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Computer Simulations as a Complementary Educational Tool in Practical Work: Application of Monte-Carlo Simulation to Estimate the Kinetic Parameters for Chemical Reactions

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ABSTRACT

From the point of view of educational environments technological innovation, teaching has stopped to be based on theory without the practical manipulations, providing new complementary educational services through different tools, computer modeling and simulations are necessary in order to encourage the university student's skills acquisition. In kinetics we have to estimate parameters for the catalytic chemical reactions, vapor deposition and many other reactions. Kinetic Monte Carlo is a simulation method often used when simulating how chemical systems evolve over time, for example how crystalline layers grow or evolve as atoms are deposited or hops around on a defined lattice surface or how concentrations of substrates depend on enzymatic reactions.

The work presented in this paper aims at highlighting the role of using computer simulations in the practical work of the teaching of the kinetic chemical roles, especially due to their impact on learning during the teaching process. Undoubtedly, by applying the Monte Carlo method and implementing a computer application developed in the educational setting for the simulations of the chemical reactions provides the students with the opportunity to acquire new skills and abilities, including the didactic and educational ones, enabling them, thus, to create a new dynamic that aims at optimizing the process of interaction and interactivity in the university. The analysis of the collected data is made after carrying out a survey on the impact of the integration of this new techno-pedagogic instrument on the students of the MSC course taught in third year at the Faculty of Science-Ben M'sik. The analysis is showing the usefulness of using this system in order to participate in the integration of the other platforms and applications of scientific simulations.

Key words : Chemical kinetics, Innovation, Integration, Monte-Carlo, Simulation

1. INTRODUCTION

The advances in the technology of information and communication in education require the continuous renovation of the educational systems in order to improve both teaching and learning and develop the students' academic skills through the effective use of a set of computer tools in the pedagogical concern such as the modeling and the simulation of the physical and chemical phenomena. The adoption of ICT for teaching and learning is a reporting innovation that has the most crucial role in the creation of a competitive society, ready to face competition and support economic development.

Many authors have shown that the integration of these technologies in the educational system has made the learning offered to students more active and interactive, offering them greater opportunities and helping them to develop their knowledge through different tools and technology. Accordingly, Bindu [1] has revealed that information and communication technologies have become an essential tool today to improve the quality of education. Likewise, Ziphorah [2] and Webb [3] have shown that its use helps students to learn constructivism as well as to develop their knowledge and shape their ability to think clearly.

Many other authors have shown that the educational integration of a new educational curriculum based on technology and computer creates favorable conditions for investment and the cognitive engagement of learners, particularly for the scientific subjects where the teaching of chemistry, for instance, is no exception to this trend. A new paradigm in the didactics of sciences has emerged, which is computer simulations as a supplementary teaching tool in chemistry. There are more simulations and computer models of the labs to study the concepts or chemical phenomena to the nanoscopic scale to facilitate their understanding and their explanation. Figure 1 shows Didactic Triangle with the Integration of Technology and Computer Tools

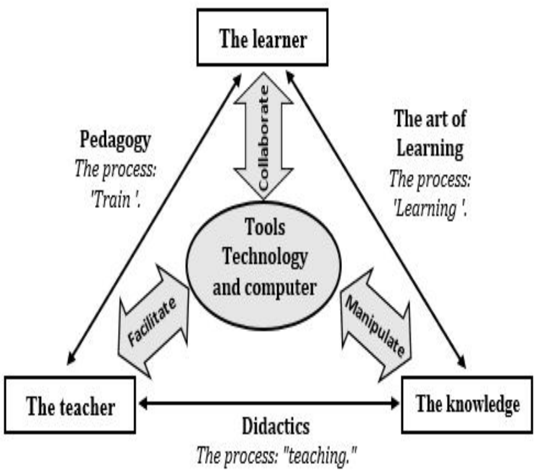

Figure 1: The Didactic Triangle with the Integration of Technology and Computer Tools

This work is part of the laws of chemical kinetics to determine the airspeed to a chemical reaction and the factors affecting them, as well as the sequence of molecular events known as the probabilistic method of Monte Carlo. The purpose of this contribution is to analyze how the development of an application on computer helps to carry out the practical work of the chemical kinetics developed by the Monte Carlo method, which can operate in a simple manner to the didactic and the pedagogical point of view.

2. THE THEORETICAL CONTEXT

It has been advanced a global HUB zero platform [4] including large-scale simulation software, educational resources. The educational systems are challenged by transforming objectives and development targets to innovate and opening up education [5,6].

This study is particularly on the use of models and computer simulations for the practical work of chemical kinetics by providing a computer application to help carry out the practical work by the method of Monte Carlo. This application has for main objective to offer a new complementary virtual environment that helps to develop the skills of student interaction with different chemical tools at the laboratory.

A. The Practical work of chemical kinetics

It is called the chemical kinetics study of the evolution in time of the chemical systems as well as the speed of chemical reactions, since during a chemical reaction, the transition from an initial state to a final State doesn't happen instantly. Thus, the laws of chemical kinetics are to determine the speed of a chemical reaction as well as the determination of the order of a reaction. Kinetics begins with the empirical kinetics, i.e. the determination of the algebraic relationships between concentration and time. Below is shown the chemical reaction takes place between two reactants A and B:

$$A + B \rightarrow C + D$$

A simple reaction speed is given by:

$$V = -\frac{d[A]}{dt} = -\frac{d[B]}{dt}$$
$$= +\frac{d[C]}{dt} = +\frac{d[D]}{dt} = k\,[A]^{n_A}\,[B]^{n_B}$$

- $n_A and n_B$are the partial order with respect to A and B
- $n_A + n_B$is the overall order of reaction
- $k$is the constant kinetics.

In the didactics of science’s practical work concerning the chemical kinetics leads the student to design an experiment to treat the measures and their interpretations in order to solve a chemical experimental problem. There are several practical chemical kinetics such as: kinetics in the liquid phase, kinetic followed by spectrophotometry, and so are simulations of chemical reactions by the Monte Carlo method.

B. The Monte Carlo Method

The usual methods of chemical kinetics usually consist in solving analytically a system of differential equations. The Monte Carlo method suppresses the resolution of differential equations. It considers the analogy between the probability that an effective shock occurs in a real reaction medium and the probability that two "objects" (numbers, letters, colored beads, etc.) are chosen simultaneously from a many more items. Each object carries a label referring to one of the chemical species of the reaction. All collisions are considered reactive, that is, the activation energy of the reaction is assumed to be zero($E_a = 0$) [7].

1) The Technical Simulation for a Second Order Reaction:$\boldsymbol{A + B \rightarrow 2C}$

A number of molecules represented by color A balls and color B balls are placed in a container. The balls are optionally diluted in solvent S molecules. One draws successively two balls taken at random. In the case where one has extracted a ball of color A and a second of color B, it is considered that there is a reactive collision so the reaction occurs; in this case the two balls are replaced by the products of the reaction, that is to say two balls C which are placed in the container before making the next choice. In the opposite case, the balls drawn are returned to the container.

Considering that a constant time interval Δt passes between two successive draws,and by taking the number of prints made, we will have a representation of the evolution of the concentrations of the different products as a function of time.The problem is the scaling of time.It is indeed solved by comparing the values of the initial speeds.We have for the reaction of order two the initial speed:

$$v_0 = k[A]_0\ [B]_0 \text{in} mol.\,l^{-1}(time)^{-1}$$

During the simulation we can express $v_0$by the variation of the number of moles of A with respect to time, from where:

$$v_0 = \frac{\Delta n_A}{\Delta t}$$

- Δn_Arepresents the number of balls A consumed in the first draw.

The final result after a theoretical demonstration is:

$$\Delta t = \frac{2\ n_B^0}{(n_A^0 + n_B^0)^2\ k\ [B]_0}$$

- $n_A^0 and n_B^0$represent $[A]_0\ and [B]_0 mole/l$

This result must be shown by the students in a review in more detail.

2) The Technical Simulation for a First Order Reaction:**A → B**

The technique used is simpler than in the case of the second order reaction. It is considered that there is effective reaction when in a run of a single ball only the reagent is extracted. The container must be filled with a specified number of color balls A.We shoot a ball in a first draw and we replace it with a ball of color B, we do after a finite number of prints. In the case where a color ball A has been extracted, it is considered that the reaction occurs; the ball is then replaced by the product of the reaction, i.e.,a ball of color B which is placed in the container before the next drawing. Otherwise, replace the ball drawn in the container.

3) The Technique of Simulation for the Simultaneous Reactions :

Either the following basic reactions:

$$(1)\boldsymbol{A} \rightarrow \boldsymbol{B}$$

$$and (2)\boldsymbol{A} \rightarrow \boldsymbol{C}$$

When we make a number of prints about the first reaction, a number of prints are made of the second reaction, such as:

$$n_1/n_2 = k_1/k_2$$

Time Δt is defined by k_1 (compared to one of the two reactions); in this case we perform$n_2 = n_1\ {k_2}/{k_1}$prints on the second reaction and it is considered that during these n_2 printshas resulted time$n_1.\Delta t$.

For example, $k_1 = 2k_2$. Two draws are then made for the first reaction,we note the result and we put the corresponding balls,then we make a single draw relative to the second reaction and we note the result by replacing the ball.The balance sheet of this draw is then determined.

C. Computer Simulations and Didactic Principles

Simulations refer to a set of computer programs that run on computer and which are based on the implementation of models theoretical or practices in experimentation to simulate a physical phenomenon or chemical real or complex.
In the process of teaching and learning of science subjects and especially the science of chemistry, computer simulations as a part of a complementary teaching approach, provide opportunities to create environments of learning as support of:

- Visualization of scientific phenomena;
- Communication for scientific information ;
- Collaboration on the discussion and the scientific argument;
- Data capture and representation.

Such computer tool saves time spent on shoots and Filling of real balls in the laboratory where the student can demonstrate the mathematical formulas and equations needed to calculate the velocities and orders of reactions of chemical kinetics.

3. METHODOLOGY

In a pedagogical axis computer simulation of practical work create favorable conditions for investment and the cognitive engagement of learners. This contribution is intended to develop a computer application on computer that operates according to a Client/Server architecture for educational use in learners that promotes autonomy, develop their spirit of initiative and values their activities.
The application allows the chemical reaction simulation by Monte Carlo method. It is a new technical tool that allows creating a virtual container and filling it with balls and performing the suitable number of prints for each model explained above, so that the representation of the results found after each draw. The application of simulation allows the generation of files representing the results of the manipulation performed by a student after authentication to access the system.
The design of an educational program is a process which aims to formalize all the preliminary stages of developing a system to make this development more faithful to the needs of the learner [8,9]. The computer design of the application developed in this research will follow three major phases:

Table 1: The Stages of the Design of the Application.

Functional analysis	We study the specification of the problem of the TP encountered in the laboratory with respect to the constraints of time, materials, from the point of view of learning. In this phase apply the modeling techniques, the description of the database and the definition of the architecture of the application.
Realization and programming	This phase involves the programming of the application and the tests to be performed as well as an optimization of the code.
Integration	A pedagogical integration of the computer simulation tool is in the last part. Students access the application and realize their manipulations under the guidance and follow-up of their teachers.

Our architecture is distributed at the level of the back-end, to organize the manipulation of data, the onset of treatment and their sequences. So:

- The presentation layer modeled by a set of graphical interfaces "WinForms" that are included in the .NET framework.
- The business layer that ensures the communication between the lowest layer and the more rise, developed by the C# programming language included in the Visual Studio environment.
- The persistence layer to ensure communication with the database created and managed by Oracle using SqlServer which is a management system database in SQL language incorporating among other things an RDBMS developed and marketed by the company Microsoft.

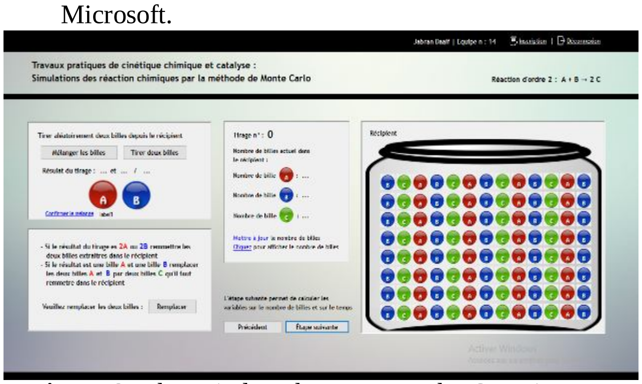

Figure 2: The Window that Presents the Container as Well as the Results of the Draws

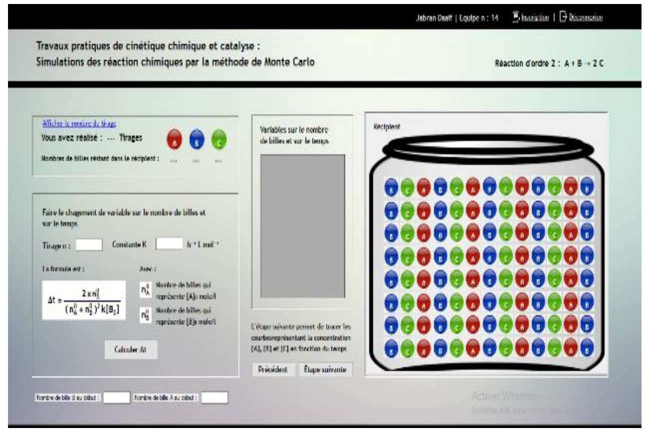

Figure 3: The Window with the Container, the Area to Calculate the Mathematical Formula and the results

Figure shows the Window that Presents the Container as Well as the Results of the Draws. Figure 3 shows the Window with the Container, the Area to Calculate the Mathematical Formula and the results.We adopted a second development architecture to better understand, predict, manage and optimize our system. The goals of an architecture are the understanding of the system studied by defining its limits and managing its growth. It includes MVC architecture is to adopt more efficient architecture:

Table 2: The Elements of the MVC Architecture.

The Model	The View	The Controller
The management layer of an application, presents classes for creating objects containing business data handled by the application through processing, constituting the business services.	It constitutes the interface users (teachers and students) elements.	It allows to control the application, it interprets the actions to realize and orders their execution (reading, data processing and updates).

Table 2: The Elements of the MVC Architecture.

4. EVALUATION AND EXPERIENCE

In the process of evaluating our add-on computer application as a teaching tool helping to carry out the practices works of the chemical kinetics by the Monte Carlo method; SMC students enrolled in the third year in the Faculty of science Ben M’sik made several manipulations to the laboratory of chemistry and physical materials in order to capture the perceptions of teachers and their students for our new tool for simulation farms.

A. The Experimental Study of the Reaction of Order 2

1) Fill the container that appears in the first window by 70 balls A and 70 balls B;
2) Make a first draw: If the result displayed is 2A or 2B put the two balls in the container (no reaction). If the result is A ball and B ball replace the two marbles A and B by two balls C. it takes to put it back in the container;
3) Do the same for 70 shoots;
4) The number of marbles A and B and the number of balls C obtained is automatically saved in a table relative to the number of draws;
5) The mathematical formula that allows to make the change of variable to the number of balls and the time is calculated and is registered;
6) Plot theoretical curves representing the concentrations of chemicals based on time;
7) Generate a Pdf file that represents the results found at the end of the manipulation in order to interpret them.

B. The Experimental Study of the Reaction of Order 1.

1) Place 70 balls type A;
2) Make 70 shoots;
3) Draw the curve of concentration simulated based on time;
4) Generate a PDF file that contains the curve for conclude.

5. THE RESULTS AND THE DISCUSSION

The questionnaire survey we did is an essential step in our study that allows to make a survey on the educational integration of computer simulation by the Monte Carlo method. We have selected a sample of 300 students enrolled in the third year S5 and 10 teachers of chemistry at question and establish a survey questionnaire.

Questionnaires represented students and teachers include preliminary questions about the experimental practice on computer time resulted with manipulation of the TP, the availability of different virtual in objects application, and the results of the TP digital generation. The questionnaire includes questions of satisfaction on the improvement of the understanding of the phenomena of chemical reactions and the interaction with the new virtual environment represented by our software solution in the laboratory. The results were favorable and will to achieve the educational objectives recommended for efficient use of the system.

According to the statistics of the results collected on the use of the application, 93% of students working on the manipulation of chemical kinetics by the method of Monte Carlo have won more than a 1/3 of the overall time of the TP using the application of simulation; it allows to enjoy the remaining time demonstrating algebraically mathematical equations represented in the theory course. Learners have had time to think, answering the questions of their teachers and then discuss the results generated by other teams from the simulation application [10].

Teachers reported that this new tool is beneficial at the educational level as more than 87% of students according to the survey have actually tried to interact with the TP in the laboratory, and develop their imaginations to know the understanding of chemical kinetics by a virtual simulation by computer. Such a process simulation and modeling is powered by the initial characteristics of learners: skills, abilities, knowledge and representations.

Computational thinking is a term that has received attention of the scientific community in recent years, much due to the lack of agreement on the definition and strategies involving the development of this kind of thinking [11,12].

In pedagogical innovation, the use of digital means represents a substantial portion, which will lead us to study other practical work for best integrations of computer simulations.

6. CONCLUSION

Based on the fact that new technologies are increasingly used in university teaching, we wanted to suggest as part of this work, the implementation of a computer application for educational use in the breast of the Laboratory of physical chemistry of materials for the probabilistic method of Monte Carlo based on the laws of chemical kinetics. The real work environment virtualization allows the adaptation of a set of graphical interfaces suitable for practical experience. This approach fits in a logic optimization and renovation of teaching practices in the context of science teaching.

As perspective of this work, it is proposed to implement a virtual lab online within the faculty to work results and the progress reports of the different TP in the laboratory for a better sharing of knowledge.

The motivation to pursue the integration of the technologies of information and communication such as software simulations is influenced by various educational factors to innovate and improve the quality of the academic training of our nation.

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