Model-based simulation design for the students’ conceptual understanding of introductory thermodynamics

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Abstract. The present study refers to the design principles of an educational simulation for the introductory physics level and their application on a recently developed simulation (IGasES: Ideal Gas Educational Simulation) for classical thermodynamics and specifically for the First Law of Thermodynamics. These principles rely on three modeling aspects (physics teaching, learning and educational simulations) and their convergence for the construction of a model-based educational simulation. The study also reviews some of the issues that commonly used simulations encounter for the teaching and learning of this topic. For addressing these issues, we choose the energy chain model as a proper representation of a thermodynamic system for mediating between the phenomenology and the mathematical expression of the First Law. In conclusion, this study draws attention on the characteristics of the educational software rather than the way they are put in use and also to the modeling procedures than can facilitate the student's conceptual understanding.

1. Introduction

Computer simulations have been making their way into every educational level for the last four decades and by now they are widely integrated in numerous formal science instruction settings and particularly in physics teaching and learning [1]. A straightforward definition of an instructional simulation is ‘an interactive representation of the system to be studied, based on a model of the system’ [2]. This type of educational software has drawn many researchers’ attention. As the relevant research grows, some equivocal results emerge regarding the simulations’ cognitive impact on the learners’ conceptual understanding in physics. Several researchers have reported successful outcomes in various physics topics and educational levels [3,4]. Conversely, other works mention indiscernible variances between simulation instruction and more conventional teaching methods to a greater or lesser degree [5,6]. Simulations are usually by nature plug-and-play software, but using them efficiently in instruction requires more than that. The studies that engage in the use of simulations in educational settings do not usually mention the background of the software they deploy. It is important to know, for example, whether the specific simulation was meant to be educational and, in that case, which deep and superficial educational features it integrates. The specifics of the software’s design, primarily in regard to the underlying conceptual models it promotes and the way it attempts to convey them, remain implicit or unexplored.

One reason that partially justifies this lack of information is that the instructor and the (educational) technologist do not usually interact sufficiently in order to create a solid product for educational purposes. It is rather reasonable that science education researchers or instructors, who want to integrate simulations in their teaching procedures, are not required to be software programmers as
well; therefore, they can neither create a complex simulation on their own or penetrate to the computational code of the existing ones. As a consequence, they more often than not have to settle for a series of elements that a plug-and-play simulation has to offer and make the best of it by designing an appropriate method of instruction. As Ren [7] notes, not only the application of educational technologies, but their design and development as well should be at the place where learning theories meet technological advancements. In other words, this should be a “transdisciplinary process” [7] or “multidisciplinary approach” [8] between different professionals or the instructors themselves could be the developers of their own “tailor-made” simulations.

2. Research objectives
The aim of this study is to present the grounded theory on educational models and to expand this theory in order to link it with the field of educational simulations. On this account, we present the design principles that can facilitate the development of an effective simulation for physics teaching and learning. As an application of these principles, we introduce the educational simulation IGasES (Ideal Gas Educational Simulation) for the topic of introductory thermodynamics and more specifically for the instruction of the First Law of Thermodynamics (FLT).

3. The three aspects of modeling for the design of the simulation
In the definition of educational simulations (see Section 1), the concept of “model” is central. According to Tiberghien [9], “models consists of qualitative and quantitative functional relations (implying mathematical formalisms) between physical quantities in order to represent the selected aspects of a set of material situations” (p. 74). Students need to engage in modeling processes so as to effectively create relations between naïve phenomenology and mathematical equations [10]. The model attempts to bridge the gap between the levels of objects and events that the learner notices and the scientific concepts that they pursue to comprehend and handle. In other words, models stand in between the experimental field of an applied science, like physics, and the respective theory of that science [11]. For the interpretation of the phenomena that are of interest to a particular teaching intervention, we do not expound the whole of a theory, but instead use models corresponding to the experimental cases in hand.

3.1. Models in physics teaching
Qualitative “pragmatic” models of the respective objects-events should take precedence in a physics education environment [12,13], as such representations of physical phenomena can sufficiently communicate fundamental physics concepts, i.e. the conservation of energy [14]. A qualitative construction can provide very translucent forms of knowledge by exposing specific relations and therefore it can facilitate the learners’ internal inquiring regarding the phenomena [11]. Nonetheless, quantitative modeling is also an essential aspect of physics education [15]. It is vastly connected to mathematical formalism [13], which is used to describe real phenomena and abstract ideas and suggests a distinct type of “pragmatic” modeling [16]. In physics teaching this practice is commonly defined as ‘mathematization’ [17]. Although mathematical formalism undoubtedly contributes to advanced physics modeling, it troubles physics learners at a great extend; these difficulties appear mainly during problem solving, within which the choice, modification and application of mathematized expressions is usually a challenge [18]. However, even the correct use of the formulas does not suggest successful quantitative modeling, because whenever the learner fails to assemble the multiple meanings that lie behind the utilized mathematic expressions, the latters end up deprived of content and functionality [19].

3.2. Models in physics learning
The second aspect of modeling concerns the pedagogical features of the model as an explanatory mechanism, which Seel [16] characterizes as the “constructivist” approach (pp. 466-467), and addresses the mental role of a model. In short, “mental models are internal representations people
commonly use to comprehend, reason about, and predict events in the world” [20]. In this case, the learner constructs a “model for” something [21]. From a perspective closer to physics learning, the learner engages in interpreting or predicting the situation at hand [22,23] by constructing a personalized model of the included objects-events, in view of their pre-existing knowledge and available reasoning skills [9,16].

A mental model that is formulated after the interaction between the learner and a material situation is usually functional, but, more often than not, is scientifically imprecise [24]. This inference emerges from the comparison between the mental model and the conceptual model (or “target” model), which is scientifically accepted [23]. The conceptual models provide an accurate, consistent and complete representation [22] of the objects-events level for each physics domain. Mental models are unstable constructions in the sense that they are subject to change, if they failed to correspond with the comparative conceptual model. However, the learner’s mental model can be very persistent and therefore certain measures should be taken for successful physics learning.

3.3. Models in physics educational simulations

Simulations by nature integrate the “pragmatic” aspect of a model as a key epistemological choice, namely they provide the user with an idealized part of the reality to handle. A “simulation model” carries its unique characteristics; it is a structure meant to generate a physical situation’s behaviour, which should reproduce some aspects of the its evolution in time and space, and create a variety of behaviours based on the user’s decisions [20,23]. Therefore it seems that the real challenge for an educational simulation is to integrate pedagogical features too, thus facilitating the formation of a “constructivist” model for the learner by initiating from the “pragmatic” one. This can be further enhanced by simulations that offer simultaneous handling of multiple representations on the same screen [25].

During the teaching process, providing students with model-relevant information is substantial for the construction of their own mental models [26] that pertain to both the qualitative and quantitative dimensions and lead them gradually to the targeted conceptual model. “Learning by modeling” assists students in building their individual mental models; this process results to a profound conceptual level of comprehending the content, the practices and the problem solving requirements [16]. In order for an educational simulation to enable the learner’s modeling activities, it should autonomously promote “learning by modeling” as a stand-alone educational tool, although it is highly advised to be part of a coherent teaching sequence in order to maximize its impact [6].

4. Introductory classical thermodynamics instruction with simulation scaffolding

4.1. Thermodynamics in education and educational simulations

It has been a matter of concern since the ‘70s whether thermodynamics, at introductory level, should be taught in schools and in which manner [27,28]. Four decades later the answer to the first question is definitely positive; however, the way in which thermodynamics should be introduced in education is still under investigation [29]. The relevant research reveals that the students face many difficulties in comprehending basic concepts of thermodynamics, such as heat and temperature [30], they bear alternative frameworks [31] that have certain homogeneities [32] and they struggle with the required reasoning skills [33].

Educational technologies and simulations in particular took up the challenge for accurate conceptual knowledge on introductory thermodynamics and more specifically on the FLT and the ideal gas law. There are virtual labs (i.e. PhET, Thermolab) and representations of physical systems with the option for modification of variables and generation of graphs (i.e. Physlets). Although these simulations seem to have positive contribution to the teaching and learning of physics [34], they render a fundamental epistemological issue. This refers to the blending of classical and statistical thermodynamics, mainly through the statistical interpretation of the macroscopic laws of the theory. It suggests a juxtaposition of different conceptual models [12] that calls in question the appropriateness of the selected reality
reduction, which is challenged to serve two separate frameworks. This mixing possibly enhances the students’ alternative frameworks and additionally it can give distorted impressions regarding the nature of science [35].

Concerning the pedagogical features of the above-mentioned simulations, they conceal the underlying conceptual model thus allowing the user to speculate and usually to indulge in misconceptions. Another characteristic is the depreciation of qualitative “pragmatic” modeling and the focus on quantitative “pragmatic” modeling without gradually passing from one to another through semi-quantitative “constructivist” models. Virtual labs embed some philosophical issues, as they can lead the learner towards a positivistic approach, namely to extract conclusions deriving merely from data and observations, which is scientifically inaccurate for thermodynamics. Additionally, the carefully pre-arranged digital lab equipment (i.e. a Bunsen burner, various substances in vessels, a thermometer) can work behaviourally for the novice learner [36]. Finally, the learners’ linear causal reasoning is not regularly taken into account in the simulation’s functions; namely, the software is neither attentive to the way the user reasons nor it efficiently challenges this type of reasoning whenever it is proven to be ineffective [37].

4.2. Proposal for the design principles of an educational simulation in thermodynamics

In order to tackle the issues mentioned above, we take a series of measures for the design of a simulation that addresses the teaching and learning of introductory classical thermodynamics, in an attempt to put into effect the three-dimensional principles of modeling. To begin with, we follow the approach of “system dynamics”, which refers to a field that shows potential in regard to model-based learning [16]. Physics commonly deals with physical or technological systems that change dynamically in time, while a phenomenon evolves within the system. A system is defined as “a quantity of matter or a region in space chosen for study” [38]. In physics learning, one strives to interpret and/or manipulate the changes in the system; this endeavour lies in the core of the conceptual understanding of physics.

The “pragmatic” model of a classical thermodynamic system represents a macroscopic version of the system, including only those elements of the objects -events that are relevant with the targeted conceptual knowledge. Technical thermodynamics offers a variety of such representations, although it originally addresses to engineers. However, the representation of the “constructivist” model is not widely used. For this matter, we suggest the energy chain model (ECM), which is a pedagogical approach for dealing with the energy concept within a thermodynamic system and can be the “constructivist” model lying in the core of a simulation. the energy chains offer a foundation for the understanding of the conceptual model through their functions: storage, transfer and transformation of energy are explicitly represented, while the conservation of energy is also embedded, but in a more implicit manner. The energy chains connect the conceptual model with the material situation, since the evolution of the phenomenon (that takes place within the system) at the “pragmatic” qualitative representation corresponds progressively to the dynamic changes in the “constructivist” representation of the ECM [10]. The EMC suggests a semi-quantitative “constructivist” model for the distribution of energy within a system; it restores a dialectic relationship between qualitative and quantitative “pragmatic” modeling [12], which can facilitate bridging the material situation with meaningful mathematical expressions [13]. On the one hand, the EMC can provide essential qualitative information on the energy quantities playing a role in the phenomenon, as well as on the changes they undergo. On the other hand, it supports the formation of preliminary hypotheses regarding the quantitative fluctuation of these quantities during the evolution of the phenomenon and the mathematical relations that link them.

5. Application of the design principles in IGasES

5.1. Description of IGasES
IGasES is proposed for the teaching and learning of the macroscopic elements of ideal gases. More specifically, it presents and operates the main four thermodynamic processes of the ideal gases (isothermal, isochoric, isobaric and adiabatic) and links them to the FLT. Considering the prime “pragmatic” aspect of the modeling, IGasES integrates selected features of the level of objects-events related to the macroscopic properties of the ideal gases. The choice of ideal gases instead of pragmatic ones corresponds to the limitation of the excessive theory, which would be unnecessary for the introductory level. The gases are dealt with as restrained in a vessel, allowed to exchange energy with a certain thermal and/or mechanical environment; this consists a deliberate reduction of the respective phenomenological field.

In regard to the embedded objects, the representation isolates a tube with a movable seal, which is filled with an ideal gas. The tube works as a volumetric vessel and is constantly connected to a manometer and a thermometer; however, none of these instruments records actual numeric data. Depending on the specific thermodynamic process, more objects can appear (Bunsen burner, extra weight on the seal, tank with water). As for the simulated events, the user can choose the preferred thermodynamic process and then specify among expansion/compression and heating/cooling, in order the respective objects to appear. While the phenomena are evolving, the depicted “measurement” instruments for volume, pressure and temperature go through simple qualitative changes; these are considered sufficient for the introduction of the ideal gas processes. Figure 1 presents the initial state of an isochoric heating.

![Figure 1. Snapshot of IGasES: initial state of isochoric heating.](image)

In addition, IGasES embeds the FLT in its mathematized form \( Q=\Delta U+\Delta W \), which suggests another side of the “pragmatic” modeling for thermodynamic processes. This formula attempts to bring into play the quantitative perspective of the phenomena. It corresponds to the selected process and therefore it “changes” respectively. Additionally, the user can insert specific numbers for each variable and execute calculations. This course of actions can work the other way around; this means that the form of the mathematic formula or the inserted numbers can define the type of the thermodynamic process that will be simulated.

However, meaningfully bridging of these two aspects of “pragmatic” modeling is a painstaking procedure that requires much more than the targeted representation of the involved elements. It calls for the adaptation of intermediate “constructivist” models, such as the ECM. This suggests an exposition of the underlying conceptual model, which should be translucent regarding its presentation, but opaque in terms of interactivity; this choice can adjust the learner’s interpretation of the system,
without requiring any interference that could distort the underlying conceptual model. This addresses the need for introducing to the students specific meta-concepts regarding the notion of the model [25]. Figure 2 presents a screenshot of both the mathematical expressions of the FLT and the ECM without any processes being selected.

![Figure 2. Snapshot of IGasES: showing all screens without the selection of a process.](image)

5.2. Use of IGasES

The role of IGasES is to enhance the mental modeling procedure and help the learner to create a mental simulation of the thermodynamic processes with the use of the ECM, in order to predict or explain the behaviour of energy, understand the underlying conceptual model and advance from the level of objects-events to the FLT formula in a meaningful way.

The various thermodynamic processes are represented simultaneously at the “pragmatic” level of digital objects-events and the “constructivist” level of the energy chain; the purpose is for the learner to realize the spatial associations and the absence of time delays between the phenomena and the energy changes. The energy is being transferred between the boxes through the arrows in a semi-quantitative way: it appears to reduce or increase in each box while being transferred through the arrows and the “sum” of the energy in the boxes and the arrows is constant at every step, but there is no numeric indication for these amounts of energy. Thus, the EMC promotes a semi-quantitative notion of the conservation of energy, which is a key aspect of the FLT. At the end of the dynamic development of both the representations, the energy chain is supplemented by the quantity symbols ($Q$, $\Delta U$ and $W$) appearing at their proper places as intermediate variables, so the learner can make a connection between the ECM and the mathematized expression of the FLT.

In figures 3 and 4 one can see the initial and the final state of an adiabatic expansion respectively. The “pragmatic” qualitative model represents the vessel full of gas, which is gradually expanding due to the internal energy that is saved in the gas. At the same time, the “constructivist” model of the energy chain is also operational. At the beginning of the process, the system’s energy appears to initiate from the gas, thus the respective box is filled, while the others are empty. By the end of the process, an amount of energy has been transferred in the form of work to the mechanical environment (the uplifted weight on the seal); the sum of energy in these boxes corresponds to the initial amount of energy. Regarding the symbols of the energy quantities and the formula of the FLT, when the phenomenon begins there is no suggestion for either of these. Only after the phenomenon is fully developed and the system reaches an equilibrium state, the symbols appear on the energy chain, the correct form of the FLT is selected and IGasES is ready for calculations.
6. Discussion
In the present work we have presented the main axes for the design of a modeling simulation for physics teaching and learning. In particular, we developed a simulation (IGasES) for the instruction of introductory classical thermodynamics with focus on the FLT for the thermodynamic processes of an ideal gas. The emphasis has been given to the three modeling types that should be embedded in such an educational tool, in order to assist the learners’ conceptual understanding, namely to help them to accurately interpret the phenomena and associate them with the proper mathematical expressions in a meaningful way.

In IGasES the targeted conceptual knowledge, which is the FLT, has been facilitated by the vast reduction of the “pragmatic” modeling; this refers to the qualitative representation of the object-events level as well as the quantitative representation of the mathematical expression. As result, IGasES is
not an opulent simulation in terms of appearances, since it focuses to the point; that is the students’ conceptual understanding of a fundamental physics concept for which they strive a lot [30,31,35]. Another essential aspect of IGasES for achieving this goal is the use of the intermediate “constructivist” ECM. The exposition of this model to the learners resulted to the development of a semi-transparent simulation, which is not common in simulation-using [39]. Although the ECM has been used before in physics teaching and learning [10], so far it has not been embedded in a simulation that allows dynamic development of the energy chain in correspondence to the depicted phenomenon. We believe that the proposed “constructivist” model, enhanced with the above-mentioned qualities, will facilitate the students’ mental modeling and help them create themselves a mental simulation for the thermodynamic processes.

Our next step is to bring IGasES into class as part of a suitable teaching and learning sequence in order to fully assess its potentiality for conceptual understanding and, also, to detect its limitations and adjustment needs. It is quite certain that the classroom environment will point out more latent uses for the software. We consider that IGasES in its current version is set as an instructional tool, namely for the presentation of the targeted conceptual model by the teacher to the students. Although this version carries some scaffolding characteristics, such as definitions of the thermodynamic processes and error messages, we would like to improve them in the future in order to make the software more suitable for individualized use.

7. References
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