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SIMULATION-BASED METHODOLOGY FOR IMPROVING CHEMISTRY TEACHING DESIGN MODELS

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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.

Keywords: 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 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). [1]

However, most learning activities are still based on static demonstrations, which do not allow students to actively investigate chemical processes.[2] 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. [3]

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). [4]

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.[5]

Moreover, although learning frameworks based on models consider the construction, testing, and development of models as essential there is a lack of empirical studies on how these frameworks can be applied in the context of analytical chemistry problems, especially in spectroscopic models (Justi & Gilbert, 2015; Carroll, 2024),[6]

Another limitation in the current literature is related to the evaluation of analytical competencies. While various studies emphasize the enhancement of higher-order thinking skills by inquiry-based learning (Ibnu et al., 2020; Orosz et al., 2023), there are relatively fewer studies that explore the impact of simulation-based modeling on competencies related to data structuring, parameter optimization, and model validation based on quantitative parameters such as RMSD. [7]

Thus, the limitation is not that there is a lack of simulation studies, but that there is no systematic and methodology-driven framework that combines imitation modeling, digital spectral analysis, computational thinking, and competency-based evaluation to create a comprehensive design for 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.[8][9]

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. [10]

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.[11]

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.[12]

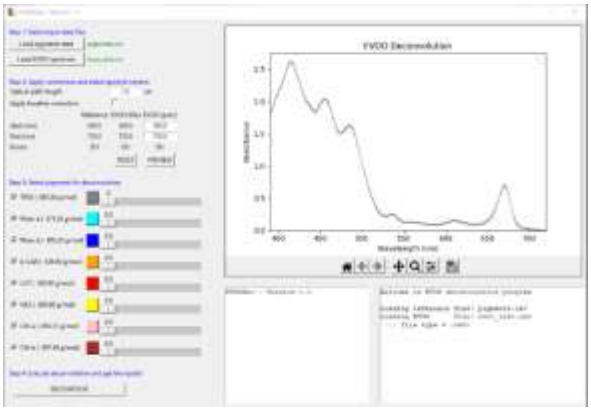


Figure 1. Initial view of EVOODec after running the executable program.

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. [13][14]

In this stage, spectral information is translated into organized forms (CSV or Excel) that can be processed by simulation software. Baseline correction is used to eliminate instrumental errors and facilitate the alignment of experimental and reference spectra. The choice of spectral window (for example, 400-700 nm) suppresses computational noise and restricts the fitting process to chemically meaningful absorption areas. In digital deconvolution, students choose pigments from a reference library and engage in manual or automatic fitting.[15] A spectrum of each pigment corresponds to a

molar extinction coefficient profile with 1 nm resolution. The sum of the modeled spectrum is mathematically reconstructed as a linear combination of individual pigment spectra. Changes to parameters directly affect concentration coefficients, enabling students to discern quantitative links between spectral intensity and pigment composition. This stage translates abstract mathematical fitting into a visually meaningful process. [16]The novelty of the framework is in its holistic integration of experimental control, data preprocessing, modeling, and validation as a unified instructional sequence. Instead of viewing simulation as a secondary visualization technique, the model sees it as a primary analytical tool that bridges physical observation and theoretical thinking.[17]

Input data structure and data management skills

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.

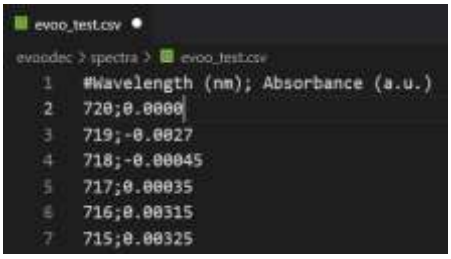


Figure 2. Example of input spectrum file in CSV format

	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

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 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. [18]

In the CSV format (Figure 2), each line corresponds to a unique data point (λ, 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.[19]

The accuracy of spectral deconvolution was directly proportional to the quality and organization of the

reference pigment database incorporated into the simulation software.

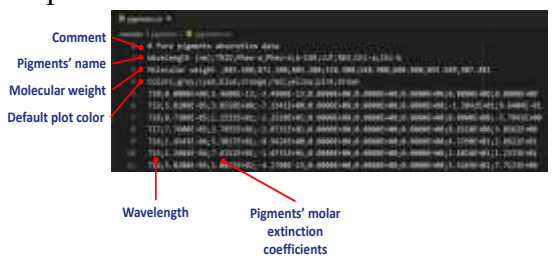


Figure 4. Structure of pigments' reference data file

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.[20]

The incorporation of molar extinction coefficients instead of absorbance measurements is a methodologically important aspect. Absorbance measurements are concentration- and path length-dependent (A = εcl), whereas 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 coefficient.

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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