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PAPER

SIMULATION-BASED METHODOLOGY FOR IMPROVING CHEMISTRY TEACHING DESIGN MODELS

Firuza Davronova[1,*]

[1]PhD student of Faculty of Pedagogy Karshi State University, Uzbekistan

*firuzadavronova612@gmail.com

Abstract

This study proposes a simulation-based approach to enhance the design of chemistry teaching by integrating imitation models and computer-based analytical tools. Contemporary chemistry education is often challenged by the problem of relating abstract theoretical constructs to observable phenomena in experiments, resulting in poor conceptual understanding of the subject by learners. The aim of this research is to design and implement an instructional model that integrates UV-Vis spectral analysis, computer simulation, and guided analysis to enhance conceptual learning and scientific reasoning. The study used a design-based approach to education using simulation software and learning tasks. The students engaged in spectrum analysis, parameter variation, and model adjustment tasks using computer simulation software. The findings show that simulation-enhanced instruction led to a significant improvement in students' capacity to interpret spectral information, understand variable relationships, and apply modeling concepts in chemistry learning. Rubric analysis showed improved performance in model interpretation and data analysis skills compared to conventional learning methods. The study concludes that simulation models based on imitation provide an efficient pedagogical tool for designing modern chemistry education for conceptual understanding, analytical reasoning, and model learning skills.

Key words: chemistry education, imitation model, model-based learning, simulation-based instruction, UV-Vis analysis.

Introduction

Modern chemistry education focuses on conceptual understanding and scientific reasoning rather than memorization of isolated facts. Nevertheless, one of the most significant challenges in chemistry education is the difference between theoretical explanations and experimentally observable phenomena (Carroll 2024; Valeeva et al., 2023). Students often face difficulties in understanding abstract concepts such as molecular interactions, spectral properties, and quantitative relationships

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between chemical variables. Recent studies in education have emphasized the role of model-based learning as a method that helps learners build knowledge by interacting with scientific models. Simulation and imitation models enable students to change parameters and analyze changes in real time, as well as improve their analytical thinking skills (Justi & Gilbert, 2016). However, most learning activities are still based on static demonstrations, which do not allow students to actively investigate chemical processes. Previous studies have proposed the use of digital technology for visual representation of chemical processes, but the development of imitation models for designing chemistry learning is still in its infancy (Chan & Fok, 2021; Ortega et al., 2024). The integration of spectral analysis and modeling into chemistry learning needs methodological development. Despite the growing use of simulation software and virtual labs in chemistry education, current studies on the topic are mostly concerned with the effect of simulation tools and virtual labs on student engagement, visualization, or learning outcomes (Chan & Fok, 2021; Ortega et al., 2024). Most studies consider simulations as additional learning resources in teaching design. Consequently, little attention has been paid to the systematic integration of imitation simulation models into the methodological framework of chemistry education.

Method

Research design.

The research used a design-based research method, concentrating on simulation-supported chemistry learning. The learning design combined experimental observation, computer modeling, and analytical interpretation. The research targeted undergraduate students studying introductory analytical chemistry courses. The data was gathered using:

-UV-Vis spectrum analysis tasks;

-simulation-based model manipulation exercises;

-directed analytical queries;

-performance assessment using a rubric.

The students utilized a computer simulation package that supported spectral deconvolution and parameter variation. The software package enabled the students to explore the effect of pigment concentration and optical factors on spectral profiles and fitting outcomes. Analysis of the data was done in three successive phases to assess the performance of the students and the efficacy of the simulation-based instructional model. The performance of the students was measured using a rubric that had four dimensions of evaluation: conceptual understanding, interpretation of models, manual deconvolution skills, and data analysis skills. The criteria were scored on a scale of 0 to 10. The scores were statistically analyzed using descriptive statistics such as mean scores, standard deviation, minimum scores, maximum scores, and percentage distribution. The scores were used to determine the performance trends and the aspects of learning that were most affected by the simulation-based instructional model. To assess the instructional efficacy of the imitation model, the performance of the students in two instructional settings was compared: traditional instruction and simulation-based instruction. The comparison was done by analyzing the differences in the average scores of the rubric between the two groups. The improvement percentages were also calculated to determine the gains in learning. The comparison was done specifically on the students' ability to interpret spectral information, modify model parameters, and describe the relationship between experimental data and theoretical models.

The spectral deconvolution quality achieved in the simulation tasks was assessed for quality using the Root Mean Square Deviation (RMSD) parameter. The RMSD parameter was determined based on the difference between experimental and simulated spectra, ensuring that the accuracy of fitting was measured. Smaller RMSD values indicated higher accuracy between the calculated model and the experimental data. The students were required to analyze the RMSD parameter during analysis tasks, ensuring that the ability of the students to determine the reliability of the model and analyze fitting artifacts such as overfitting and negative concentration values was determined. The outcome of the statistical analysis, comparative analysis, and RMSD analysis was used to determine the effectiveness of the proposed simulation-based methodology.

Result and discussion

Prior to the simulation activity, oil samples were processed based on standardized spectroscopic techniques to ensure accurate absorption data. Solid particles were filtered out using rapid filtration to reduce scattering effects and avoid spectral distortion. The simulation environment offered the students a graphical representation of spectral fitting and pigment decomposition.

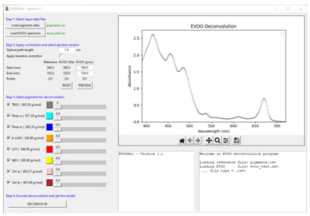


Figure 1. Initial view of EVOODec after running the executable program.

Figure 1 above shows a five-step instructional model intended to facilitate the simulation-based spectral modeling approach in chemistry education. The five steps are a measurable instructional function that logically relates to both the accuracy of experimental results and cognitive development. The first step involves the filtration of oil samples and the adjustment of the optical path length (0.2-0.5 cm). The filtration process removes suspended particles in the oil samples that cause light scattering, which would otherwise result in an increase in absorbance values beyond the Beer-Lambert law linearity. The reduction in optical path length ensures that the absorbance values are within the valid range of the instrument (generally below 2.0 AU), thus maintaining the proportionality between concentration and absorbance.

The students were asked to organize the raw data from the UV-Vis spectrophotometer into a form that is amenable to the simulation software. This process was not only a necessary step in preparing for the simulation, but it was also an important analytical task that reinforced the concepts of data representation.

Figures 2 and 3 above show two acceptable input data structures. These include semicolon-delimited CSV files and two-column Excel files. In both cases, the first column represents the wavelength, which is measured in nanometers (nm), while the second

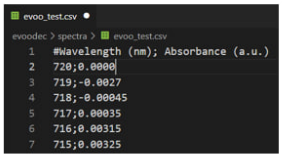


Figure 2. Example of input spectrum file in CSV format

	A	B
1	Wavelength	Absorbance
2	720	0.00000
3	719	-0.00270
4	718	-0.00045
5	717	0.00035
6	716	0.00315
7	715	0.00325
8	714	0.00285
9	713	0.00515

Figure 3. Example of input spectrum file in Excel format

column represents the corresponding absorbance (A). The requirement that the input data be in two columns eliminates any possibility of confusion regarding which column represents which variable, and it also ensures that the data is properly parsed by the simulation algorithm.

In the CSV format (Figure 2), each line corresponds to a unique data point (, A). The use of the semicolon as a delimiter was necessary to prevent regional decimal point notation from causing ambiguity. The use of comment lines marked with the "" symbol allowed the software parser to ignore comments, which could then be used for metadata without affecting calculations. This requirement taught students to distinguish between data and comments, which is a critical skill in scientific data management.

In the Excel format (Figure 3), students were required to enter wavelength data in column A and corresponding absorbance values in column B, with a header row indicating units of measurement. This requirement ensured that units were consistent across measurements, which would have otherwise led to dimensional errors. The need for consistent unit labeling reinforced the importance of measurement standards and reproducibility. From a computational standpoint, correct formatting was necessary because the simulation algorithm requires spectral interpolation at a resolution of 1 nm. Missing data points, repeated wavelengths, or incorrect delimiters led to errors in fitting or unstable deconvolution. Students were thus forced

to check for monotonic wavelength increments and uniform spacing before importing the data.

This activity reinforced a number of tangible skills:

– the ability to organize numerical data within the constraints of an algorithm.

– the ability to recognize inconsistencies in formatting that lead to errors in computation.

– the recognition that absorbance is a function of wavelength.

– the ability to take experimental results and translate them into a form suitable for simulation.

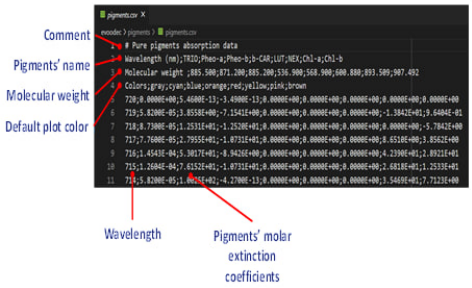


Figure 4. Structure of pigments' reference data file

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Figure 4 shows the organized structure of the reference pigment data file. The data file includes values of wavelengths in the first column (370–720 nm with a resolution of 1 nm) and molar extinction coefficients (ε) for each pigment in the remaining columns. The first three rows contain metadata: pigment names, molecular weights (g/mol), and default display colors for visualization.

The incorporation of molar extinction coefficients instead of absorbance measurements is a methodologically important aspect. Absorbance measurements are concentration- and path length-dependent, as shown by the equation: $A = \varepsilon clwhereA$ is absorbance, ε is the molar extinction coefficient, c is the concentration, and l is the path length. In contrast, extinction coefficients are molecular absorption properties that are independent of experimental conditions. This enabled students to recognize that the simulation software does not merely plot empirical curves but calculates the entire spectrum according to molecular parameters and concentration coefficients.

Students analyzed the spectral patterns of fresh and aged oils. They noted the decrease in peaks related to chlorophyll in aged samples and explained the chemical degradation mechanisms for pigment stability. The guided discussion approach forced students to make every modeling step justified by experimental data. For example, when excluding a pigment from the fitting process, students were compelled to justify their action based on RMSD values and peak discrepancies. This approach changed the paradigm of learning from software procedure to evidence-based reasoning. In contrast to open-ended questioning, the guided analytical approach was directly connected to specific competency areas: quantitative reasoning, awareness of variable control, and accuracy of spectral interpretation. The discussion component of the approach thus served as an overt transition from computational manipulation to chemical conceptualization. The guided analytical approach ensured that simulation exercises were not merely reduced to fitting procedures but rather facilitated systematic scientific thinking based on observable data.

The performance of the students was evaluated using a structured analysis rubric that was adapted from the evaluation scheme provided in the supporting materials.

As students reformatted data, removed baselines, chose spectral windows, and resolved resolution constraints, they practiced essential skills of analytical chemistry (data cleaning, visualization, and validation). This "data realism" enhances conceptual learning because students are forced to validate chemical assertions (e.g., pigment identification, concentration variation) based directly on spectral data. This strategy is justified by the EVOODec case study, which deliberately employs spectral deconvolution as a learning scenario for both high school and college levels.

In terms of modeling, the most productive aspect from an educational point of view was the assumption of linear combination in deconvolution, namely that the total spectrum can be reconstructed from weighted pigment reference spectra. Students' strongest performance in "model interpretation" can be attributed to the fact that variations in parameters (coefficients of pigments) produce immediate and localized effects in the spectral regions, thereby creating a cause-and-effect

relationship. This is in line with studies on modeling in laboratory classes, where modeling activities facilitate scientific practice when students are required to explain how representations are linked to mechanisms and measurements (Margolin et al., 2022)

Conclusion

Crucially, our findings show that the greatest benefits lie in the area of data interpretation and model reasoning, rather than simple content recall. This is in line with what has been found in other simulation studies, namely that the benefits of simulations are greater when the learning objectives are set at a higher level of reasoning (interpretation, evaluation, troubleshooting) rather than at a procedural level. In the area of chemistry education, it has been suggested in a number of recent reviews that simulations need to be embedded in a structured learning sequence, otherwise the technology becomes simply a visualization tool with little effect. This is reflected in the design shown in Figure 1, where preprocessing and validation are made mandatory steps that directly affect the quality of model output. Rubric-assisted assessment was critical for two reasons. First, it allowed for construct-aligned assessment of modeling performance (conceptual understanding, deconvolution reasoning, RMSD interpretation, technical proficiency) rather than relying on grades or student self-assessment. Second, the rubric criteria provided clear performance goals that likely mitigated shallow "button-clicking" activity and supported reflective explanation (e.g., pointing out negative concentrations as non-physical artifacts). This is in line with research that shows well-crafted rubrics can enhance the reliability of inquiry and modeling competency assessment (Lu et al., 2024)

Finally, the framework supports computational literacy skills by requiring students to work with data as machine-readable objects (format constraints, delimiters, resolution, metadata management). This is directly in line with the emerging trend of computational thinking integration into school subjects, where modeling, debugging, and data reasoning are viewed as core practices rather than secondary digital literacy skills. There is evidence to suggest that when computational thinking is integrated into subject learning, students' analytical problem-solving skills are enhanced—following the same pattern we saw in modeling and interpretation scores.

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