Innovative: International Multi-disciplinary Journal of Applied Technology
(ISSN 2995-486X) VOLUME 4 ISSUE 4, 2026

SIMULATION MODELING AS THE BASIS FOR AN INTEGRATIVE MODEL OF CHEMISTRY INSTRUCTIONAL DESIGN

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Abstract:
This article presents a model for integrative instructional design in chemistry using simulation modeling, based on competency-based education theory. This model systematically integrates target competencies, structured content requiring visualization, digital modeling technologies, a methodological sequence, and measurable learning outcomes into a unified learning system. A quasi-experimental design with control and experimental groups was used to evaluate the model's effectiveness. Students in the experimental group worked in a virtual laboratory using simulations and modeling, while the control group used traditional methods. Quantitative data were collected using a t-test, which showed significant improvements in students' conceptual knowledge, research skills, and abstract thinking when using simulation modeling. Qualitative observations revealed significant improvements in cognitive engagement and motivation for learning. The use of integrative instructional design using simulations enhanced the quality of instruction in chemistry, helping students develop cognitive skills in a learning environment based on STEAM approach.

Keywords: simulation modeling, chemical education, development of educational materials, integrative model, virtual laboratory, STEAM education

Introduction

The ongoing digital transformation of education has significantly reshaped expectations regarding the design of instructional materials and pedagogical practices. In science education, particularly in chemistry, this transformation has highlighted the need for innovative approaches that make invisible and abstract processes cognitively accessible to learners. Chemistry operates at the microscopic

level, where atoms, molecules, reaction mechanisms, and energy changes cannot be directly observed. As a result, students often struggle to construct coherent mental models of chemical phenomena.[1][2] Although traditional laboratory instruction remains important, it does not always guarantee deep conceptual understanding. Real laboratory experiments are constrained by time, safety regulations, equipment availability, and limited opportunities for repeated observation of processes at the molecular level. Consequently, students may perform experimental procedures without fully understanding the underlying mechanisms. Simulation modeling offers a pedagogically promising alternative. By recreating chemical processes in digital simulation environments, it becomes possible to visualize atomic interactions, manipulate reaction parameters, and observe dynamic changes in real time. Such environments provide controlled, reproducible, and safe learning conditions. In this context, the aim of this study is to develop and empirically validate an integrative model for designing chemistry instruction based on simulation modeling (Bybee, 2013; Mayer, 2020).[2][3]

In education, simulation modeling can be understood as the structured representation of real-world processes through digital simulations and interactive virtual environments. Unlike static visual aids, simulation-based systems enable learners to interact actively with modeled phenomena, modify variables, and observe the consequences of their actions. In chemistry education, this approach supports several important instructional functions. First, it facilitates the visualization of processes at the microscopic level.[4] Students can observe molecular motion, bond formation and breaking, reaction pathways, and energy transformations—processes that would otherwise remain abstract and inaccessible.[5] Second, simulation environments enable safe experimentation. Students can conduct virtual experiments involving hazardous substances or complex procedures without physical risk. Third, simulation modeling promotes interactive hypothesis testing. Students can formulate predictions, adjust reaction conditions, and evaluate the results immediately. Finally, these environments foster the development of analytical and systems thinking, as learners interpret simulation data and connect microscopic representations with macroscopic observations (Clark & Mayer, 2020).[6]

The integrative approach adopted in this study is based on the principle of systemic coherence.[7] Effective instructional design requires alignment among educational objectives, content selection, technological tools, methodological strategies, and expected learning outcomes.[8] When these elements function as an interconnected system rather than as isolated components, instructional effectiveness is enhanced. Within this framework, simulation modeling is viewed not merely as a technological supplement but as a structural element integrated into the overall architecture of instruction.[9]

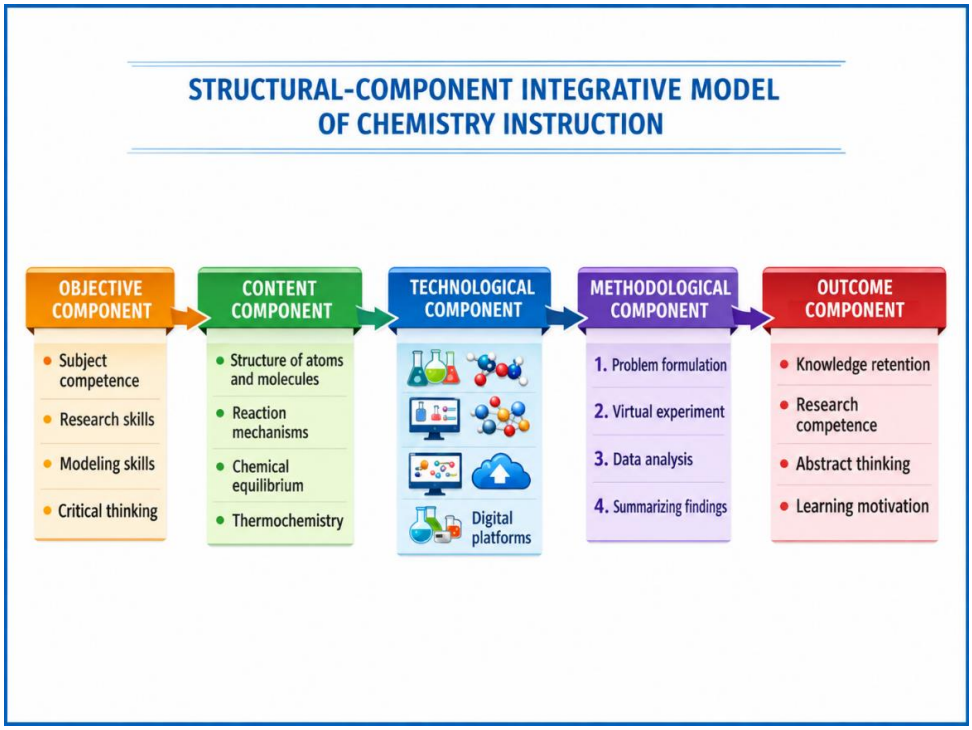


Figure 1. Integrative Structural-Component Model for Chemistry Instructional Design.

The proposed model is structured as a system of five interrelated components, each of which performs a specific pedagogical function while maintaining logical continuity with the others. The first element is the **objective (competency-based) component.** [10] It defines educational goals in terms of measurable competencies rather than knowledge acquisition alone. These competencies include conceptual understanding of chemical phenomena, research skills, modeling skills, and critical thinking. [11] The second element is the **content component.** It encompasses areas of chemistry that particularly benefit from visualization and simulation, such as atomic structure, molecular geometry, reaction mechanisms, chemical equilibrium, kinetics, and thermochemical processes. Content selection is guided by the principles of conceptual complexity and the need for dynamic representation. The third element is the **technological component.** It integrates digital simulation platforms, virtual laboratories, and interactive modeling tools that enable students to manipulate variables and observe changes in real time. In this model, technology is not an end in itself but rather a means of promoting conceptual clarity and active inquiry. The fourth element is the **methodological component.** It organizes the learning process into sequential stages: problem formulation, simulation-based investigation, experimental manipulation in a virtual environment, data analysis, and reflective synthesis. This step-by-step organization facilitates cognitive progression from observation to abstraction. [12]

Finally, the **outcome component** reflects measurable educational results. These include improved knowledge retention, strengthened research competencies, enhanced abstract thinking, and increased learning motivation. The effectiveness of the model is evaluated through empirical assessment and statistical analysis. Together, these five components form a coherent integrative system in which objectives determine content, content guides technology selection, technology supports methodological implementation, and methodology leads to measurable learning outcomes. The structural logic of the model reflects the systemic nature of instructional design in contemporary chemistry education.[13]

Materials and Methods

A quasi-experimental research design was employed to investigate the effectiveness of the proposed integrative model. The study was conducted over one academic semester at a higher education institution. A total of 120 students participated in the study and were divided into two groups: an experimental group (n = 60) and a control group (n = 60). The control group received traditional

instruction based on lectures and standard laboratory sessions. [14] The experimental group was taught using the integrative model based on simulation modeling. Instruction in the experimental group included virtual laboratory simulations, dynamic molecular modeling tools, and structured inquiry-based tasks supported by simulations. Data were collected through pre-tests and post-tests designed to measure students' conceptual understanding, problem-solving abilities, and research competencies in chemistry. The assessment instruments included multiple-choice conceptual questions, open-ended analytical tasks, and scenario-based modeling problems. The reliability of the instruments was assessed using Cronbach's alpha coefficient ($\alpha = 0.81$), indicating acceptable internal consistency. [15]

Quantitative data were analyzed using Student's *t*-test to determine statistically significant differences between the two groups. The significance level was set at $p < 0.05$. The methodological approach is consistent with established practices in educational research involving simulation-based learning (Rutten et al., 2012; de Jong et al., 2013). [16]

Results

The results revealed a clear difference in learning outcomes between the two groups. Although both groups demonstrated improvement from pre-test to post-test, the increase was substantially greater in the experimental group. Students who received instruction using simulation-based methods demonstrated a deeper conceptual understanding of reaction mechanisms, molecular interactions, and thermodynamic processes. [17] Their ability to interpret graphical simulation results and explain microscopic phenomena in terms of macroscopic observations improved considerably.

Statistical analysis confirmed that the differences between the groups were statistically significant ($t = 3.87$, $p < 0.01$). This finding suggests that the integrative simulation-based model had a measurable positive effect on learning outcomes. Similar patterns have been reported in previous studies comparing virtual and traditional laboratory environments (Hofstein & Lunetta, 2004; Zacharia, 2007). Furthermore, observational data and student feedback indicated higher levels of engagement and intrinsic motivation in the experimental group. Students reported that simulation tools helped them "see" chemical processes rather than merely memorize isolated facts. This finding is consistent with the theory of multimedia learning, which emphasizes the cognitive benefits of visual and dynamic representations (Mayer, 2020). [18]

Table 1. Pre-test and Post-test results

Groups	Mean score (pre-test)	Mean score (post-test)	Score gain
Experimental	56,4	82,7	+26,3
Control	57,1	68,9	+11,8

The experimental group demonstrated significantly greater positive progress compared with the control group. The distribution of research competency proficiency levels is presented in Table 2.

Table 2. Levels of Research Competency Development (%)

Level	Experimental group	Control group
High	48	21
Intermediate	42	46
Low	10	33

The data indicate a substantial increase in the proportion of students demonstrating a high level of competency in the experimental group. Statistical analysis was performed using the independent-samples Student's *t*-test. The mean gain in scores in the experimental group was 26.3 points ($SD = 10.2$), compared with 11.8 points ($SD = 9.5$) in the control group. With sample sizes of $n_1 = 60$ and $n_2 = 60$, the calculated *t*-value was 8.06, with $df = 118$, exceeding the critical value at the $p < 0.01$ significance level. Additionally, the effect size was calculated using Cohen's *d*, yielding a value of *d*

= 1.47, which indicates a large effect. These findings suggest that the integrative model had a substantial positive impact on learning outcomes.[19]

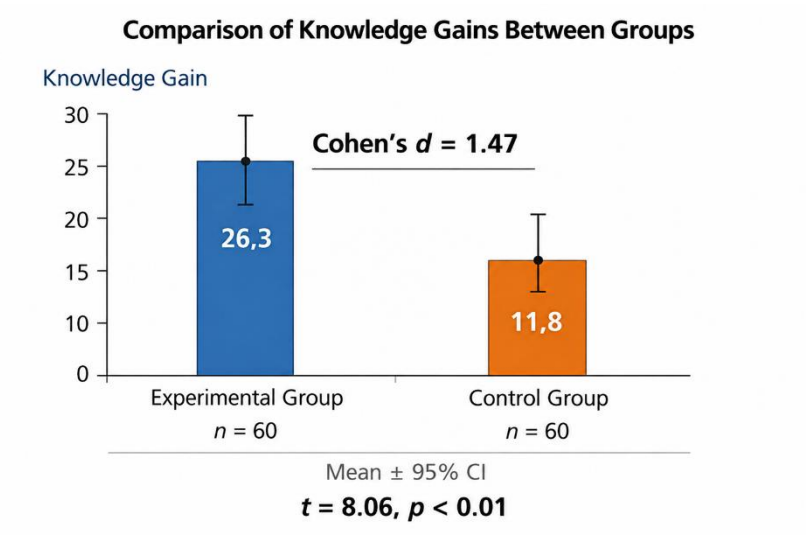


Figure 2

Discussion

The findings support the theoretical assumption that simulation modeling enhances conceptual learning in chemistry by bridging the gap between abstract symbolic representations and observable phenomena. The integration of simulation technologies into a structured instructional model appears to strengthen not only knowledge acquisition but also higher-order cognitive processes. The effectiveness of the model can be explained by several pedagogical mechanisms. First, dynamic visualization reduces cognitive load by facilitating dual-channel information processing (Clark & Mayer, 2020). Second, interactive manipulation of variables promotes active knowledge construction, which is consistent with constructivist learning theory (Bransford et al., 2000). Third, simulation-based experimentation enables repeated exposure to complex processes, thereby facilitating deeper encoding and retention of information. Importantly, the findings indicate that technology alone does not guarantee improved learning outcomes. Rather, its impact depends on systematic integration with clearly defined learning objectives and methodological stages. The integrative framework of the model ensures alignment between pedagogical design and technological implementation.

These findings contribute to the ongoing discussion of the role of digital transformation in science education and support the growing body of research advocating the use of simulations in instructional design (Bybee, 2013; Rutten et al., 2012).

Conclusion

This study developed and empirically validated an integrative model for chemistry instructional design based on simulation modeling. The results provide compelling evidence that the systematic incorporation of simulation-based technologies into the learning process significantly improves students' conceptual understanding, research competencies, and overall engagement in learning. The statistically significant differences observed between the experimental and control groups confirm the pedagogical effectiveness of the proposed model. The key contribution of this study lies in demonstrating that technological innovations alone do not automatically lead to improved learning outcomes. Rather, positive effects emerge when digital tools are embedded within a coherent pedagogical framework that ensures alignment among learning objectives, content complexity, methodological sequencing, and assessment strategies. The integrative nature of the model enables students to progress gradually from observation to experimentation, from experimentation to analysis, and from analysis to conceptual generalization. Furthermore, the study demonstrated that simulation modeling facilitates the visualization of abstract microscopic processes, thereby reducing

the cognitive barriers commonly associated with learning chemistry. The structured use of virtual simulations supports deeper knowledge construction, stimulates analytical thinking, and strengthens the connection between theoretical concepts and observable phenomena. Despite these positive findings, the study is limited to short-term learning outcomes within a single academic context. Future research should investigate long-term knowledge retention, the transfer of knowledge to novel problem-solving situations, and the scalability of the model across different educational levels. In addition, integrating artificial intelligence-based adaptive simulations may further enhance personalization and responsiveness in simulation-based learning environments.

In conclusion, the proposed integrative model provides a viable framework for modernizing chemistry education in the context of digital transformation and competency-based learning.

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