ineffective in promoting conceptual change and understanding. As a result, students come to HIEs with an incomplete understanding of systems, kinetic models of ideal gases, energy, heat, and work done. First-year university general physics bridges high school and university such that students

come to physics lectures with pre-conceptions about thermodynamics and kinetics. Bain and Towns (2016) suggested that pre-conceptions affect learning as they become integrated into the cognitive structures.

Research in science education (Bain et al., 2018; Dreyfus et al., 2015) relating to students' conceptions of thermodynamics and kinetics, has shown that high school and university students have similar alternative conceptions. At the university level, studying thermodynamics requires a student to comprehend abstract and complex concepts, such as the statistical approximations of particle collisions and the kinetic theory of gases (Bain et al., 2014). Furthermore, the abstract microscopic nature of thermodynamics makes it difficult for students to understand its concepts. Thermodynamics also involves complex differential equations.

Research conducted over the past ten years has demonstrated that PhET computer simulations significantly improve instructional effectiveness in science education for both high school and university students (Banda & Nzabahimana, 2021). The effectiveness of the simulations has been reported to progress when inquiry-based teaching strategies are used. However, in the global south simulations have been used using a lecture-centred approach as a demonstration (Chinaka, 2021; Ramnarain & Moosa, 2017). Inquiry-based approaches can prove futile with large classes in HEIs in South Africa. South Africa is a country that has endured apartheid past injustices for a long time. In a quest to increase access and equity to education at Higher Education Institutions (HEI) this has led to massification, and large classes have become a reality. While the size of large classes varies among different universities, in a rural and comprehensive university context, a large class can mean more than 200 students in a lecture room. The high enrolments in HEIs started in 2012 when the South African Department of Higher Education and Training (DHET) published its Green Paper encouraging enrolments to increase from 900,000 to 1.5 million by 2030 (Green Paper on Post-School Education and Training, 2012).

1.2. Purpose of study

The recurrent difficulty experienced by first-year students, resulting in poor marks in Natural Science and Technology, underpins this research. The conceptual challenges that students face in college, which stem from high school, are not likely to be overcome anytime soon, therefore universities need to figure out how to meet the demands of their students. They may need to reconsider the current lecture formats and curriculum structure. This study explores an alternative instructional approach for teaching the First Law of Thermodynamics using the PhET gas and properties simulation, guided by the Johnstone triangle framework.

2. METHODS AND MATERIALS

This study employs a novel instructional methodology to teach the First Law of Thermodynamics, leveraging the PhET gas and properties simulation alongside the Johnstone triangle framework. Traditional, lecture-based teaching approaches in contexts like South Africa often lead to misconceptions about thermodynamic concepts, particularly due to their heavy reliance on mathematical formulations. By using the PhET simulation, this methodology offers a visual and interactive exploration of core principles like heat, temperature, and internal energy, allowing students to develop a clearer, sub-microscopic understanding without overwhelming them with calculations.

3. RESULTS

3.1. The first law of thermodynamics

The first law of thermodynamics is based on the principle of conservation of energy, which states that energy can be converted from one form to another but cannot be created or destroyed. The validity of the First Law of Thermodynamics is challenging to establish when assessing the total energy of the universe. In the field of chemistry, this involves calculating the kinetic energy of electrons in atoms and ions, along with the potential energy associated with the atomic nuclei. The First Law can be validated by measuring changes in a system's internal energy, which encompasses mechanical energy as the sum of kinetic and potential energy. However, students often find it difficult to differentiate between kinetic, mechanical, thermal, and internal energy. Maskiewicz and Lineback (2013) suggest that these challenges arise from the students' everyday understanding of the concepts of "heat" and "work."

In introductory physics and chemistry, Nilsson and Niedderer (2012) reported that students struggled to identify how work is done by and on the system. Furthermore, students have challenges with the relationship between the system and their surroundings. In a similar study, Bain and Towns (2016) found that students have difficulties in using the first law equation $\Delta U = q + w$. Most students thought that the internal energy is conserved only through the initial and final states. Several researchers (Hadfield & Wieman, 2010; Abell & Brezt, 2019) have reported that using mathematical problem-solving still poses difficulties among first-year students. Three equations: $w = -\int PdV$; $q = \int CvdT$; $\Delta U = q + w$, that represents the first law are treated separately by most students. Furthermore, how equations represent both the conversion and conservation of energy challenges the students.

While many students are adept at performing numerical calculations with ideal gas laws during high school, they often struggle to connect these mathematical equations to the curves depicted in PV diagrams (Iyengar & deSouza, 2014). PV diagrams allow students to derive fundamental gas laws, such as the relationship between pressure and volume for ideal gases at a constant temperature, which can be illustrated using xy plots. A consistent theme in the literature indicates that, despite formal instruction, some students do not transition to a more scientifically accurate understanding of energy, heat, temperature, and related concepts. The integration of everyday ideas such as work, heat, and energy can further complicate their comprehension of thermodynamic principles.

Several teaching approaches have been reported on introducing thermodynamics (Xing et al., 2023, de Souza & Iyengar, 2013, Finkenstaedt-Quinn et al., 2020). To introduce the Pressure vs Volume graphs (de Souza & Iyengar, 2013) used pictorially integration to explain work and state functions. The thrust of the study was to distinguish between state functions and non-state functions. PV diagrams were also employed to explain entropy and provide a microscopic perspective using the Maxwell-Boltzmann distribution. The First Law of Thermodynamics was introduced through the classic textbook example of a gas contained in a cylinder with a moving piston. This approach was underpinned by the macroscopic fundamentals of thermodynamics and kinetics concepts. One advantage of this approach was to use graphs first followed by a strong mathematical basis to explain state functions and non-functions.

Finkenstaedt-Quinn et al., (2020) used the Writing to Learn assignment to capture students' conceptions of thermodynamics and kinetics. This approach is grounded in the constructivist perspective of learning, where students initially interact with knowledge through two external representations. Additionally, the students are supplied with articles where they apply their conceptual knowledge. The researchers reported that the approach allowed the students to interact with their peers and they also got anonymous feedback. In addition to capturing students' knowledge, the writing itself facilitates peer-to-peer knowledge construction (Klein and Leacock, 2012) as feedback is a very important continuous reoccurring stage in learning (Lu et al., 2022). Anonymous feedback was based on laws of thermodynamics and entropy. The results of this study reported learning gains in the students' abilities to describe thermodynamics and kinetics concepts. Students performed well in areas that have been deemed difficult in research. The WLT showed that when students are offered more opportunities on important concepts of thermodynamics their conceptual understanding improves.

Schwedler and Kaldewey (2020) used a simulation Bridging Imagination and Representation (BIRC). The simulation was designed to provide first years with a learning opportunity in physical chemistry. The simulation used molecular dynamics to improve the student's mental model on the sub-microscopic level. It also targeted the microlevel to connect them to equations and PV diagrams. The results of the study revealed that the BIRC improved the conceptual understanding of thermodynamics concepts. The students were also able to link the abstract representations to other concepts in Physical chemistry.

3.2. The standard approach

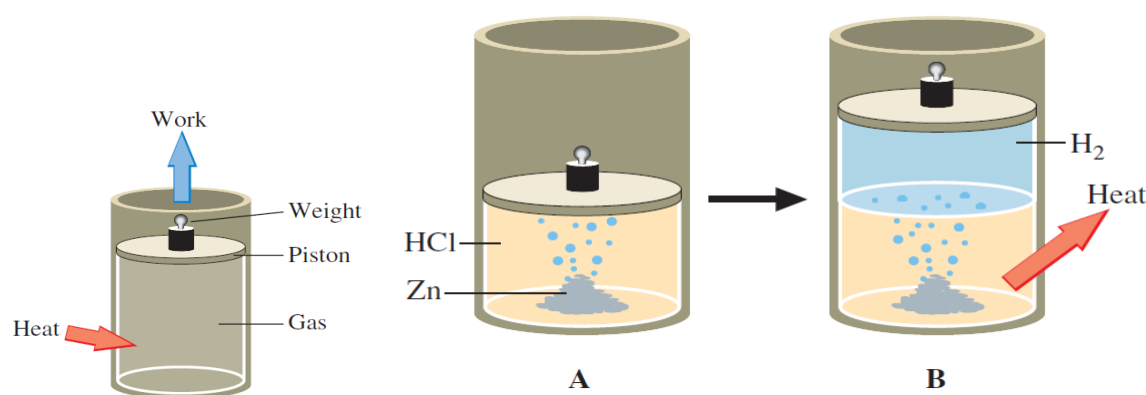
The first law of thermodynamics is introduced using the lecture-centered approach. About two hundred students are enrolled every year. Two college physics textbooks are used as resources Cutnell and Johnson 11th Edition (Cutnell and Johnson, 2009) and Giancoli Physics with Applications 7th Edition (Giancoli, 2013). The lecturer presents the lecture using Microsoft PowerPoint slides and YouTube videos. The first part of call involves defining thermal energy and explaining the difference between heat and temperature. Heat has many

definitions that can be reduced and focus on energy transferred due to a temperature gradient. Next, internal energy (U) is defined as the total energy of all the molecules within the system. It encompasses both the kinetic and potential energies of its atoms and molecules. Changes in a system's internal energy occur as a result of heat transfer and work, which serve as the foundation for the First Law of thermodynamics.

In chemistry, kinetics refers to the energy associated with the motion of electrons, nuclei, and molecules. Potential energy, on the other hand, is derived from the chemical bonds between atoms and the attractions between molecules. At this point, internal energy is introduced as a state function, which is a property of a system that relies solely on its current state. Path functions, on the other hand, are those that depend on the path between two points. The state function refers to values based on the state of the substance, such as temperature, pressure, or amount. This is followed by introducing a path function work. Work done is the exchange of energy that results when a force is displaced.

Figure 1

Work done by system adapted from Ebbing and Gammon (2007)



The diagrams above (Figure 1) are used to explain the work done. The First Law is dependent on two state functions (ΔU , H) and path-dependent Work done. ΔU in the system (Figure 1) gains internal energy from the heat absorbed and loses internal energy via the work done.

3.3. Johnstone triangle

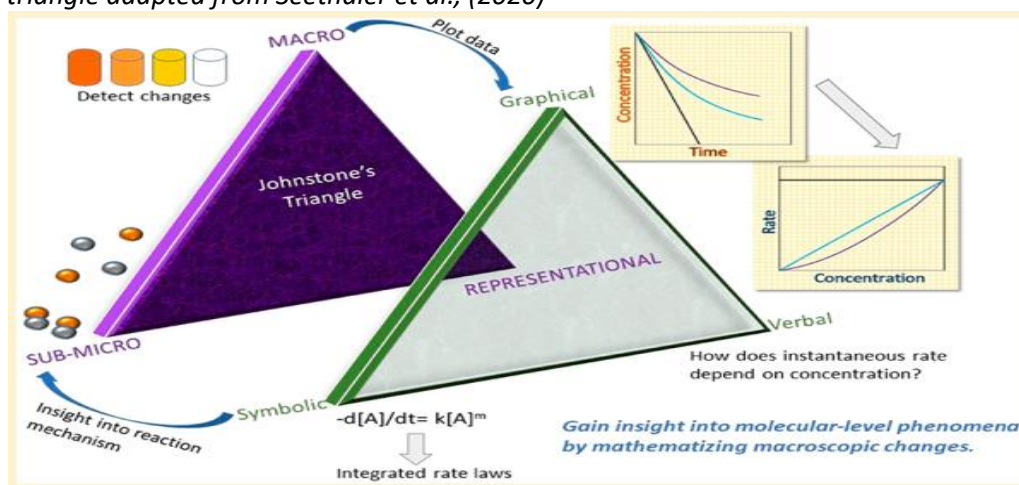
Johnstone (2010) proposed that knowledge in physics and chemistry can be understood through three fundamental "levels" or "representations": macroscopic, symbolic, and sub-microscopic. The macroscopic level encompasses everything that can be perceived through the senses, such as sights, smells, and tactile experiences, which include practical investigations and observations. The sub-microscopic level refers to the dynamic nature of atoms, molecules, and ions involved in reactions, which is not directly observable and relies on explanatory models. The symbolic level consists of representations such as symbols, equations, mathematical formulas, graphs, and diagrams. While scientific phenomena are often observed at the macroscopic level, their explanations typically involve abstract concepts that are not visible. Johnstone (2010) states that an expert chemist can operate at all three levels with ease. He postulates that experts in chemistry view any subject topic at three levels, and "jump freely from level to level in a series of mental gymnastics". However, students struggle to operate at all three levels simultaneously, and as a result, they end up making some misinterpretations.

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Figure 2

Johnstone triangle adapted from Seethaler et al., (2020)

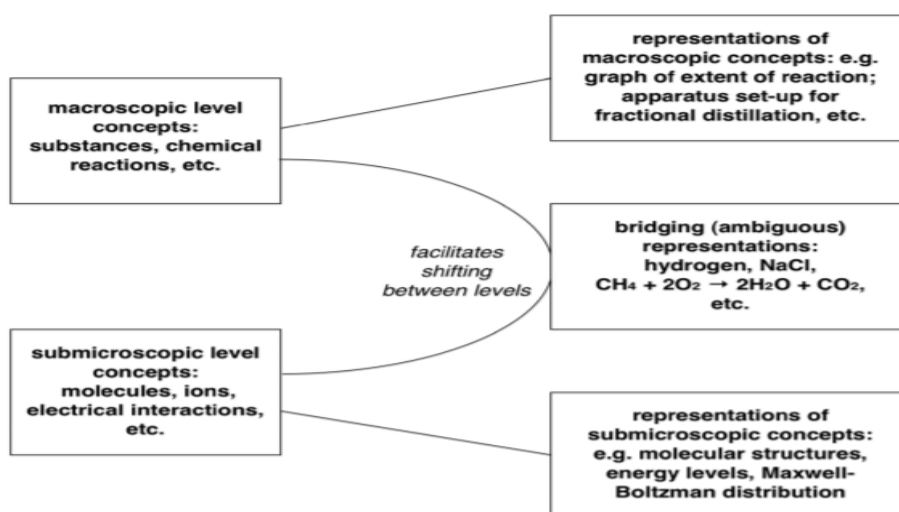


Johnstone's triangle framework (figure 2) is applicable beyond just chemistry. For instance, Wright et al. (2016) employed this model to analyze how students interpret graphs related to catalysis. This theory categorizes various components found within chemistry's three levels, and utilizing these levels as models aids in student comprehension by simplifying the interpretation of concepts and enhancing their understanding of chemical kinetics (Ainsworth et al., 2011). However, Treagust and Chandrasegaran (2009) note that students frequently encounter challenges in grasping and utilizing the interactions among the triangle's levels. On the other hand, Taber (2012) contends that the symbolic or representational level functions as the language for communicating and depicting chemical concepts, asserting that it should not be treated as an isolated "level" of chemical knowledge but rather as an essential part of the ontological triad encompassing the macroscopic, sub-microscopic, and symbolic dimensions.

Taber (2012) views two levels (Figure 3) the macroscopic and sub-microscopic, to be of vital importance when learning chemistry, and the representation or symbolic level facilitates the shift. Thus, representations such as graphs are treated as facilitators that enable students to shift between the macro and sub-microscopic levels. However, the present study views the symbolic representation as critical in interpreting graphs. Graphical representation is fundamental in interpreting chemical or physical phenomena.

Figure 3

The symbolic domain



According to Taber (2012), the macroscopic peak of Johnstone's triangle presents its own set of challenges. Although chemistry is crucial for understanding and creating materials, introductory chemistry courses often overlook the materials that learners already encounter in their daily lives. Chemistry fundamentally deals with substances, which are significant abstractions from real-world experiences (Taber, 2012). Consequently, the macroscopic level itself incorporates a degree of abstraction that is also present in the sub-microscopic domain. In the context of introductory physics, students are taught to simplify and abstract concepts like frictionless bearings, perfectly rigid supports, and negligible air resistance, further illustrating this notion.

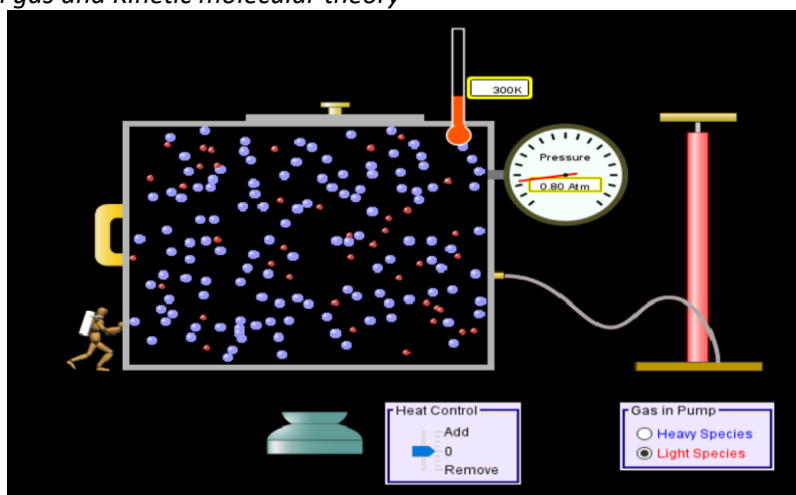
In chemistry education, the tangible aspects of materials are often distilled into the study of pure substances. This approach presents an inherent abstraction, as students must bridge the gap between these theoretical concepts and the real-world phenomena they observe, which often involve various substances, many of which bear unfamiliar names, and the reactions they participate in. Thus, Taber (2012) suggests that there is high conceptual demand even at the 'macroscopic' corner of the triangle. In analyzing the domains of chemical knowledge offered above, symbolic knowledge cannot easily be separated from both macroscopic and sub-microscopic knowledge, since it depicts and communicates the concepts and models developed at these two levels.

3.4. The new approach

The new approach I suggest here uses the PhET simulation Gas properties (Ideal Gas Law | Kinetic Molecular Theory). The simulation can be used to explain thermal energy. Kinetic energy linked to atoms' and molecules' random motion is called thermal energy. It can also be defined as the energy possessed by a system due to the movement of particles within a system. The dynamic nature of the molecules or particles at the microscopic level can be explained well using the simulation. Thermal energy is an important concept that forms the foundation for distinguishing the difference between heat and temperature. The simulation also shows the system and the environment. A clear distinction between the system and the environment is important in elucidating the First Law, especially in emphasizing the conservation of energy.

Figure 4

Gas Properties Ideal gas and Kinetic molecular theory

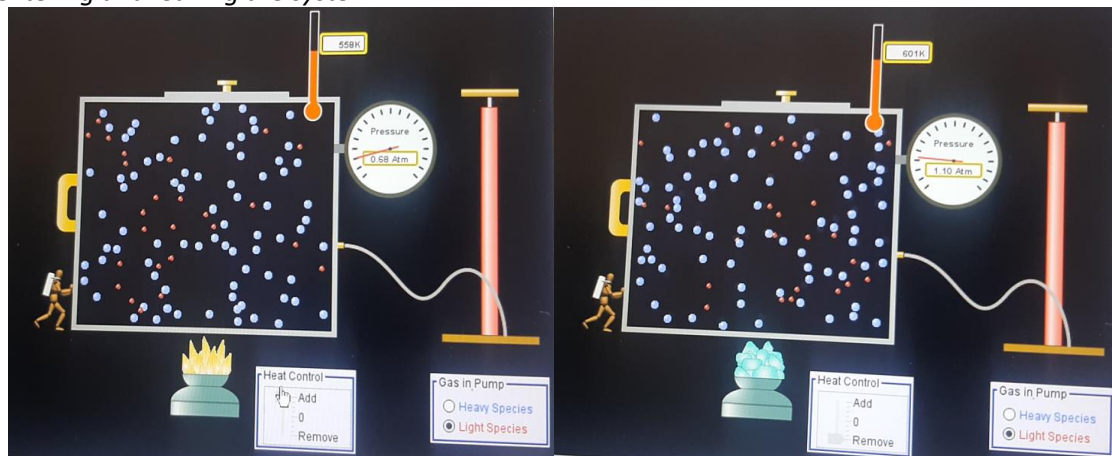


Students from rural schools where the chalk and talk had been the main instructional method might reach university with incorrect conceptions of the system. From Figure (4) the temperature (kelvins) and pressure of the ideal gas are shown on the thermometer and barometer. The interactive and dynamic nature of the particles cannot be explained using still pictures in textbooks. The most important concepts are heat and temperature. The simulation can be used to elucidate the difference. Temperature is the average kinetic energy of the molecules. Using thermal energy and the thermometer the temperature of the system can be defined and explained. Heat is defined as the spontaneous transfer of energy due to a temperature gradient. There must be a temperature gradient between the system and the environment. Figure 5 shows how heat can enter or leave the system due to a temperature gradient. At this juncture, it is important to clearly distinguish

between heat and temperature. The addition of heat doesn't necessarily have to be the flame or ice blocks. The energy can come from the sun, chemical reactions, or the surroundings. The ice blocks show a temperature gradient between the system and the environment.

Figure 5

Heat entering and leaving the system

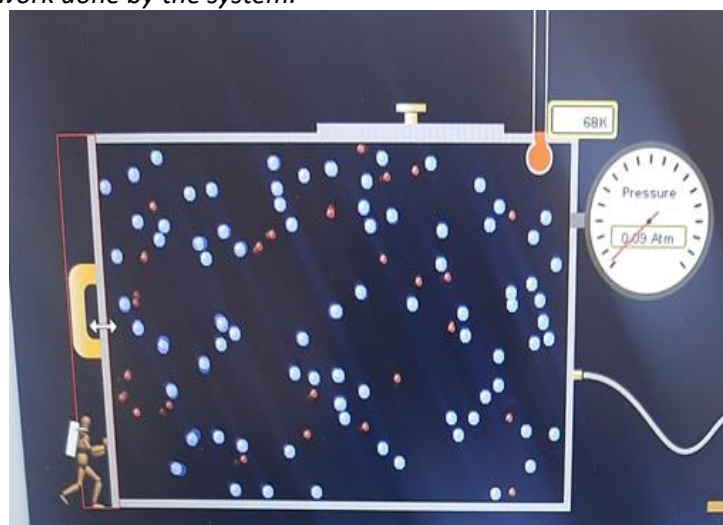


Students must comprehend how energy enters and exits a system to lay the groundwork for the First Law. The system's internal energy is another crucial idea. The sum of the energy of the molecules that make up a system is its internal energy. The total of the kinetic and potential energies of a system's atoms and molecules is its internal energy or U . It is the total of the mechanical energy of atoms and molecules. The system's overall kinetic and potential energies, as well as the difficulty of measuring internal energy, are best illustrated by the dynamic movement of the molecules within it. The logical method to see how heat and work affect the system is to look at the change in internal energy. Therefore, the work done on the system or by the system can result from a change in the internal energy. Lastly, when heat is added to the system, it changes the thermal energy of the energy which in turn does work by pushing the man on the system backward (work done by the system) or inwards (work done on the system). The area of the system that results from the translation is the work done.

The area represented by the red rectangle shows the work done by the system. This method sidesteps the use of mathematics especially calculus which involves partial differential equations. Thus, this new approach is another route from the traditional cylinders used in most textbooks. The area is mainly given as $W = -P\Delta V$, here the area is a rectangle.

Figure 6

Area of the rectangle work done by the system.



4. Potential advancements

The use of the simulation has the advantage of mimicking real-life experiments. It also improves the visualization of the abstract concepts in physics and chemistry. The PhET simulation improves the visualization of the ideal gas at the microscopical level. At the university level, studying kinetics requires a student to comprehend abstract and complex concepts, such as the statistical approximations of particle collisions and the kinetic theory of gases (Bain et al., 2014). Khumalo and Maphalala (2018) reported that the dominant instructional approach remains teacher-centered in high schools. Thus, students arrive at university with incorrect conceptions of thermodynamics. First-year university general chemistry and physics bridges high school and university such that students come to lectures with pre-conceptions about thermodynamics. Yan and Subramaniam (2018) suggested that pre-conceptions affect learning as they become integrated into the cognitive structures. In this alternative approach to the PhET simulation, the microscopic level and its dynamic nature are elucidated. Though Taber (2012) argued that learning science involves shifting between macroscopic and microscopic, the simulation mainly focuses on the microscopic.

Another important potential advantage is the distinction between two important terms heat and temperature. Students struggle to distinguish between heat, work, and internal energy (Greenbowe & Meltzer, 2003; Bain et al., 2014; Turányi & Tóth, 2013). Furthermore, students struggle to identify heat flow in and out of the system and its surroundings. The PhET simulation can be used to explain heat flow, temperature, and internal energy. It should be noted that at this stage the PhET simulation is being used as a demonstration. The simulation also captures thermal energy in its dynamic nature which cannot be captured in physics or chemistry textbooks. Internal energy is critical in thermodynamics since its measurement can be difficult to measure but its change can be used. Heat flows in and out of the system and is exchanged between the system and the environment due to a temperature gradient. Heat flows spontaneously due to a temperature slope thus using a flame and ice blocks in the simulation to affect a temperature gradient between the system and environment. The flow of heat in and out of the system also affects the thermal energy of the system which also to changes in temperature.

The simulation also sidesteps the contentious issue of mathematics in thermodynamics. Christensen and Thompson (2010) reported that students may have difficulties interpreting physical meaning from mathematical expressions. In addition, students have difficulties with the notion of holding variables fixed in a partial derivative. The potential of the simulation also shows that the area in the rectangle is the work done. This breaks from the traditional cylinders that are used in the textbooks. The cylinders use $W = -P\Delta V$ but the simulation shows that $W = l \times b$. Several studies in thermodynamics have shown that students have difficulty executing the mathematical operations necessary to understand thermodynamics.

The PhET simulation approach can be extended to drawing PV diagrams. It's important to note that the simulation lays bare the idea of an isolated system. The variables are there on the simulation such as temperature, pressure, volume, and heat. Finkenstaedt-Quinn et al., (2020) bemoaned the lack of conceptual understanding of thermodynamic phenomena among university students. The reliance of students on rote skills risks thermodynamics becoming just a mnemonic exercise. Lecturers should strive to teach a conceptual understanding that may lead to better retention even in large classes.

The issue of big classes of roughly two hundred students in the module has led to the usage of the simulation as a demonstration of this new technique. Similar to the conventional teaching method, the demonstrative approach is lecturer-centered. When it comes to teaching with technology, South Africa and higher education in general face several fundamental obstacles. According to numerous scholars in this sector (Burnapp 2011; Khoza 2011; Sharpe et al., 2010), pedagogical knowledge continues to be a barrier to the efficient use of emerging technologies, despite their growing popularity among educators and students.

"How can we, in a volatile higher education environment that is struggling to come to grips with transforming an oppressive system, move beyond using technology as an incidental adjunct?" and "How do we cater to an increasingly diverse student population with varying levels of technological ability, while overcoming our fear and frustration with "technologies that become obsolete as quickly as they arrive?" are two questions written

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by Pratt (2014) that highlight the difficulties of integrating technology as a pedagogy. The Technological Pedagogical and Content Knowledge (TPACK) framework developed by Mishra and Koehler (2006) provides a helpful framework for examining some of the difficulties in integrating technology into education as a pedagogy. As a result, using the PhET simulation may need to incorporate technology into instruction.

5. CONCLUSION

The study introduced an alternative approach to introducing the First Law of Thermodynamics. In the global South high school is characterized by the traditional teacher-centred instructional approach. The chalk and talk coupled with a lack of teaching resources led to incorrect conceptions of thermodynamics. Students reach university with alternative conceptions. At university large classes also lead lecturers to use lecture-centred approaches. The PhET simulation is proposed as a demonstration. According to the Johnstone triangle, the students must translate the three domains (macro, representation, and sub-micro) to understand thermodynamic phenomena. The PhET simulation gas and properties operate mainly at sub micro level.

The students can make shifts from the sub-micro level to the representation and macro levels. Important concepts in thermodynamics heat, temperature, thermal energy, and internal energy must be taught at sub micro level. Textbooks do not provide the dynamic movement of the particles instead pictures are used. The simulation discussed in this study provides an alternative approach to understanding two terms that are used in everyday life heat and temperature. One limitation of the approach is that lecturers must integrate the simulation as a pedagogy. Implications for practice is to use PhET simulations in large classes.

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Ethical Approval: The study adheres to the ethical guidelines for conducting research.

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