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THE ROLE OF DYNAMIC SIMULATION MODELS IN CHEMISTRY EDUCATION

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Abstract
This paper focuses on the integration of dynamic simulation models and chemistry lessons and its importance in education. In addition, the advantages of dynamic simulation models and the types of applications are presented. The advantages of integrated lessons over traditional lessons, the results achieved when organizing integrated lessons. An overview of dynamic simulation models is presented, identifying their important aspects and significance in practice, ways of using dynamic simulation models and solving problems arising in chemical education using simulation models.

Keywords: Exothermic, endothermic, simulation-based, integrated learning.

Introduction

In modern education the use of information and communication technologies is actively developing, the integration of lesson processes with simulation models is increasing. The most popular and promising directions are the introduction of multimedia technologies. They allow us to access different forms of information presentation and actively interact with them. Stimulation of the visual apparatus and hearing, activation of various channels of perception and processing of information makes the educational process more intensive, easy, effective, colorful and subjective.

Computer simulation helps to develop and expand professional knowledge, strengthen students' professional thinking and reasoning abilities, and realize new ideas. The combination of experiential learning with theoretical learning is encouraged through computer simulation [1].

Simulation models can take many forms. For example, "dynamic simulation models" are modeling systems used to simulate how variables and their interactions change over time. These models are widely used to understand, predict, and optimize the dynamics of complex systems and processes. The main features of dynamic simulation modeling are as follows:

1.Dynamic models act as a critical time variable and show how the results change over time. This helps in predicting the future state of the system.

2.These models identify the relationships and effects between elements within a system. For example, it shows how one change in economic, environmental, biological, chemical or social systems can affect other elements.

3. Dynamic simulation models can model complex systems, their internal dynamics and how they respond to external influences. They can also show how a system adapts to changing conditions.

4. Dynamic simulation models can use continuous (continuous) or continuous variables over time. Continuous models are usually expressed using differential equations, whereas discontinuous models are used to track a sequence of events or steps. Dynamic simulation modeling provides an accurate representation of internal complexity and dynamics, making it a valuable decision-making tool for researchers and engineers.

Molecular dynamics models are a promising class of computational models with broad applications in science education. Molecular dynamics models use classical mechanics and the atomic force approximation to calculate the motion of sets of atoms and molecules in two or three dimensions. Many of the basic ideas of thermodynamics can be seen in molecular dynamics models, such as temperature, conservation of energy, increasing entropy (the idea that the most disordered state is the most likely), and the equipartition principle (average kinetic energy of all states, objects in thermal equilibrium are identical) and the ergodic hypothesis (the time average of some parameter, such as kinetic energy, is equal to the average of all particles in the system at a point in time). Many of the behaviors of complex systems that were previously predictable only through complex statistical calculations can now be seen in dynamic models of fewer than 100 atoms. Examples include the ideal gas law, thermal equilibrium, phase changes, latent heat, crystal structure, diffusion, thermal expansion, osmosis, compressibility, absorption of gases by solids, and solubility. In the language of complexity theory, these large-scale phenomena “emerge” from simple rules that govern the actors (atoms and molecules) that make up the system. An animation of an atomic-scale system can be very similar to the results of one of the computational models. In both cases, the user sees many atoms or molecules moving across the screen. The difference between animation and computer models is flexibility and interactivity. An animation may be run simply as a video clip, or it may consist of several video clips selected to match some input signal. For example, a popular atomic-scale animation shows different pieces of atoms moving at speeds depending on temperature settings. In contrast, molecular models of atomic motion are calculated based on details of atomic motions and interactions. As a result, students can experiment with the system and create accurate models endlessly. However, much can be learned from studies using animated atomic-scale models [2].

In most scientific and engineering fields, there are two main types of computer models: data models and process models. Molecular visualization is an example of the limitations of using only static data models in education. Models help us understand the dynamics of real-world text processes by providing computer simulations of the real but simplified forces that are assumed to give rise to system behavior. Computer modeling becomes “dynamic” not only when the feedback processes between system components are fixed in time, but also when model development is based on the dynamic exchange of data and information between a group of modelers and a group of users [4]. Today, science educators have access to sophisticated multimedia models that allow students to view and interact with models of phenomena and processes. These simulations can provide students with visual representations of dynamic theoretical entities that are difficult to visualize in the static environment of a science textbook, but are important for understanding why materials behave the way they do [5].

Until the early 1990s, computer technology was used in chemistry education primarily as a means to assist teachers in carrying out repetitive teaching activities and as a means of transferring "traditional" teaching and learning activities to computers. In the early 1990s, behaviorist approaches were still evident and digital learning technologies were mainly used to provide teaching aids and "learn and practice" environments, but later new approaches such as "computer-assisted learning" emerged [6]. Since the invention of molecular graphics, a subject focused on visualizing molecules using three-dimensional computer graphics, chemists have used molecular visualization tools that allow them to quickly display molecular structures and view them from different perspectives. Several free tools have been developed to display molecules on web pages [3]. Chemical concepts related to fluid equilibrium mechanics are often explained with static diagrams in many textbooks, but in most cases The learning process is not complete until the students are done. Visualize the molecular dynamics of a phenomenon. Ultra-fine visualization using particle/molecule animation. It is an effective way to describe phenomena involving moving molecules. These visualizations are helpful. Students overcome learning barriers to visualize and understand how complex dynamic chemistry can be. A process is happening [7].

Molecular dynamics simulations using forward potentials from electronic structure theory have recently been shown to open new reaction pathways in complex chemistry and allow the investigation of high-temperature and high-pressure conditions where fine-grained mechanisms are difficult to resolve experimentally. Researchers have also discovered ways to use neural networks to predict the chemical reactions of reactants and reagents. Combined with these methods for finding new reactions, our statistical systems will eventually lead to building comprehensive Monte Carlo kinetic models for complex chemistry. It can be used to It can be refined to include more fundamental reactions and higher rates and then systematically scaled down to suit the specific system of interest, enabling rapid simulation capabilities for a wide range of chemical compositions and thermodynamic conditions [8].

Materials and Methods

For the research design, I chose the topic "Exothermic and Endothermic Reactions" and chose 2 different teaching methods to cover this topic. 2 groups (30 students in each group) agreed to participate in the study. I named the groups A and B. Group A's lesson traditionally began with a presentation and ended with writing on the board. To Group B, the topic of energy absorption and release in reactions was explained using dynamic simulation models. Initially a kinetic model was used to correctly determine the period of the reaction process. As a result, it can be seen that an increase in internal temperature may be required to allow energy movement as long as the change is detected during the reaction. The next step is the selection of thermodynamic models. Because it has been shown that endothermic reactions require an increase in temperature and exothermic reactions require a decrease in temperature. Then in order to study random angles we chose Monte Carlo models. Using this model facilitates to study the dynamics of reactions. Next step is choosing Computational Fluid Dynamics (CFD) model explains how gases or liquids change during the reaction. In a reaction, temperature is the change in pressure and different masses. This sequence is useful for explaining and analyzing the absorption or release of heat in reactions.

Results and its Discussion

Initial implementation ideas were explored for both groups at the beginning of the study. The study assesses students' initial skills in developing simulations and integrating chemistry. The students said that they face difficulties in subjects unrelated to their major, such as chemistry. But they noted that integrated education increases their interest and develops their analytical skills. After additional questions about how to identify the development stages of integrated education, it became clear that they had incorrect information. Students stated that it would be difficult to learn the topic orally. It is very helpful to present the material sequentially to increase student interest in all aspects of science. For example, when teaching the topic "Law of Conservation of Mass" instead of providing the concept only through the area of science, connecting it to mathematical thinking skills such as analysis and inference using dynamic modeling, the rate of learning was higher. As a result of the study teaching self-critical thinking and data analysis using simulations showed the importance of integrated learning in the classroom. The development of lessons in chemistry classes based on simulation models and the results of comparison of students' knowledge, skills and abilities with traditional lessons are presented in Figure 1.

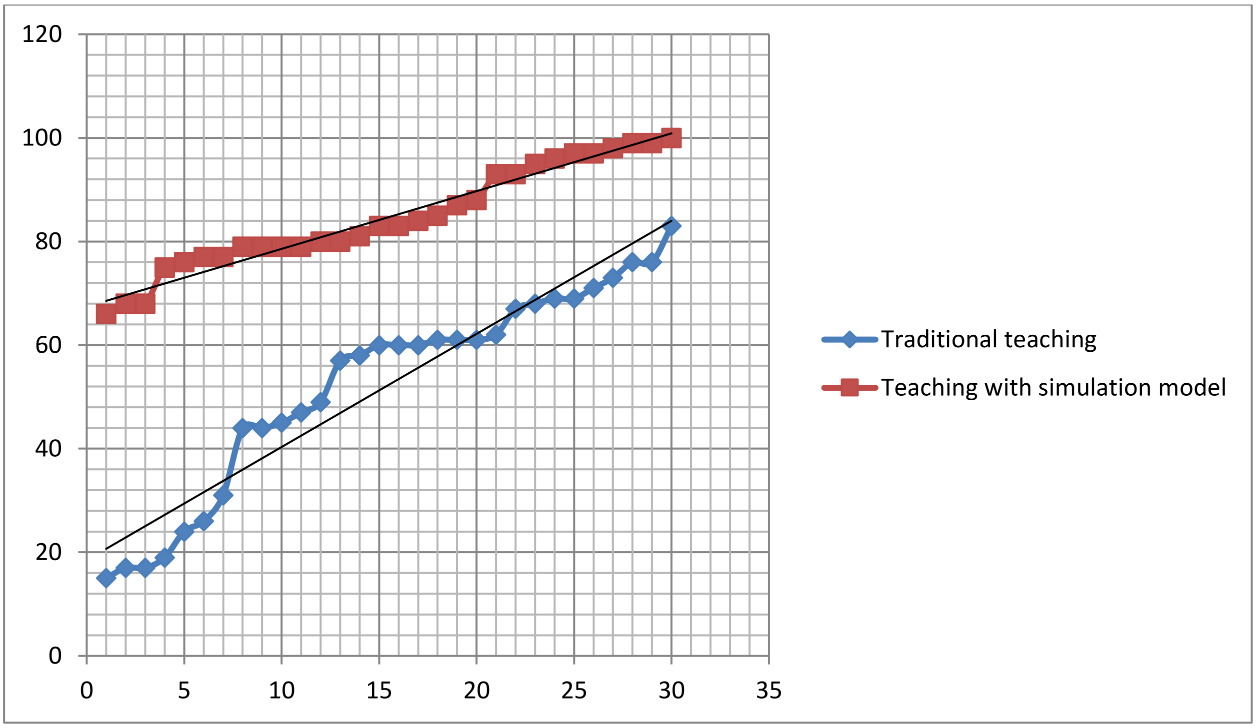

Figure 1. Red lines represent lessons organized with simulations. Accordingly, the blue lines show the results of conventional chemistry teaching.

Group A	Traditional teaching			
	Student number	Result (out of 100 points)	Student number	Result (out of 100 points)
	1	15	16	60
	2	17	17	60
	3	17	18	61
	4	19	19	61
	5	24	20	61
	6	26	21	62
	7	31	22	67
	8	44	23	68
	9	44	24	69
	10	45	25	69
	11	47	26	71
	12	49	27	73
	13	57	28	76
	14	58	29	76
	15	60	30	83

Figure 2

Group B	Teaching with simulation model			
	Student number	Result (out of 100 points)	Student number	Result (out of 100 points)
	1	66	16	83
	2	68	17	84
	3	68	18	85
	4	75	19	87
	5	76	20	88
	6	77	21	93
	7	77	22	93
	8	79	23	95
	9	79	24	96
	10	79	25	97
	11	79	26	97
	12	80	27	98
	13	80	28	99
	14	81	29	99
	15	83	30	100

Figure 3

As a result of the observation, it was found that the integration of chemistry with simulations showed a significant advantage. Figures 2(group A) and 3(group B) shows the number of students in both groups and their level of achievement according to the results of the test (calculated as 100%).

When implementing integrated learning using simulation models in chemistry education, students often encounter various problems in the teaching practice of college, school. The problem is that teachers fail to develop integrated learning, and it affects students' grasp of concepts. Students become more active if the teacher achieves integration with simulation models in the college-school teaching process. Based on the results obtained from the study, the following conclusions can be drawn. Here by complex material we mean identifying the basic concepts that can be taught in science, identifying and analyzing the energies absorbed and released during a reaction, and differentiating them from each other. This method also helps students make decisions and identify alternative strategies when they encounter difficulties in understanding.

Conclusion

In conclusion, simulation-based learning is important for further developing students' understanding, especially for self-assessment and analysis of knowledge gained. This study fills a gap in traditional teaching. Because the analysis and teaching of self-knowledge is activated by students having the opportunity to solve real-life problems through lessons organized in the framework of integrated science education.

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