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Importance of using Simulation in Chemistry: the Case of Batteries, Accumulators and Electrolysis

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Abstract*: In this work we focus on the study of the degree of effectiveness of simulation programs in teaching few skills of the lesson "Stacks and Energy Accumulation" in Chemical Sciences, "Daniell stack" experiment, for students in 3rd year of secondary qualified classes of the Regional Direction of Moulay Rchid-Sidi Othman. This work analyzes the importance of the use of simulation to develop some targeted skills in chemistry, through a survey, to answer a simple question: How effective is the simulation in the teaching of chemistry lessons?

***Keywords* : Education, chemistry, effectiveness, stack, electrolysis, Morocco**

I. INTRODUCTION

The technological revolution that was launched in the world at high speed has been the product of the progress of science in our contemporary world unparalleled progress, "The contemporary realities and the outlook for the future confirm that we are on the verge of a new era radically different from today's world. The enormous developments and changes in the depth, breadth and impact on various aspects of life and in different fields and locations: economic, social, political, scientific and educational". Sakrane, 1999, P.25.

The use of computers has become necessary in our lives, and what we are witnessing is a huge and fast development in computer technology that calls for its activation in the field of education in an innovative way, as it is no longer a field of knowledge except for the computer, has an important role in it, among the scientific technological revolution, "which influenced the teaching of computer simulation technology and patterns of use such as virtual reality and artificial intelligence and expert systems and the need to take advantage of these technologies in the development of modern education and the service of the teacher and learner, which is reflected in improving the efficiency of the educational process" Taoufik, 2003, P.246

Simulation refers to the imitation of real-world activities and processes in a safe environment, it aims to provide an experience as close to the 'real thing' as possible; however, a simulated activity has the advantage of allowing learners to 'reset' the scenario and try alternative strategies and approaches. This allows learners to develop experience of specific situations by applying their wider learning and knowledge [1].

No one can neglect the importance of experience or simulation in the teaching of chemical sciences. However, some people think that simulation in some cases can effectively represent physical or chemical phenomena, at the microscopic and even temporal scale.

Simulations are a term used for those programs or models that experts design to represent or replicate the real system, whether existing or intended to be created. It aims at knowing and familiarizing all the expected results with a set of other sciences, Mathematics, information science, physics and other information.

It is very important to say that it is easy to use simulation programs: to move an atom or a charge carrier, zoom in, repeat, speed up or slow down a chemical reaction in a simple single click.

In the case of the use of simulation programs in chemistry, it is particularly necessary to see, model or predict the microscopic changes.

Different uses of simulation:

- Computer simulation: which is done using certain software programs, and the JAVA software programs are the most popular software.
- Model Building: The model is a replica of the original form but is small in size.

What are the benefits of using it?

- Provide material cost for some expensive reactions.
- It is used to study complex matters, formulate them, and observe changes that may occur.

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- Lead students to study the system clearly, and show the results that will be obtained after with a single click.
- Used as a method in academic study of evaluation in some cases, in order to save time.
- They are also used to study the behavior of an object being produced under certain rare circumstances.
- They are also used to study and observe changes over the slow chemical transformations.
- It is also used to study future results that may arise from the use of a particular object.
- The simulation is also used to make students gain high efficiency during lessons.
- Its use is to give students greater and better experience without any harm.
- Therefore, the simulation is done as a test for a product, instrument or device, before actually testing it on the ground.

Before using any simulation or technology, there's some questions need to be asked, in order to properly frame the situation.

- Where in the course/module would this approach work best? What are the targeted skills?
- What situations would the student benefit from being able to explore in a controlled environment?
- What timescale should be used? Real-time? Faster? Slower?
- Are the students ready for this?

II. PROBLEM

Simulation has recently become a practical tool in the teaching of some subjects precisely scientific subjects, especially at the microscopic scale (rearrangement of atoms, model of the atom, displacement of charge carriers ...) or at the level of slow reactions, explosive or toxic, for the students of the 3rd year of secondary qualified classes, in the regional direction of Moulay Rchid-Sidi othman. This work aims to answer a simple question: What is the degree of efficiency of the simulation in the teaching of chemical sciences?

Several questions can be derived from the main question:

- What are the skills targeted by the use of simulation in this part of the course?
- What are the reasons for this use?
- What kind of simulation program? What kind of use of simulation?
- Can simulation replace experience and especially in this part of lesson?
- To what extent can we say that simulation has almost been the reality?
- Is there really a correlation between the scores obtained and the use of the simulation?

III. LITERATURE REVIEW

In philosophy of education, Olivier Reboul (1980) showed that simulation is not just a practice, it is also the founding principle of school organization: « The problems of school are analogous to those of life, but without their consequences; in real life, a badly written letter is not a cause of refusal to hire, a miscalculation does not ruin anyone, a clumsy manipulation is without real danger. The driving school is a school only because driving mistakes do not cause an accident » (P.10) [2].

Modeling and simulation represent a vast field for research related to scientific and technological education, explored for several decades now (Giordan & Martinand, 1987). The oldest works on science modeling have been listed by Drouin (1992) who proposed nearly 250 references based on epistemology, cognitive psychology or science didactics [3]. The simulation seems to be a response to the increasing demand for operationality, or even employability, of people leaving training. (Apprendre par la simulation, de l'analyse du travail aux apprentissages professionnels. Pierre Pastré, 2005).

Hebenstreit (1992) mentions that users may confuse a real phenomenon with its representation in simulation. To avoid such a risk, Richoux & al. (2002) insist that it is necessary to clearly separate reality and theories. In this sense, according to these authors, simulation can be presented as an interesting intermediate state to facilitate the transition between reality and theories [4].

Mark (1982) notes that simulations necessarily omit certain factors; we run the risk that students forget the existence of these additional factors. Thomas and Hooper (1991) add that in some situations, the contribution of the simulations is uncertain or even nil. Indeed, when the student can not find the solution, he can not know which aspects of his model of the system are inappropriate [4].

IV. METHOD

To answer the study questions, we used descriptive analytical and structural methods. The sample of the study was selected from students of the 3rd year of secondary qualified classes. Four divisions were selected: Life and Earth Sciences LES, Physical Sciences PS, technical sciences mechanical option TSM and technical sciences electric TSE option at "Jaafar el fassi" high School of the Regional Direction Moulay Rachid – Sidi Othman, the sample were 90 boys and 90 girls. The independent variable "effectiveness of simulation" was subjected to experimentation and its effect was measured on "development of targeted skills" variable. The study was implemented during the second semester of the 2017/2018 academic year.

To achieve the objectives of the study, a list of targeted competencies was prepared during the paragraphs included in the curriculum of the third year of secondary qualification education within "stacks and energy accumulation" lesson.

The sample is divided into 6 groups of 30; 3 groups were taught by the traditional method by drawing on the blackboard, and by speaking, the others were taught by the official simulation program made by the ministry of education "Edumedia" and other simulation from the internet, using computer and video-projector.

After a one-hour session, each group received a small test consisting of a few questions to test the achievement of the targeted goals.

The treatment of data was made by SPSS statistics 20.

V. THEORITICAL FRAMEWORK

The educational process has changed since the discovery and use of the computer. It becomes more dependent and related to the new information and communication technologies, specially computer and internet. Andrew Molnar 1997.

However, the reality of the Digital Divide - the gap between those who have access to and control of technology and those who do not - means that the introduction and integration of ICTs at different levels and in various types of education will be a most challenging undertaking. Failure to meet the challenge would mean a further widening of the knowledge gap and the deepening of existing economic and social inequalities [5].

Technology has impacted almost every aspect of life today, and education is no exception. Or is it? In some ways, education seems much the same as it has been for many years. Just a little difference in some details (the content is the same, but the way of teaching/learning has upgraded). Indeed, the possibility of using modeling in younger students is not unanimous and was debated (Tytler & Peterson, 2004).

Sort of experience, intellectual or theoretical tool of analysis, or intermediate between theory and experience and source of information on the nature of things, the epistemological status of simulations is controversial among scientists and epistemologists (Parrochia, 2000, Varenne, 2006).

Before integrating any technology in our classes, we must question its validity, efficiency and its impact on our educational system.

VI. RESULTS & DISCUSSION

There is a fort correlation between using simulation and achieving the goals ($\alpha \leq 0,05$), that means is “effectiveness of simulation” is related to “development of targeted skills”, that clears the outperformance of students using simulation over others.

A. Advance knowledge

- Oxidation-reduction reactions for metal ion / metal pairs

B. Knowledge and skills required

- Schematize a stack.
- Use the criterion of spontaneous evolution to determine the direction of movement of the charge carriers in a stack.
- Write the equation of the reaction for each electrode (2 arrows), and the balance equation during the operation of the stack (1 arrow only).
- Interpret the operation of a battery by having one of the following information: direction of flow of electric current, electromotive force e.m.f, reactions to electrodes, polarity of electrodes or movement of charge carriers.
- Write the reactions to the electrodes and relate the quantities of matter of the species formed or consumed to the intensity of the current and the duration of the transformation, in a pile.

C. Method using traditional drawing on board

For educational reasons this theoretical part is borrowed from a French educational site [6].

a. Experimental Highlighting

Q1. Indicate the material used in the experiment

A copper blade immersed in a solution of $Cu^{2+}_{(aq)}$ + SO_4^{2-}(aq) and a zinc blade dipped in a solution of $Zn^{2+}_{(aq)}$ + $SO_4^{2-}{}_{(aq)}$ (see Fig. 1).

b. Observations

Q2. What indicates that there is a chemical reaction? An orange-brown deposit not present initially appears and the color of the copper sulphate (blue) disappears. So something is happening in the beaker.

c. Reagent identification

Q3. What does the discoloration of the solution indicate? This indicates that $Cu^{2+}_{(aq)}$ ions (they are the ones that give the blue color to the solution) have disappeared.

Q4. What is the other reagent? As the SO_4^{2-} ions are spectators, they do not participate in the reaction. Zinc Zn is the other reagent.

d. Product identification

Q5. What is the nature of the observed orange deposit? The orange-brown color shows that this deposit is copper.

It is admitted that ions $Zn^{2+}_{(aq)}$ (colorless) appeared in the beaker.

e. Assessment of the chemical transformation

Reagent 1 + Reagent 2 = Product 1 + Product 2

$$\mathbf{Cu^{2+} + Zn = Cu + Zn^{2+}}$$

f. Interpretation of the transformation

Q6. What happened to the reagent Zn? Zn atom turned into $Zn^{2+}_{(aq)}$ by losing 2 electrons.

Q7. Choose the right equation for the corresponding transformation. Q8. What is the type of reaction? Zn = $Zn^{2+}_{(aq)}$ + 2 e- , it's an oxidation.

Q9. What happened to the reagent Cu^{2+}? Cu^{2+} ion was transformed into Cu by gaining 2 electrons.

Q10. Choose the right equation for the corresponding transformation. $Cu^{2+}_{(aq)}$ + 2 e- = Cu

Q11. What is the type of reaction? $Cu^{2+}_{(aq)}$ + 2 e- = Cu, it's a reduction.

So during the transformation, the $Cu^{2+}_{(aq)}$ ion captured the 2 electrons released by the zinc atom to form a copper atom.

g. Conclusion

Q12. Choose the right total equation for the corresponding transformation.

$Cu^{2+}_{(aq)} + 2e^- = Cu_{(s)}$ Cu appears: the copper blade thickens.

$Zn_{(s)} = Zn^{2+}_{(aq)} + 2e^-$ Zn disappears: the zinc blade wears out.

$Cu^{2+}_{(aq)} + Zn_{(s)} = Zn^{2+}_{(aq)} + Cu_{(s)}$

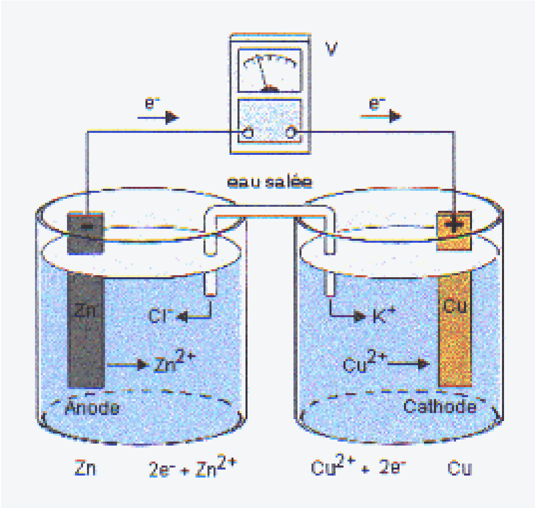

Fig. 1.Example of drawing on the board, by hand [7].

h. Why does the battery wear?

40% of students failed in this question, for a lack of imagination, what's really happening in both beakers, the surfaces of the two blades and in the salt bridge.

Q13. After a certain period of use, the battery can no longer supply current. In your opinion, why?

If the battery can no longer supply current, it means that:

- Either there is no zinc to supply the electrons; the reaction can not take place anymore.
- There are no more Cu2+ copper ions to recover the electrons; the reaction can not take place anymore.

The battery will stop when one of the two reagents Zn or Cu2+ will be missing.

D. Method using Simulation programs

The EduMedia program of the Moroccan Ministry of Education contains a very important simulation, free and easy to use. It displays the complete assembly of the experiment (the blades, voltmeter, wires, beakers, salt bridge, lamp ...), see Fig. 2.

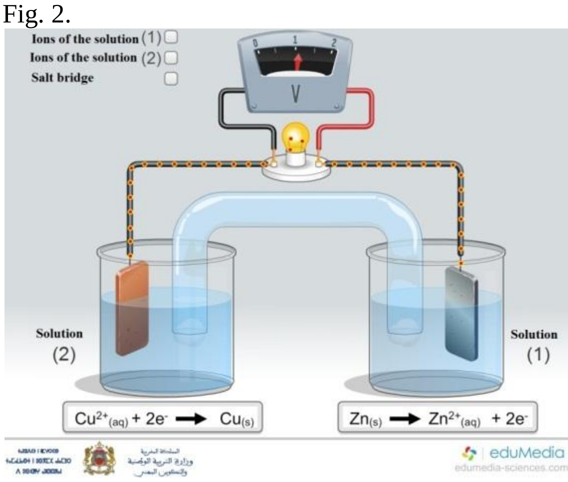

Fig. 2.Simulation program of the EduMedia platform.

Checking the various options available in the EduMedia simulation, we can see the different ions in both solutions and in the salt bridge even their direction of movement, see the Fig. 3.

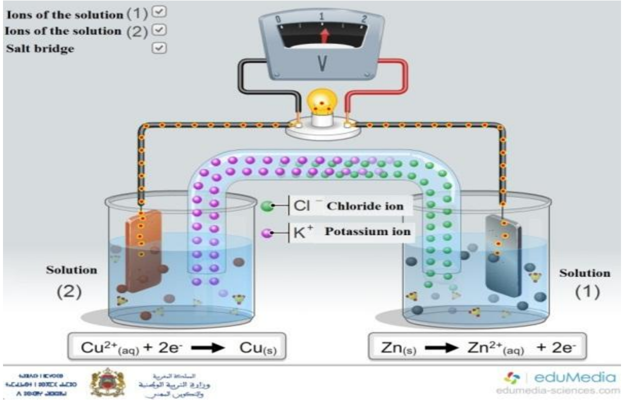

Fig. 3.Check the ion display options.

It is clear that in the final state the simulation showed the difference of the masses of the two blades in a very short time interval, see Fig. 4. "Normally it takes several hours depending on the initial concentration of ions in the solution". Unfortunately this simulation does not take into account the change of the coloring of the solution while using the battery.

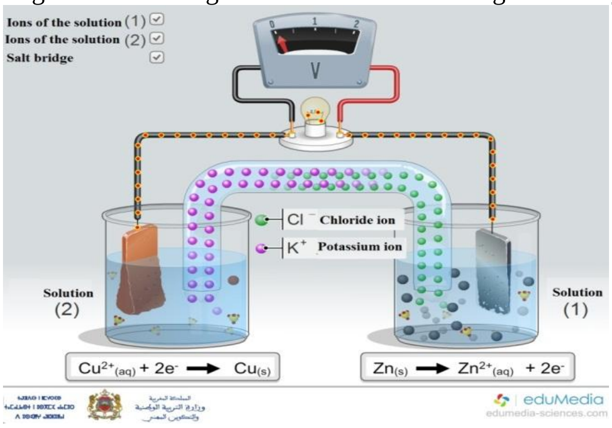

Fig. 4.The simulation in the final state.

There is another fascinating simulation program [6], [8] available on internet (see Fig. 5), that gives a new experience, exposing new ways of teaching allowing students to see what's really going on the solution and at the surface of the two blades "exchange of electrons and transformations metal/ion".

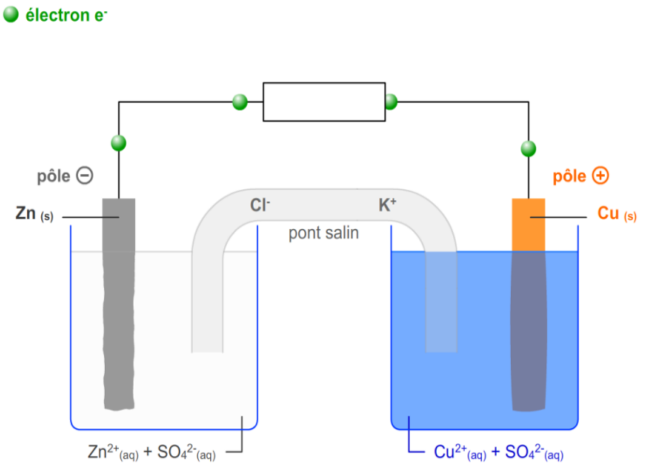

Fig. 5. First look on simulation, in initial state [6], [8].

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This simulation fortunately does take into account the change of the coloring of the solution, and more, it can show the difference of the masses of the two blades (see Fig. 5 and 6).

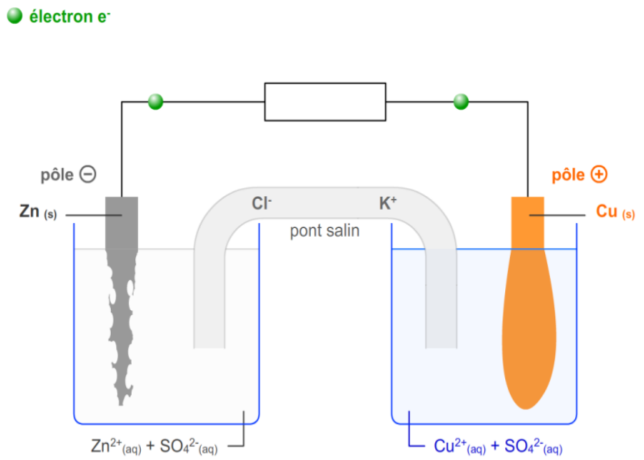

Fig. 6.Battery is in use.

Another amazing option integrated in this simulation, is the “Magnifying glass option”, which gives 3 options (see Fig. 7). The first option (1) allows the student to see the transformation of Zinc metal to zinc ion Zn^{2+}, emitting 2 electrons in the form of electric currents (see Fig. 8). The second option (2) allows the student to see the transformation of Cu^{2+} ion to copper metal Cu, receiving 2 electrons cent by the first transformation, in the form of electric currents (see Fig .9), which helps to explain why the copper blade thickens, and why the zinc blade wears out, and why 90% of the selected students have successfully answered the **Q13**, against 60% of students of the traditional method.

83% of the selected students have successfully answered the **Q2,3,4,5**, because it’s easy to remember the (blue) color of Cu^{2+} just by the look for example, and link it to the disappearance of those ions, against 59% of other groups.

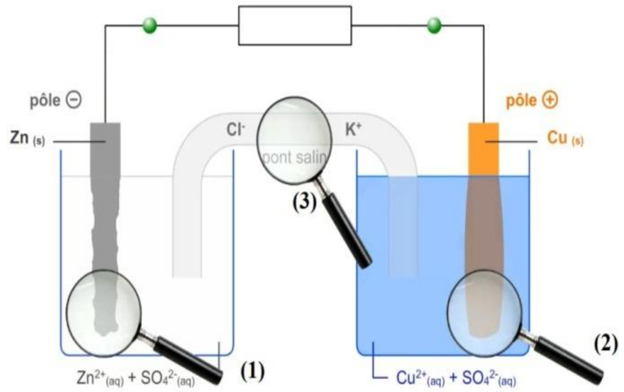

Fig. 7.Zoom in option.

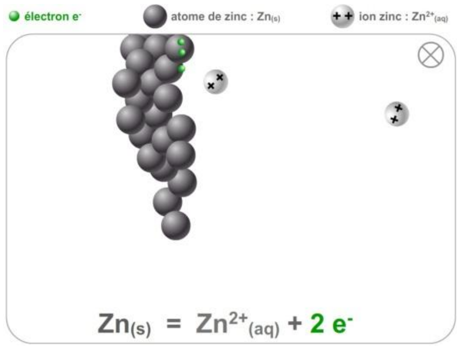

Fig. 8.Transformation on the surface of the cathode (2)..

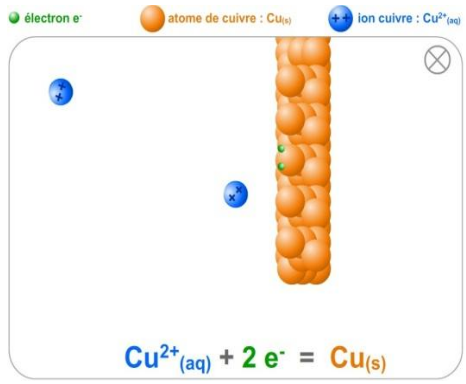

Fig. 9. Transformation on the surface of the anode (1).

The third option (3) allows the student to observe the movement of ions in the salt bridge, in different directions, than interpret the direction of each ion.

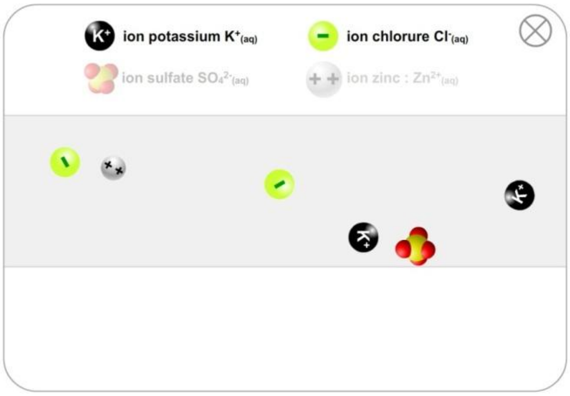

Fig. 10. Zoom in salt bridge (3).

The CCI (chemical concepts inventory) is a multiple choice instrument that can be used to indicate the level of chemistry misconceptions held by students. The inventory is a multiple choice instrument composed of one- and two-tiered non-mathematical conceptual questions (22 questions total). Each wrong choice for each question corresponds to the specific concepts on the stack and its operation, used as tools to measure conceptual understanding. Data from this study are analyzed using descriptive statistics and the t test8 for comparisons of data from the two experimental control groups and with the use of simulation. This study showed that students in the simulation group for an average of ($a \sim 0.39$) scored better than the control group ($a \sim 0.18$). The difference between the standardized learning gains of the two groups is statistically very significant ($p < 0.05$). There is also a fort correlation between using simulation and achieving the goals ($\alpha \leq 0, 05$), that means is “effectiveness of simulation” is related to “development of targeted skills”, that clears the outperformance of students using simulation over others.

We group in the following the main results recorded:

- 72% of participants say that the simulation offered them the opportunity to start again if they made a mistake.
- All participants say that the simulation allowed them to explore what’s really happening in the two beakers (98%).
- All participants (99%) say that the simulation allowed them to visualize the data in the form of images and colors.
- The majority of participants (86%) say that the simulation allowed them to gain time by speeding the process.

VII. CONCLUSION

It is clear that simulation can not replace the experiment, but sometime it could be used as a complementary tool for slow, toxic or explosive chemical reactions or to explain phenomenon on the microscopic scale. The aim of this study was to identify the leverage of an imitation-based technical program in developing some metacognitive skills in the science curriculum. The synthesis of the effectiveness of simulations for science learning, highlighted by this work, allows us to say that simulation can be considered as a support for new activities in the context of scientific education of skills, especially in chemistry: the emphasis is on the one hand on the utility, the play of representations, both graphic and mental, the visualization of scientific phenomena and the efficiency of the simulations used. it is important that students really approach more complex phenomena and scientific concepts "that can not be seen in the classroom by 'naked eye'", and experiment for the exploration and construction of models.

We believe that simulation is a powerful tool that could be very beneficial to learning and a key element in designing innovative learning environments that focus on the needs of learners and integrate ICT at the right time and for the right activity. However, in the development framework of education, simulation will eventually take a very large part of the scientific lessons, to give it a fun and enjoyable character, which we have missed in our classes.

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