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AN ONTOLOGICAL AND EPISTEMOLOGICAL ANALYSIS OF THE PRESENTATION OF THE FIRST LAW OF THERMODYNAMICS IN SCHOOL AND UNIVERSITY TEXTBOOKS

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Abstract

Considering the relevance of thermodynamics to the scientific discipline of chemistry and the curriculum of the Western school system, the philosophical system of Mario Bunge, particularly his ontology and epistemology, is used herein to analyze the presentation of the first law of thermodynamics in 15 school and university textbooks. The ontological analysis shows that the concepts heat “q” and work “w” are categorized as processes, while the concepts of internal energy “U”, pressure “P”, volume “V” and temperature “T” are categorized as properties. The results reveal that 8 of the 15 textbooks incorrectly present work “w” as a property, while 7 textbooks incorrectly present heat “q” as a property. Furthermore, 3 textbooks present the concept of energy as a property and assign it a merely operational definition as the capacity to do work. The analysis also examined patterns of causality and the mechanism used to explain the connection between the variables of cause and effect in three thermodynamic systems. The results indicated that only 2 textbooks contain such a mechanism.

Introduction

In the natural sciences, the concepts of theory, hypothesis and law are generally confused by both professional scientists and science teachers (Lederman, Abd-El-Khalick, Bell, & Schwartz, 2002). One of the most influential philosophies for defining these concepts within the natural sciences is scientific realism, whose principle exponent, according to the journal Science, is Mario Bunge (Michel et al., 2011). One of the most notable features of this philosophy is the fact that it is not simply epistemological but also logical, ontological, axiological and metaphysical (Bunge, 1974a, 1974b; Bunge, 1977, 1979, 1983a, 1983b).

The proposal defines the concepts of theory, law and hypothesis as follows. A scientific hypothesis is an idea, i.e., a statement, regarding a given material reality, which should have a basis and be empirically verifiable. Supporting evidence will then validate the idea as a scientifically legitimate hypothesis. A law is a subcategory of a hypothesis and identifies a pattern of causality and a proven mechanism that connects the variables of cause and effect. Finally, a scientific theory is a system comprising hypotheses logically connected by a relationship of deductibility, wherein the most general hypotheses are known as posits or axioms (Bunge, 2007).

Therefore, in this philosophy, the concepts of hypothesis, law and theory are closely linked, not only in how they are formed (epistemology) but also in their natural or material reference points (ontology and metaphysics). The ontology and the materialist metaphysics of this system offer important semantic tools for clarifying scientific concepts for teaching purposes. For example, in 2000, Mario Bunge clarified the concept of energy from an epistemological, an ontological and a metaphysical perspective. He categorized energy as the only property applicable to all material objects, thereby implying the mutability of reality (Bunge, 2000).

Using ontology and realist epistemology to analyze scientific concepts, in a previous study, our research group analyzed Boyle’s Law from an ontological perspective, identifying the variables of pressure and volume as properties of a gaseous system, where the volume is the cause and the pressure of the gas is the effect. This perspective is consistent with the proven mechanism of molecular collisions. Analyzing 14 university-level general chemistry books from this perspective showed that 13 of the books contained serious ontological errors, such as omitting the pattern of causality or presenting it erroneously, namely by identifying pressure as the cause and volume as the effect (Quiroz & Rubilar, 2015). In a subsequent study, our group analyzed the concept of osmosis and its presentation in university-level biology and chemistry textbooks. The results showed that more than 50% of the books identifies osmosis as a process associated only with the property of concentration, thus reducing it to a mere diffusional process, without mentioning the state of equilibrium and the property of osmotic pressure (Spinelli Barria, Morales, Merino, & Quiroz, 2016).

Many complex concepts can benefit from Bunge's ontology and metaphysics to ensure their correct presentation. It is clear that the evaluation of Mario Bunge's systematic philosophy provides an opportunity for science education(Matthews, 2012). However despite its great influence on the philosophy of science, the application of this philosophical system for the analysis of scientific concepts in science education studies has been comparatively minor and limited to a few works of Deleporte about the concept of "specie" in biology (Deleporte, 2012), a Bunge work on the concept of energy(Bunge, 2000) and our previous works about Boyle´s law(Quiroz & Rubilar, 2015)and the concept of "Osmosis" (Spinelli Barria et al., 2016). In more general terms, beyond the philosophical system of Mario Bunge, the use of ontology as a tool for the analysis of scientific concepts in science education studies are mostly limited to the work of chi and colleagues about conceptual change and its relationship with ontology (Michelene T. H. Chi, 2008; M. T. H. Chi, Roscoe, Slotta, Roy, & Chase, 2012) . The same problem arises in the case of the use of epistemology for the analysis of scientific laws where the only work we have found in literature is from Kipnis related to Ohm's law(Kipnis, 2009). Considering the core relevance of classical thermodynamics to chemistry as a scientific discipline and the importance of chemistry knowledge in the Western school system, we deemed it relevant to apply this tool for analyzing the presentation of these concepts in science textbooks. Accordingly, this study aims to ontologically and epistemologically analyze the presentation of the first law of thermodynamics in chemistry textbooks used in universities and schools.

Classical Thermodynamics

Logically and epistemologically, classical thermodynamics is a theory comprising four general scientific hypotheses, or axioms, all of which are laws. The first two laws are known as the zeroth and the first laws and are mentioned in most general chemistry textbooks and the Chilean secondary education system.

To analyze the presentation of these laws in scientific and school textbooks, we must first establish their ontology, i.e., the material references of their concepts, and their patterns of causality.

The zeroth law of thermodynamics states that a thermodynamic property called temperature exists. This law defines the state of thermal equilibrium as the point at which the temperatures of the two systems in contact are identical (Engel et al., 2007). The first law defines a second property of a system, namely internal energy. Depending on the conditions, changes in internal energy (ΔU) can occur from or to the environment through the processes of heat and/or work. Mathematically, these changes are presented in the following way in most textbooks, as shown in Equation 1.

$$\Delta U = q + w \quad (1)$$

where "q" and "w" are the concepts of heat and work, respectively.

The present study aims to visualize how the first law of thermodynamics is presented in university and school textbooks, while, if possible, discerning whether the law is presented with the correct pattern of causality and the mechanism responsible for generating a particular effect. It is also important in this study to identify the ontological definition attributed to this law and how concepts associated with it are used, such as internal energy, heat, work, volume, pressure and temperature. Considering the universal application of this law, our analysis focuses on perfect gases and reversible processes, which are the most common systems used to develop and explain this law in chemistry textbooks.

Ontological classification of the concepts of internal energy, temperature, heat and work

Mario Bunge's philosophy defines the following five ontological categories: "things or material objects", "properties", "processes", "events" and "states" (Bunge, 1977). As explained below, the two categories relevant to the laws of thermodynamics are properties and processes.

A property refers to a characteristic or an attribute of an object or a thing. Therefore, properties do not exist of their own accord. In the zeroth law, the concepts of temperature and internal energy "U" are properties because, as Mario Bunge explains, energy does not exist of its own accord; rather, an object with energy exists. This explanation is consistent with the evolution of caloric theory, which regards energy as an object, whereas contemporary thermodynamics regards it as a property (Levine, 2014). The same rationale holds for the concept of temperature "T". That is, temperature does not exist; instead, objects with temperature exist, as specified by this law.

The most complex concepts to categorize ontologically are heat and work.

The concept of heat "q" can be explained as follows:

> *[…] the term "heat" is that it's like "hotness." "Hotness," as we illustrated above, refers to molecular motion, and motion is a Process. But the technical term heat, although a noun, actually refers not just to the motion of the molecules, but to the transfer of "hotness." That is, heat is defined as "the transfer of energy" or energy in transit from one object or substance to another, and is therefore a Process*. Chi et al. (Michelene T. H. Chi, 2008)

Given our perspective, we classified both work and heat as processes. For Mario Bunge, a process is a successive and sequential change in the state of an object, whereas a state is a set of properties that define an object at a given moment.

The concept of heat "q" therefore refers to a process of energy transfer that occurs when a system moves from an initial state of thermal disequilibrium to a final state of thermal equilibrium. Clearly, this concept is associated with states, the properties of energy and temperature and changes over time. Our classification is aligned with this reasoning. The concept of heat is not classified ontologically as a "form of energy", as this classification would imply that heat is a property, i.e., an attribute of a material object, similarly to pressure or volume. Heat characterizes the change from a state of thermal disequilibrium to a state of thermal equilibrium. Thus, it is not an attribute of an object, but a manifestation of a change in internal energy based on differences in temperature. Heat refers to the process, whereas temperature and internal energy are properties of the different states, and the material object is the physiochemical system in which the process occurs.

The concept of work is also related to changes in states within a thermodynamic system. These states can be clearly identified in certain cases, for example, in the case represented below by the graph of volume "V" vs. pressure "P", both of which variables, together with temperature T, describe the current state of the system. These variables change over time due to energy exchanges. As with the concept of heat, the concept of work is intrinsically connected to states, properties and changes. Accordingly, our classification of work as a process stems from this understanding of connectedness.

Therefore, proposing that a body "possesses" heat is as incorrect as stating that a body possesses work. Properties, not processes, are possessed, and they are possessed by material objects. Our ontological classification is summarized in Table 1.

Table 1 Ontological classifications of implicit and explicit concepts in the zeroth and first laws of thermodynamics

Variable	Ontological classification
U	Property
q	Process
w	Process
T	Property
P	Property
V	Property

Pattern of causality of the zeroth law

The zeroth and first laws of thermodynamics hypothesize a pattern of causality. A semantic analysis of these laws within the framework of the materialist ontology of Mario Bunge's philosophy establishes the variables of cause and effect and the mechanisms responsible for forming the patterns of causality.

For the zeroth law, the analysis is simple in that the law states that given two systems in contact and of identical temperature, thermal equilibrium is established, thereby implying that given two bodies with the same temperature (cause), the effect is that the difference in internal energy is zero ($\Delta E=0$), assuming no other energy transfer is occurring.

Similarly, given two bodies with different values of mass, m_1 and m_2, and different temperatures, T_1 and $T_{2,}$ such that $T_1 > T_2$, an energy transfer will occur from the body with higher temperature to the body with lower temperature until thermal equilibrium is achieved at a final temperature $T_{f,}$ as expressed by Equation 2:

$$m_2c_2(T_2-T_f)=m_1c_1(T_f-T_1)\equiv q \quad (2)$$

where c_1 and c_2 are the specific heat capacity of both bodies. The cause variable is T, a property, and the effect variable is the transfer of energy E, also a property. The mechanism associated with the process of heat "q" occurs at a microscopic level and involves the movement of particles that collide with the system walls. Contact between the bodies permits energy exchanges, which are manifested in the aforementioned process. The patterns of causality of the zeroth and first laws are therefore closely linked.

Pattern of causality of the first law of thermodynamics

Because the first law explicitly involves three variables, ΔU, q and w, and implicitly involves T, P and V, analyzing its pattern of causality is complex and cannot be performed without considering the specific material system. The following section analyzes the patterns of causality for different specific systems.

System with a mobile adiabatic wall

Consider a system consisting of an occluded gas in a chamber with a mobile but thermally isolated wall. Here, energy exchange does not occur via heat. Therefore, q=0, so the first law is reducible to Equation 3:

$$\Delta U=w \quad (3)$$

During an infinitesimal change of temperature, the heat capacity of a gas remains nearly constant. Because any change in internal energy depends only on a change in temperature, the relationship between internal energy and temperature can be expressed by Equation 4:

$$\frac{dU}{dT} = C_v \quad dU = dTC_v \text{ (4)}$$

Considering a mobile wall, the value of work “w” can be expressed as Equation 5:

$$w = -PdV \text{ (5)}$$

Inserting Equations 4 and 5 into Equation 3 and considering the ideal gas equation, where $P = \frac{nRT}{V}$, yields

$$dTC_v = -PdV$$

$$dTC_v = -\frac{nRT}{V}dV$$

$$C_v\frac{dT}{T} = -nR\frac{dV}{V}\text{(6)}$$

For a process resulting in a change of state 1 (T_1, V_1) to state 2 (T_2, V_2), Equation 7 applies:

$C_v\int_{T_1}^{T_2}\frac{dT}{T} = -nR\int_{V_1}^{V_2}\frac{dV}{V}$(7). This equation can be subsequently integrated into Equations 8 and 9.

$$ln\left(\frac{T_2}{T_1}\right) = ln\left(\frac{V_1}{V_2}\right)^{\frac{R}{Cv}} \text{ (8)}$$

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\frac{R}{Cv}}\text{(9)}$$

In a reversible process, P could be maintained to be relatively constant. Consequently, the causal relationship would be initiated by a change in the gas Volume “V”, followed by work “w” changing the gas temperature “T” without heat “q”, and finally, a change in internal energy (U). However, the variation of V, T and P it happens simultaneously according to equations 8 and 9. Anyway, ΔV in this case is the cause and ΔU is the effect.

ΔU (effect) ← ΔV (cause)

A system with rigid diathermal walls

For the case of an occluded gas within rigid but thermally conductive walls, w = 0 because the volume does not vary. If this system is placed in contact with a system of a different temperature, then an energy transfer will occur via the heat process, represented by Equation 10:

ΔU = q (10)

When an infinitesimal quantity of energy is transferred by differences of temperature until a body of mass m and specific heat capacity C (at constant volume), the heat process can be obtained by Equation 11:

$$dq_v = mc_v dT \quad (11)$$

Thus, the magnitude of the heat can be calculated with Equation 12:

$$q_p = m\int_{T_1}^{T_2} c_v dT \quad (12)$$

where T_2 and T_1 differ in terms of the cause and ΔU, the effect. The choice of T as the cause is not arbitrary, but based on the implicit mechanism. Because the temperatures of the occluded gas and its environment differ, an energy transfer occurs until thermal equilibrium is attained. The initial cause of the entire process is the temperature T in the two systems, thereby provoking the effect "q", which causes a variation in the internal energy of the system, ΔU. If the system is at a lower temperature T than the environment is, then its internal energy will increase due to the energy transfer, and vice versa. As T increases, the kinetic energy (E_k) of the molecules increases, as expressed in Equation 13:

$$E_k = \frac{3}{2}kT \quad (13)$$

As E_k increases, the average velocity of the gas molecules of mass "m" increases, as expressed in Equation 14:

$$E_k = \frac{1}{2}mv^2 \quad (14)$$

where v is the average velocity of the molecules. Finally, after the average velocity of the molecules increases, the gas pressure increases, as represented by Equation 15:

$$P = N\frac{m\,v^2}{V} \quad (15)$$

where P is the gas pressure, and V is the gas volume, which remains constant in a system with rigid walls. This mechanism is related to the Gay-Lussac Law.

Hence, it is evident that if the system is isolated and has rigid walls, then the variation in internal energy is zero because the internal energy of the system remains constant, as specified by Equation 16.

$$\Delta U = 0 \quad (16)$$

This equation represents how the law is presented in many textbooks. It implies that no physical processes are possible, an implication that is also a universal statement and therefore does not contradict the law. Rather, it concurs with established knowledge, namely the general law of energy conservation.

A closed system with mobile and thermally conductive walls

In a closed system with mobile and thermally conductive walls in which heat and work can be present in different proportions, the first law in Equation 1 is a valid mathematical expression in that the two processes, heat and work, are generated based on the initial and final conditions of the states involved.

The cause variable for this type of system is established, which in certain cases, may be V, where a variation of this property generates an energy transfer via w, consequently varying the internal energy U. Thus, if the initial and final temperatures of the system are not identical, then the heat process is initiated.

The latter occurs because the original cause variable can be temperature or volume, depending on the conditions of the given material system. That is, a difference in temperature will spur an energy transfer, culminating spontaneously upon attaining thermal equilibrium. Depending on the final gas volume, which will depend on the external pressure, work "w" will be generated, and its magnitude will in turn depend on the distance the wall moves. The remaining energy will increase or decrease q and internal energy U. Table 2 shows the patterns of causality and the mechanisms on which they are based within the context of this proposal.

Table 2 Patterns of causality of the first law of thermodynamics and their associated mechanisms

System	**Cause**	**Effect**	**Mechanism**	**Expression**
Diathermal	T	ΔU	$T \to q \to P \to \Delta U$	$\Delta U = q$
Adiabatic	V	ΔU	$V \to P \to w \to T \to \Delta U$	$\Delta U = w$
Isolated	-	-	No process occurs	$\Delta U = 0$
Closed	T,V	ΔU w	$T \to V \to P \to w(q^*) \to \Delta U$	$\Delta U = q + w$

* The magnitude of q depends on the initial and final temperature of the system.

Teaching thermodynamics in the school system

In teaching chemistry, how a scientific idea is communicated to students is crucial, particularly when the goal is the scientific literacy of the public, in other words:

> A process of "focused investigation" that ignores conceptual reductionism to allow students to participate in the scientific adventure of facing relevant problems and (re)building scientific knowledge that teaching normally presents already built, thus favoring more efficient and more significant learning (Sabariego del Castillo, 2006)

Current science teaching focuses on transmitting established scientific knowledge. The challenge today, however, is ensuring this transmission includes processes of reflection and constant questioning whereby students can internalize the acquired knowledge, while rebuilding and using their initial conceptions as starting points to gain a fuller understanding of a particular topic. "*The presence of these ideas in students is thus very relevant in the process of building knowledge, given that students learn based on what they already know"* (Mahmud & Gutiérrez, 2010).

Students formulate different conceptions of a subject, based on their interaction with reality through their senses, the means by which common knowledge increasingly acquires its basis and structure and which will eventually be expressed through everyday language and thus communicated within society. Can we use everyday language to refer to scientific concepts, facts or phenomena? We know the answer, and we know that the use of everyday language, on many occasions, is incompatible with the concepts representing scientific knowledge. Thus, the language used to express a scientific idea must be articulated to communicate the underlying concept correctly so that the concept can be clearly and precisely understood, as described by Neus Sanmartí (1999): "*A characteristic of this type of language is the specific vocabulary it possesses*". Terms are often used whose everyday connotation refers to the precise object. Moreover, in specific cases, such as heat and temperature, terms are used in the same contexts, but no differentiation is made in everyday language. This lack of differentiation can influence the ideas students form about the concepts.

About the concepts underlying the first law of thermodynamics it is important to mention that the ontological relationships between energy, work and heat is complicated and have evolved from the work of joule in 19 century(Rosenberg, 2010). Therefore is not surprising that both teachers and students generate alternative ideas about the concepts of energy, work and heat.

For example, Kean et. al demonstrate that a significant number of seniors in chemical and mechanical engineering do not understand how temperature and energy are related (Kean et al., 2008). On the other hand Niaz evaluate the ability of science major freshman students to differentiate between heat energy and temperature demonstrating that even after having studied thermochemistry, students still have considerable difficulty in differentiating those thermodynamics concepts(Niaz, 2006). In 2013 Wattanakasiwich et. al develop a conceptual survey for assessing the understanding of more than 2000 student from Australia and Thailand of fundamental principles in thermodynamics. The results demonstrate that students have more difficulties in the integration of concepts related with the first law of thermodynamics and processes related(Wattanakasiwich, Taleab, Sharma, & Johnston, 2013). Another study of Laburu and Niaz they propose a Lakatosian philosophical approach for the differentiation between heat energy in 32 ninth-grade students in a public school in Londrina, Brazil. Results demonstrate that some students were able to question the "hard-core" of their beliefs about heat, energy and temperature to construct a transitory model that increase progressively in their heuristic/explanatory further towards the scientific model(Laburú & Niaz, 2002).

An study among students aged 12 to 23 years on alternative ideas related to the concepts of heat and temperature and learned that a large proportion of students had incorrect prior conceptions, such as “*the body has heat*”, and “*temperature is heat*”. The study concluded that the influence of everyday language persists in the use and verbalization of many ideas associated with heat and temperature (Mahmud & Gutiérrez, 2010). This study is noteworthy because the first quote highlights the ontological confusion between a process (heat) and a property that is emphasized by the phrase “has heat”. The second quote equates temperature and heat, thus revealing an ontological confusion between property (temperature) and the process that triggers it (heat).

A study conducted at Ahi Evran University found that “*of a sample of 60 second grade students at the department of sciences of the Faculty of Education, 38% do not comprehend the difference between the concepts of heat and temperature, using the different contexts indistinctly, which is in agreement with several studies in this area (.; McDermott, 2003)”* (Kartal, Öztürk, & Yalvaç, 2011). Finally in an excellent review of Wong, Chu and Yap about alternative conceptions of the concept of heat they find that can be classified in five categories: “residing in object,” “ontological”, “movement,” “cause and effect,” and “condition” which may be traceable to the linguistic usage or definitions in textbooks. In this work they demonstrate that even among scientists and science educators still are some disagreement on the definition of heat considering as an adjective, a nuon, a verb, a process, a “form of energy”, thermal energy and molecular kinetic energy(Wong, Chu, & Yap, 2016).

According to Carrascosa (2005), the origins of the alternative conceptions vary, but they can nevertheless be classified as follows:

> The influence of everyday experiences in which the reiterative, sensorial and direct nature of these experiences and, fundamentally, the habitual way they are interpreted though the use of ordinary thought, lead to the internalization of certain explanations as unquestionable evidence.

As mentioned, the influence of verbal, visual and written communication is based on the premise that common language comprises words whose meaning is the fruit of everyday experiences transmitted by previous generations. Therefore, occasionally, this process of transmission can engender or perpetuate alternative ideas.

Thus, these conceptions are articulated coherently through our mental structure. They remain persistent in a field and resist conceptual change, thus prompting the following question: How can we refocus these conceptions and build a coherent scientific notion based on science? Although answering this question requires analysis from several different viewpoints, in the current context, one viewpoint is particularly relevant. This viewpoint encourages correctly using scientific language in science classes. It simultaneously recommends providing adequate tools and strategies to contend more critically and more reflexively with the reality presented in the literature or in scientific textbooks, based on the idea that all knowledge can be questioned and that questioning information obtained from different sources is the process that has generated scientific knowledge throughout history (Greenbowe, 2003).

We have discussed in general how articulating scientific language acquires importance in science teaching and how alternative conceptions can arise through personal experience. It is important to mention a third origin of these conceptions, as it is the focus of the present study, namely the conceptual errors or omissions in textbooks in the body of the text, images, or the captions accompanying the images. Conceptions can arise in secondary education and persist throughout higher education. They can also be reinforced by specific university textbooks such that the concepts formed prior to university learning are not refocused into accepted scientific knowledge, but remain, generating alterative conceptions. Therefore, it is important to analyze a scientific text from a more critical and reflective viewpoint, which teachers should likewise encourage by providing students with adequate conceptual tools.

Because this study focuses, moreover, on the ontological classification of concepts, it is important to analyze the relevance of ontology and student misconceptions based on the existing literature. (M. T. H. Chi et al., 2012) propose:

> […] that misconceptions are largely flawed inter-level causal explanations of the patterns of processes, and they are flawed in ‘‘structure’’ (and perhaps also incorrect in other ways, such as the technical details). By flawed in ‘‘structure,’’ we mean that the ‘‘type’’ of explanations might manifest an inter-level attribute that is ontologically inappropriate […]

Building on this argument, Slotta, Chi & Joram propose that:

> “students may classify science concepts according to these ontological categories (Material substances and processes) and then rely on these classifications in subsequent learning as a source of inference or sense making. To the extent that students are mistaken in their ontological categorization of a particular concept, we propose that they exhibit characteristic misconceptions”.(Slotta, Chi, & Joram, 1995)

It is clear thermodynamics is a central issue in education in physics, chemistry, and biology. About that Dreyfus et. al states that *“coordination between and among disciplines would be fruitful”* (Dreyfus, Geller, Meltzer, & Sawtelle, 2015). We believe that the common discourse among these three scientific disciplines can be achieved through a materialistic ontology and also this ontology allows us to understand how introductory-level undergraduate students understand the central concepts to thermodynamics.

We believe that the ontological categories implicitly assigned to scientific concepts may generate alternative conceptions. For instance, it can be difficult to correctly learn that the concept of heat refers to a process of energy transfer, not to a material object or a property.

The current science curriculum provides a large amount of information, prompting the following questions: It is necessary to provide so much information? Are we encouraging student learning? Are we prioritizing significant and/or sustainable learning or mere memorization? We could continue asking similar questions that should be asked by anyone in the teaching profession.

In the context of thermodynamics and considering how its curriculum is defined, we identify several subject areas and concepts that are presented to students in the penultimate year of secondary education. These concepts include energy, heat, work, and temperature. They are defined in the area of physical chemistry and constitute the basis for comprehending several macroscopic phenomena and a wide range of physical and chemical processes.

Therefore, they must be taught correctly so that other chemistry concepts can be understood with a solid, correct and coherently structured conceptual basis, thereby allowing the student to more effectively comprehend other science subjects in the curriculum and thus build a body of knowledge that is adapted to the current demands of science and society. All of the named teaching considerations constitute a challenge for anyone involved in delivering science teaching and must be addressed to achieve significant advancements in the scientific literacy of the general public.

Text analysis

Textbook selection criteria

The criteria used to select textbooks were based on the work of Binn and Bell (Binns & Bell, 2015), Vesterinen et al. (Vesterinen, Aksela, & Lavonen, 2013) and Niaz and Fernandez (2008). The criteria are as follows:

a) The availability of the textbooks in universities, nearby libraries and high schools
b) Textbooks were used in previous years
c) Textbooks that have been published in several editions and have been accepted by the science education community
d) Consultations with colleagues teaching in different parts of the world revealed that various textbooks selected for this study are used as translations
e) Various studies published in science education journals have used these textbooks
f) Textbooks are regularly used by science teachers in the Chilean school system

The present study aims to evaluate the ontological classification and patterns of causality of the first law of thermodynamics by analyzing the presentation of the concepts of energy, internal energy, heat and work in the textbooks. From a pedagogical standpoint, it is also necessary to reflect on how this subject matter in specific physical chemistry textbooks may promote inferior levels of education because of possible errors contained in the textbooks and by identifying the major differences between the textbooks. Although the content of the university and school textbooks cannot be evaluated using identical criteria, due to the expected use of the books, we accept the idea that in science, concessions (e.g., simplifications) are permitted so that a scientific idea can be understood on different educational levels. However, this allowance is acceptable only when the underlying concept remains unaltered in an explanation and its meaning and interpretation do not generate errors and eventual alternative conceptions.

To achieve this aim, 15 textbooks from different educational levels were selected. As Table 3 shows, four textbooks are used in physical chemistry, eight textbooks are used in general chemistry, and three textbooks are used in secondary school education.

Table 3 Textbooks consulted for analysis

Text	Publisher	Author	Year	Pages	ID
Química Física	Pearson Educación	Engel, T., Reid, P., Hehre, W.J.	2006	13-18, 22-23	L1
Química física	Médica Panamericana	De Paula, A., & De	2007	28-40	L2

		Paula, J			
Fisicoquímica	McGraw-Hill Interamericana de España S.L.	Chang, R.	2008	76-84	L3
Fisicoquímica	Compañía Editorial Continental.	Laidler, K. J., & Meiser, J. H.	1997	45-54	L4
Principios de química: los caminos del descubrimiento	Médica Panamericana.	Atkins, P. W., & Jones, L.	2006	198-207	L5
Principios y reacciones	Thomson Paraninfo	W. L. Masterton, C.N. Hurley	2004	212, 229-231	L6
Química la Ciencia Central	Pearson educación	H. E. L. Theodore L. Brown, Jr., Bruce E. Bursten, Julia R. Burdge.	2004	152-162	L7
Química y reactividad química	Thomson Paraninfo	J. C. Kotz, P. M. Treichel, G. C. Weaver	2005	203-220	L8
Química	McGraw - Hill	K. W. Whitten, K. D. Gailey, R. E. Davis	2008	547-551, 566-569	L9
Química	McGraw - Hill	R. Chang	2007	224-234	L10
Principios de química	Panamericana	P. Atkins, L. jones	2012	235-249	L11
Química	McGraw - Hill	R. Chang & K. Goldsby	2014	231-241	L12
Texto del estudiante química 3°-4° Medio	Ediciones Calycanto	Cabello, M.	2015	21-22, 26, 30-36	L13*
Química III medio	Empresa Editora Zig-Zag, S.A.	M. Contreras, G. Cordano, M. Rojas, J. Valenzuela.	2010	16-25	L14*
Química III medio	Santillana Bicentenario	N. Arancibia, O. Ortega, W. Figueroa, S. Torres, R. Pérez	2012	12-25,	L15*

* These textbooks are school-level chemistry books

Results and Discussion

To systematically analyze the presentation of the first law of thermodynamics, a tool was created to aggregate the relevant information and classify it according to the ontologically and epistemologically defined categories presented at the beginning of the article. This aggregation was performed by identifying the relevant concepts and assigning a category based on the results. The results of the categories are shown in Table 4, and the tool is shown in Fig. 1.

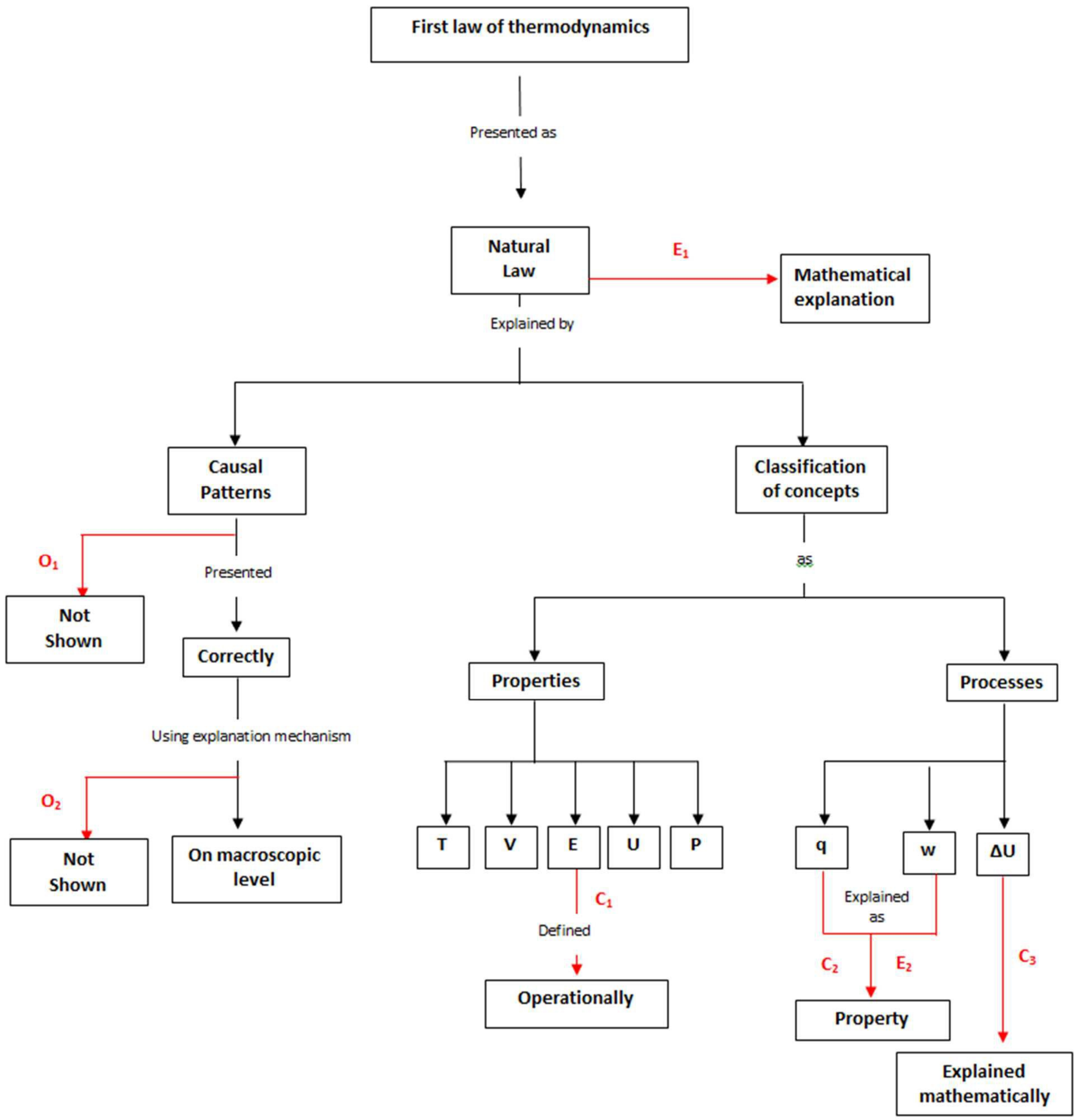

Fig. 1 Errors and omissions in the presentation of the first law of thermodynamics

Table 4 Types of ontological and epistemological errors

Classification	Errors
E_1	This error is epistemological. In the mathematical presentation of the law in association with different material systems, the variables of cause and effect are confused.
E_2	This error is ontological and arises from identifying concepts that refer to processes (i.e., q or w) as being properties (i.e., T, U).
	Contradictions
C_1	This contradiction refers to defining internal energy as a system property, whereas the concept of energy is operationally “the capacity to do work”.
C_2	This contradiction refers to defining the concepts of heat and work as processes, though when used within the text, they are explicitly identified as forms of energy.
C_3	This contradiction occurs when the state of a system is claimed as depending only on the thermodynamic properties it possesses, whereas when the process of the variation of internal energy is presented, the processes of heat and work are mentioned, thus neglecting to discuss the properties that define these states, namely P, V or T.
	Omissions
O_1	This omission occurs when the law and the underlying processes are disconnected from causal patterns.
O_2	This omission occurs when the law is presented, but not in association with an explanation mechanism that links the cause and the effect variables.

Tool Validation

A main obstacle to detecting ontological or epistemological errors, omissions or contradictions in textbooks is guaranteeing the objectivity and reproducibility of the classification. To verify both types of typological testing, a double codification of the same textbook was performed by two independent observers. A correlation between both classifications was calculated, following Eltinge and Roberts (Eltinge & Roberts, 1993) and based on the statistical tool developed by Kappa de Fleiss, Cohen, and Everitt (Fleiss, Cohen, & Everitt, 1969) which has been widely used in several text analyses (Lemoni, Lefkaditou, Stamou, Schizas, & Stamou, 2013; Lemoni, Stamou, & Stamou, 2011).

The Kappa coefficient is a measure of agreement between two observers. It was calculated within a range of 0 to 1, where 0 indicates no agreement, and 1 indicates full agreement.

The Kappa statistic is calculated by constructing a contingency table based on the classifications of each observer. Equation 17 specifies how to calculate the Kappa statistic determination.

$$K = \frac{P_0 - P_c}{1 - P_c} \quad (17)$$

where P_0 is the sum of the diagonal elements of the contingency table divided by the total sample, and P_c is the sum of the products of the sums of the rows and columns divided by the square of the total sample.

Kappa coefficient obtained by two independent observers was 0.89, which is close to 1. Thus, we have a high degree of confidence in our results.

Textbook analysis of the presentation of the First Law of Thermodynamics in perfect gas systems

The possibilities of conducting an ontological and epistemological analysis of scientific concepts are numerous. Both authors and the aforementioned investigations demonstrate some of the possibilities, for example, analyzing the evolution of the textbooks of different editions (Quiroz & Merino, 2015) and studying the presentation of the same concept in different scientific disciplines (Spinelli, Morales, Merino & Quiroz, 2016).

The analysis of the information in the selected textbooks is summarized in two tables, with different categories, thus exemplifying the first approach to the proposed study. Table 5 contains two categories of analysis (CAs). The first category indicates whether the text correctly defines the concepts energy (E), internal energy (U), heat (q) and work (w) in accordance with the ontological categories previously defined (A). The second category identifies the contradictions in the textbooks (B) regarding the processes of variation in internal energy (ΔU), heat and work. Analogously, Table 6 shows the analysis of the first law of thermodynamics in the following three systems: adiabatic with mobile walls, diathermal with rigid walls, and closed with mobile and thermally conductive walls. The analysis examines how the variation in internal energy is presented and whether an explanation mechanism (M) connecting the cause (Ca) and effect (E_f) is presented for the variation.

Table 5 Categories of analysis (CA): Ontological definition and classification (A) and the presence of contradictions regarding the processes ΔU, q and w (B) in the presentation of the first law of thermodynamics in school and university chemistry textbooks

CA		**L1**	**L2**	**L3**	**L4**	**L5**	**L6**	**L7**	**L8**	**L9**	**L10**	**L11**	**L12**	**L13**	**L14**	**L15**
A	E	C_1	C_1	P	P	C_1	C_1	C_1	C_1	C_1	C_1	C_1	C_1	P	C_1	C_1
	U	P	P	P	P	P	P	P	P	P	P	P	P	P	P	P
	q	E_2	P	P	E_2	P	E_2	E_2	E_2	P	P	E_2	P	E_2	P	P
	w	E_2	E_2	P	E_2	E_2	E_2	E_2	E_2	P	P	P	P	E_2	P	P
B	ΔU	P	P	C_3	C_3	P	C_3	C_3	C_3	C_3	C_3	P	C_3	C_3	C_3	P
	q	P	C_2	C_2	P	C_2	P	P	C_2	C_2	C_2	C_2	C_2	P	C_2	C_2
	w	P	P	P	P	P	P	P	C_2	C_2	P	C_2	P	P	C_2	C_2

O_1: No causal pattern is provided; P: Presented in the correct form; C_1: concept of energy is understood operationally; E_2: Error in ontological classification. C_2: Contradiction of processes as forms of energy; C_3: Mathematical explanation without reference to causal patterns

Table 5 shows that the most frequent results are “C_1” and “E_2”, pertaining to the ontological classification of the concepts E, U, q and w (A). For example, 11 of the 15 university textbooks define the concept of energy merely operationally, without linking it ontologically to a property. This presentation contrasts with that of the concept of internal energy, whose ontological connection to a property is present in all the textbooks. Regarding the concepts q and w, w is erroneously defined as a property in 8 of the 15 textbooks, and the same error (E_2) occurs with q in 7 of the 15 textbooks.

As described above, energy is a property possessed by all things, i.e., a universal property that also allows the mutability of all things, i.e., change. Because material properties do not exist in isolation from things or material objects, reference will always be made to the energy possessed by a certain thing. In thermodynamics, this energy is internal energy (U) (the energy of a thermodynamic system). Therefore, defining energy as the “capacity to do work” limits comprehension of the concept as merely the consequence of a body possessing energy, thus severing the concept from the definition and ontological classification that years of research have established.

Some textbooks classify the concepts of heat and work as “forms of energy” (E_2), evidenced by sentences such as “… *The energy is transferred in the form of heat or work* …” (Atkins & Jones, 2006).

This classification construes these concepts as properties. This construal is not arbitrary because if we understand energy as a property, then its manifestations acquire an identical ontological classification. However, our classification indicates that “q” and “w” are processes of energy transfer.

If we use the definition of heat and work as forms of energy and therefore, properties, we can state that a body “possesses heat or work” or that it is able to transfer heat and/or work. However, this statement generates a misunderstanding of the nature of these concepts due to an incorrect ontological classification and the incorrect use of the concept.

Similarly, regarding heat, phrases such as the following classify heat ontologically as a "thing" in claiming that it can flow or pass between systems or between the system and its surroundings: “*[…]* During the reaction, heat flows out of the system *($q < 0$),* and internal bath temperature increases to T_f *[…]* (Engel, Reid, & Hehre, 2006); and *[…]* When two systems are at different temperatures, heat can pass one to another directly *[…]”* (Laidler & Meiser, 1997).

Assigning the characteristic of flowability to heat echoes the assertion of caloric theory, which regards heat as a material substance and claims that its transfer causes temperature variations in the system. This theorization is also consistent with the following statement:

> Early chemists described heat according to the caloric theory, in which an object’s temperature was proportional to the quantity of caloric contained in the object. This early view, which attributed to the heat a substance ontology, was seen as a process of molecular excitation. (Slotta, Chi & Joram, 1995)

With regard to the presence of a pattern of causality for the processes ΔU, q and w, it can be observed that these processes are mostly presented correctly in the textbooks. That is, the textbooks explicitly state that U will vary depending on the variation of properties that define the state of the system (T, P, V). They also specify that q will accompany a state of thermal disequilibrium and that “w” will arise only when the pressures between the system and the environment differ. However, analyzing the results presented in Table 5 (B), it can be stated that many of the textbooks contain contradictions, mainly regarding what the processes “ΔU”, “q” and “w” refer to.

With regard to the first of these three processes, the most frequent contradictions relate to internal energy. Ten textbooks present a type-3 contradiction (C_3) in which the internal energy of a system is correctly defined as a property that depends on the current system state, which is determined by the properties T, P V and n. Subsequently, however, the textbooks explain that the variation in state results from heat being absorbed or released by the system or the work performed by or upon the system, disconnected from the properties that cause the variation itself. For example, consider the following statements: “*The first law can be expressed by saying that the change in the internal energy of a system, ΔU, is the sum of the heat q that enters the system and the work w that is done upon it: $\Delta U = q + w$*” (Laidler & Meiser, 1997); and “*if work is done on a system or if heat is given to it, its energy will increase*” (Masterton, Hurley, Llopis, & Cuenya, 2004). These statements, the first law is connected only with the processes causing variation in internal energy, while remaining disconnected from the causes of the variation (q and w) that generate E_1. The concept of heat is also classified as other than a process in claiming “heat that is given” and alluding to heat as transferrable between systems or between the system and the environment. Thus, heat is classified as a property.

We can therefore ask the following question: How are the variables (T, P, V and n) connected to the variation in internal energy in the presentation of the first law? Does the variation in the internal energy depend directly on q and w, or do these processes constitute part of the mechanism that generated this variation in the system? These questions are being answered throughout this article; however, it is important to reflect on them and ensure that this reflection allows us to identify the optimal presentation of the first law of thermodynamics, including the causal patterns that cause the change in the state of a particular system.

Regarding “q” and “w”, the contradictions found in the analysis are mostly of type C_2, as the concepts are described as “forms of energy”. Why are these descriptions contradictory? They are consistent with the correct ontological classification, but when a concept is used in an explanation, either in an image or within the text itself, it refers to an incorrect ontological classification. For example, the most common case is when heat and work are presented as processes of energy transfer and then used in statements such as:

- *“The work transferred to or from the system” (Kotz, Treichel, & Weaver, 2005)*
- *“The other component of the internal energy is the Heat q” (Chang & Herranz, 2007)*
- *“Therefore, heat and work with properties of direction or path and not states” (Laidler & Meiser, 1997)*
- *“If the gas absorbs heat from the environment” (Chang, 2008)*

All of these examples insinuate that “q” and “w” are properties.

In 10 of the 15 textbooks, this contradiction occurs for the concept of q and in 5 textbooks for the concept of w. As previously noted, in science, and in this case, chemistry, concessions are made. That is, certain statements help simplify explanations and allow people who do not possess in-depth knowledge of a subject area to nonetheless understand it. Notwithstanding the usefulness of concessions for learning, we believe it is important to obtain a consensus regarding a concept and its explanation. With this consensus, we can avoid altering the correct definition and/or the ontological classification, thus ensuring the meaning of the concept remains unchanged. Otherwise, conceptual errors appear because of didactic concessions. For example, several textbooks state that q is a process, but use the concept to discuss the flow of heat, thereby leaving the concept amenable to interpretation and distortion, as heat can thus be understood as a “thing” transferrable from one system to another system or a property of thermodynamic systems that describes their state.

Table 6 Analysis of the patterns of causality and the mechanisms in the presentation of the first law of thermodynamics in different systems in school and university science textbooks (Ca: Cause / M: Mechanism / Ef: Effect)

	Adiabatic system			Diathermal system			Closed system		
	Ca	M	Ef	Ca	M	Ef	Ca	M	Ef
L1	P	P	P	P	P	P	P	P	P
L2	P	P	P	P	O_2	P	E_1	P	P
L3	P	O_2	P	E_1	O_2	P	P	P	P
L4	P	P	P	E_1	O_2	P	E_1	P	P
L5	P	P	P	P	P	P	E_1	O_2	P
L6	O_1	O_2	O_1	E_1	O_2	P	E_1	O_2	P
L7	O_1	O_2	O_1	O_1	O_2	O_1	E_1	O_2	P
L8	O_1	O_2	O_1	E_1	O_2	P	E_1	O_2	P
L9	O_1	O_2	O_1	E_1	O_2	P	E_1	O_2	P
L10	O_1	O_2	O_1	E_1	O_2	P	E_1	O_2	P
L11	P	P	P	P	P	P	P	P	P
L12	O_1	O_2	O_1	E_1	O_2	P	E_1	O_2	P
L13	O_1	O_2	O_1	O_1	O_2	O_1	E_1	O_1	P
L14	O_1	O_2	O_1	O_1	O_2	O_1	E_1	O_1	P
L15	O_1	O_2	O_1	O_1	O_2	O_1	P	P	P

E_1: Error in epistemological classification; P: Presented correctly; O_1: No causal patterns provided; O_2: No explanation mechanism provided

Table 6 indicates that the presentation of the first law of thermodynamics as applied to the three types of systems exhibits a common pattern across the textbooks. Namely, no significant differences were observed in how the information is presented. Although the degree of complexity varies depending on the educational level of the students and their knowledge of the area, the errors, omissions and contradictions discovered in the analysis are similar across textbooks used in university-level physical chemistry and general chemistry courses and even in school-level textbooks.

The results show a high frequency of the presentation of the law in these three systems without an explanation mechanism connecting the variables of cause and effect (O_2). That is, the effect (ΔU) is associated with a cause, but this effect does not correspond to the properties determining the state of the system (T, V, P). Moreover, the cause described in the text is the sum of heat and work, so the first law is presented in a merely mathematical way (E_1). Hence, it impossible to clearly visualize how the internal energy of a system changes and identify which properties cause the change. Therefore, the pattern of causality is unfounded, and it is unclear which variables is the cause and which variable is the effect.

Additionally, several textbooks do not refer to the application of the first law for systems with mobile adiabatic walls or for systems with rigid diathermal walls (designated O_1 because the causal patterns of these processes are not given). This lack of reference prompts the following question: Is it important to explain this law in relation to other types of systems? We would answer that it is necessary to extend the presentation and explanation of the first law to other systems because although the law is the same, its explanation mechanism differs depending on the characteristics of a particular system (see Table 2). Therefore, if the law and thus, the mechanism linking the cause and effect variables of the system are not noted for different types of systems, it is impossible to understand the nature of the change in internal energy, i.e., to understand the actual cause of the change and the process generating the effect. Although internal energy is a function of the state and depends on not the path pursued, but the initial and final states of the system, when presenting the law and discerning its epistemological referent, the presentation of the law (a scientific hypothesis that defines a pattern of causality and links the latter to a mechanism of explanation) must clearly explain how the law manifests in material reality by specifying the cause and the associated mechanism and effect. Without these specifications, the presentation of the law remains merely a scientific hypothesis.

Presentation of the First Law of thermodynamics' proposal

Now we will make a proposal for the presentation of the first law using the appropriate ontological concepts based on our philosophical framework.

The internal energy is that estate of a thermodynamic system that represents other forms of energy (kinetic and potential energy) and that merely depends on the variables/properties that define the state of the system (P, V and T). Thermodynamics is in charge of studying the changes of internal energy that a system undergoes, directly related with noticeable macroscopic evidence related to the properties mentioned above.

The first law of thermodynamics states that the internal energy of a system can vary through the implementation of two processes, work and heat, as they are expressed in the following equation:

$$\Delta U = q + w$$

(Considering a system with diathermic mobile walls)

Both processes are triggered by the variation of some of the properties that define the state of the system (T, P and V). In relation to the heat process, it is correct to claim that it will take place, if and only if, an initial state of thermal imbalance exists between two systems, or between the system and its surrounding. In the case of the external temperature being higher than the one from the system (T surrounding > T system) the energy transference will occur from the zone of higher temperature to the one with a lower temperature, so the system´s temperature will increase with the purpose to reach a state of thermal balance. Happening this, the internal energy of the system will increase. In relation to the working process, it is correct to affirm that it will take place, if and only if, there is a difference in pressure between the system and its surrounding. In the case in which the external pressure being higher in comparison to the one from the system (P surrounding > P system) an energy transference will occur to the system with the purpose of reaching a balance between both pressures, so the decrease in the volume of the system will cause an increase in the pressure and gas temperature. Happening this, the energy from the system will increase.

Considering this, it is possible to establish an expression that represents a sign that acquires the energy transferred through those processes and the relation that they have with the variation of the internal energy of a thermodynamic system.

The internal energy of a system will increase when:

- The system increases its temperature by the transference of energy through heat process. The energy transferred acquires a positive value and can be represented as : $q > 0$
- The system increases its temperature as a product of the energy transference through the work process, producing a decrease in the volume and, pressure rise of the gas. The energy transferred acquires a positive value and can be represented as: $w>0$

On the other hand, the internal energy of a system will decrease, when:

- The system will decrease its temperature as a product of the transference of energy to its surrounding through heat process. The energy transferred acquires a negative value and can be represented as: $q < 0$
- The system will decrease its temperature as a product of the transference of energy to its surrounding through work process, producing an increase in the volume and therefore a decrease in pressure of the system. The transferred energy acquires a negative value and can be represented as: $w < 0$

By making reference to a closed system with diathermic and mobile walls, both processes of transference of energy can take place, so the variation of the internal energy of the system will depend on the sign that acquires the transferred energy according to what has been discussed beforehand.

Conclusion

The study of science education across all scientific disciplines can develop tools based on ontology and epistemology to analyze the presentation of scientific concepts in textbooks. The epistemology and ontology of Mario Bunge's philosophical system are sufficiently general and orienting for this purpose.

Our results indicate that the thermodynamic concepts heat “q” and work “w” must be presented as processes, while considering their underlying dynamic nature. The concepts of energy, internal energy “U”, volume “V”, pressure “P” and temperature “T” must be presented explicitly as properties.

To accurately present the first law of thermodynamics, we propose specifying in the text that patterns of causality and the mechanisms of this law depend considerably on the systems to which this law applies. The first law must be presented with the mechanisms and patterns of causality in the context of at least one particular system.

We believe that the ontological categorization of concepts provides one way to make learning concepts more significant because it helps establish a direct relationship between the concept and its material basis.

Ontological analysis aims to examine concepts and propositions and is a process of combining ideas within certain propositions and using ontological categories (thing, state, event, property and process) to imbue the provided information with meaning. Our ontological analysis of the concepts of heat and work indicate that these concepts are widely classified as properties either in their definition or in their application in explaining a thermodynamic unit. The concepts are explained as forms of energy and thus are classified as properties rather than processes. Consequently, the nature of the concept is incorrectly presented, as its ontological classification is erroneous for one of two reasons. First, the concept may be defined correctly and assigned the correct ontological classification. Subsequently, however, its application construes its nature as belonging to a different ontological category. Second, it is incorrectly defined, and this incorrect classification is then used to explain a particular system.

Natural laws corresponding to an epistemological category indicate patterns of causality linked through a mechanism that generates a determined effect. However, the textbooks analyzed did not completely provide this indication as follows: the first law of thermodynamics was assigned attributes that are merely mathematical or operational, thus hindering reflection on the subject matter by providing only a formula in which to substitute values and calculate the outcome of variables presented without their ontological references, i.e., without the properties and processes that arise from them. These textbooks present the first law of thermodynamics in terms of the processes that cause variations in the internal energy of the system. However, no direct link is established between the properties that describe the system state and that are the original variables, which precede changes in the state and therefore, variations in internal energy.

It was also common for the textbooks to define energy from an operational perspective, thus failing to clearly represent its ontological classification. Although energy is connected with material objects as described above, the concept of energy is associated with not a universal property, but the mutability that it supplies material systems, i.e., the changes observed in these systems following the variation of one or more properties of that system. This mutability is indicated in the definition of energy as the capacity to do work.

Due to these difficulties that have been previously recognized, is that the necessity to modify the way in which the first law of thermodynamics is presented appears, whether in scientific texts or at the moment to teach it to high-school or higher education students. To do so, we consider relevant that at the moment to present the first law of thermodynamics, the following aspects be explicitly mentioned:

- To establish a relation between the type of system that is experiencing the change, the mechanism associated to the process that is taking place, and the causative patterns implied that give origin to it.
- To connect the process of energy transference to the properties of the system (P,V and T)
- To present heat and work as transference of energy processes, which causative patterns are the properties of the system.

We believe that it is also important to be able to identify the relationship between the three levels of representation of a subject. Only by doing so is it possible to generate integrated knowledge, namely by establishing connections between perceivable facts (phenomena) and non-perceivable facts, which comprise most facts relating to reality. Although such facts are not perceived, they can be understood by encouraging actions such as conjecture, model creation, and the construction of connections between symbols and between micro- and macroscopic levels.

Finally, if we aim for our students to learn the sciences, then we must help them acquire more adequate, clearer and more precise language to ensure they are able to communicate ideas coherently and articulately. They also require the correct tools to comprehend reality from a critical and analytical viewpoint, such that questioning plays a fundamental role in their lives, consistent with the principle that all knowledge can be questioned and perfected. From our perspective, this pedagogical path is optimal.

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