

# THE APPLICATION OF ARTIFICIAL INTELLIGENCE IN CHEMISTRY EDUCATION AND THE PREDICTION OF CHEMICAL REACTIONS

Gulnara Duruskari, Gulbadam Akbarova, Khalil Naghiyev  
Baku State University, Baku, Azerbaijan

Received: 19 February 2026

Accepted: 10 April 2026

Published: 13 April 2026

---

In the modern world, the technological revolution has also triggered a transformation in the fields of science and education. Artificial intelligence and similar 21st-century technologies are no longer confined solely to computer and information sciences. They have begun to find broad applications in various fields, including chemistry, biology, and physics. Today, chemistry – as a science characterized by complex reactions and numerous variables – presents itself as an open platform for leveraging the capabilities of artificial intelligence (AI). AI introduces a range of innovations into the teaching and learning of chemistry. This study aims to explore the potential impact of artificial intelligence on education. The article analyzes the integration of AI into educational environments and examines its practical applications. In particular, it investigates the use of AI for the automation of chemical reactions. The objective is to highlight the importance of this topic from both scientific-technical and pedagogical perspectives and to illustrate how such technologies can be implemented within instructional contexts. The integration of AI into the field of chemistry should not be limited to academic or industrial research alone. Incorporating these technologies at the secondary school level can enhance students' scientific and technical literacy while also fostering essential 21st-century skills such as critical and creative thinking. A review of relevant literature has been conducted, and practical examples involving the use of ChatGPT have been presented in the paper. The significance of such research lies in its contribution to the emerging direction of AI-assisted chemistry education. The findings of this paper suggest that the use of AI in chemistry instruction makes significant contributions to the learning process and represents a modern instructional tool aimed at improving the quality of education. The application of such technologies in chemistry classes not only serves as a supportive resource for teachers and students but also plays a crucial role in enriching students' learning experiences and promoting the development of critical thinking skills.

**Keywords:** artificial intelligence, chemistry education, chemical reactions, reaction mechanisms, automation, ai in education

---

## INTRODUCTION

In a short period of time, artificial intelligence has led to rapid transformations across various industries, including the field of education. The development of AI has introduced numerous innovations with significant impacts on different areas of human life. As a key pillar of societal progress, education has inevitably been influenced by this wave of technological advancement. ChatGPT, an AI-based chatbot developed by OpenAI, was initially released on

November 30, 2022, based on the GPT-3.5 model, and later updated on March 14, 2023, using the GPT-4 model [1]. According to many experts, it is considered one of the most powerful AI tools developed to date [2].

ChatGPT is a large-scale language model based on Generative Pre-trained Transformer (GPT) technology. In addition to being a pre-trained generative neural network, it has been fine-tuned using supervised learning and reinforcement learning techniques. This approach enables the model to understand and respond to a wide range of queries with high accuracy and to engage in coherent and contextually appropriate conversations with users. ChatGPT is capable of performing various tasks. Although its responses are not flawless, the tool has reached an unprecedented level of technological innovation. Artificial intelligence and machine learning have gained significant popularity in recent years and have been widely applied in educational settings [3].

In this regard, the achievements in AI offer valuable methods for enhancing the teaching and learning process [4]. Particularly in the field of chemistry education, there is growing interest in integrating AI and machine learning into curricula. These technologies are applied in laboratory experiments, simulations, virtual laboratories, data analysis, and assessment processes [5,6]. AI is also used for a variety of purposes within educational systems. As a computer program capable of simulating human-like thinking, AI can perform complex tasks such as visual recognition, natural language understanding and generation, data analysis, and providing intelligent recommendations [7].

Teachers may also utilize this technology to develop instructional materials or simulate discussions for educational purposes, thereby expanding the pedagogical capabilities of tools like ChatGPT [8]. However, as with any technological advancement, ChatGPT is not free from potential risks. These include the generation of biased information, dissemination of misinformation, and the possibility of producing inappropriate or harmful content [9]. Additional concerns involve data privacy, security, transparency, and explainability [10]. Understanding and addressing these challenges is essential for ensuring the effective and ethical use of ChatGPT in educational contexts. This impact extends beyond technological aspects, encompassing pedagogical approaches, ethical considerations, and the professional development of educators. Likewise, technological innovation plays a significant role in enhancing chemistry education. The use of digital technologies in teaching chemistry – particularly in topics that require extensive use of molecular models – can contribute to more effective and clearer instruction [11,12].

Furthermore, integrating AI into the learning process enhances students' analytical thinking, problem-solving skills, and ability to critically evaluate experimental results. The prevention of errors in traditional laboratory settings, reduction of time and resource waste during data analysis, and adaptability to individual learning needs are among the major advantages of implementing AI in educational environments. The primary aim of this research is to examine the predictive capabilities of AI models in the context of chemical reactions – specifically the reaction between vinegar and baking soda leading to carbon dioxide generation – analyze their pedagogical implications, and demonstrate how AI technologies can be implemented in modern instructional methodologies. This approach not only contributes to the digitalization of the teaching process but also fosters interest in chemistry, supports interdisciplinary connections, and promotes the development of essential 21st-century skills.

## **EXPERIMENTAL**

The primary objective of this experiment is to examine the impact of artificial intelligence (AI) on the learning process in chemistry education and to evaluate its ability to predict the outcomes of chemical reactions. The study investigates the role of AI in education, its potential to enhance students' analytical and critical thinking skills, and how the application of modern instructional tools in chemistry classes can deepen learning and facilitate accurate and efficient experimental results. The findings of this study provide insight into the effectiveness of integrating AI into the teaching of chemistry. In the experimental phase of the

study, the amount of carbon dioxide ( $\text{CO}_2$ ) produced from the reaction between acetic acid ( $\text{CH}_3\text{COOH}$ ) and sodium bicarbonate ( $\text{NaHCO}_3$ ) was measured. Substances were mixed in various volumes and masses, and observational data were systematically recorded.

These real-world results were then analyzed using an AI-based approach. For this purpose, a simple AI algorithm was developed using the Python programming language, based on a Linear Regression model. The model was trained using the input values of vinegar and baking soda quantities, while the corresponding output was the measured volume of  $\text{CO}_2$  produced. After the training phase, the model was used to predict the amount of  $\text{CO}_2$  for new experimental conditions.

The application of AI served not only to facilitate the analysis of the experimental results but also acted as a pedagogical tool that enabled comparisons between predicted and actual outcomes. Initially, the model was trained using data from five different experiments. Subsequently, it was used to predict the volume of  $\text{CO}_2$  for combinations of reactants that had not been previously included in the training set. During the research process, experiments were also conducted under varying conditions of temperature and pressure.

Changes in temperature can affect the reaction rate and the amount of product formed, while pressure can influence the reaction environment and thereby alter the outcomes. Each of these variables plays a critical role in the prediction of  $\text{CO}_2$  volume. In practice, vinegar and baking soda were combined under different temperature conditions (e.g.,  $20^\circ\text{C}$ ,  $30^\circ\text{C}$ , and  $40^\circ\text{C}$ ) and pressure conditions (e.g., atmospheric pressure and elevated pressure). The volume of  $\text{CO}_2$  produced under each condition was measured, and the results were recorded. The collected data were analyzed using the AI model, with inputs consisting of vinegar and baking soda amounts, temperature, and pressure values, and the corresponding output being the observed  $\text{CO}_2$  volume. Once the model had been fully trained, it was used to predict the volume of  $\text{CO}_2$  for new experimental setups.

**Table 1:** Experimental Data (Real Observations)

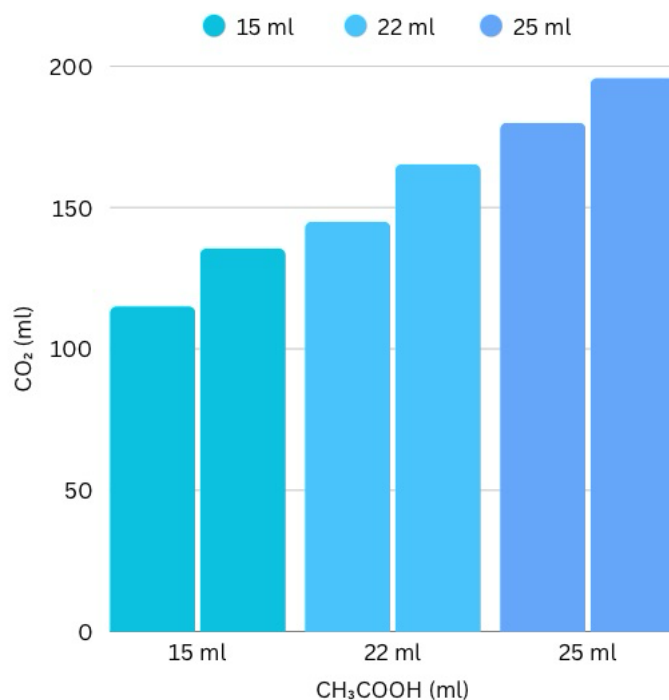
$\text{CH}_3\text{COOH}$ (ml)	$\text{NaHCO}_3$ (g)	$\text{CO}_2$ (ml)	Temperature ( $^\circ\text{C}$ )	Pressure (atm)
10	2	75	25	1
15	2.5	115	35	1
20	3	145	20	1
25	3.5	180	35	0.9

**Table 2:** Predicted Results Generated by the Artificial Intelligence Model

$\text{CH}_3\text{COOH}$ (ml)	$\text{NaHCO}_3$ (g)	Predicted $\text{CO}_2$ (ml)	Temperature ( $^\circ\text{C}$ )	Pressure (atm)
18	2.8	$\approx 135.5$	30	1
22	3.2	$\approx 165.3$	20	1
27	3.7	$\approx 195.7$	35	0.9

Based on the collected empirical data, an artificial intelligence model was developed and trained using a Linear Regression algorithm. The input variables for the model included the volumes of acetic acid and masses of sodium bicarbonate, while the output variable was the corresponding volume of carbon dioxide ( $\text{CO}_2$ ) produced. Table 2 presents the model's predicted outcomes for experimental combinations that were not previously included in the training data. For example, when 18 ml of acetic acid and 2.8 g of sodium bicarbonate were used, the model predicted approximately 135.5 ml of  $\text{CO}_2$  generation. This prediction closely aligns with the empirical data, indicating that the AI model provides reliable and accurate estimations. These findings support the conclusion that artificial intelligence can serve as an effective tool for the analysis and interpretation of chemical reactions. As illustrated in Figure 1, there is a close agreement between the experimentally measured volumes of  $\text{CO}_2$  and those predicted by the artificial intelligence model across varying concentrations of acetic acid ( $\text{CH}_3\text{COOH}$ ). For each amount of acetic acid, the first bar represents the actual experimental result, while the second corresponds to the AI-predicted value. This suggests that the model

demonstrates a reasonable level of accuracy in estimating the outcomes of the chemical reaction (Figure 1)



**Figure 1.** Comparison of real vs AI predicted CO<sub>2</sub> production

## RESULTS AND DISCUSSION

The results of the conducted study demonstrated that the application of artificial intelligence (AI) in chemistry education goes beyond the mere transmission of knowledge; it also encompasses the analysis, interpretation, and prediction of experimental outcomes, thereby making a significant contribution to the development of students' scientific and analytical skills. The primary objective of the experiment was to measure the amount of carbon dioxide (CO<sub>2</sub>) generated as a result of the chemical reaction between acetic acid (CH<sub>3</sub>COOH) and sodium bicarbonate (NaHCO<sub>3</sub>), to analyze the outcomes, and to predict future results under new conditions using artificial intelligence. In the initial phase of the study, real-life experiments were conducted using varying quantities of vinegar and baking soda. The volume of CO<sub>2</sub> produced was measured and systematically recorded. The course of the reaction was observed under different experimental conditions, including variations in temperature (20°C, 30°C, 35°C, and 40°C) and pressure (1 atm, 0.9 atm), and the influence of these factors on CO<sub>2</sub> production was analyzed.

The results clearly indicated that increasing temperature accelerated the kinetics of the reaction, leading to faster and greater gas formation. This observation is consistent with Le Chatelier's Principle and the kinetic theory. On the other hand, a decrease in pressure resulted in an increased gas volume, a phenomenon that can be evaluated in light of Boyle's Law. The experimental data were analyzed using an AI algorithm based on a Linear Regression model. The input variables included vinegar volume (ml), baking soda mass (g), temperature (°C), and pressure (atm), while the output variable was the volume of CO<sub>2</sub> (ml) produced. The model was initially trained on data from five different experimental setups and subsequently used to make predictions for new conditions not included in the training data.

The predictions made by the AI model closely aligned with the actual experimental outcomes. For instance, under the conditions of 18 ml of vinegar and 2.8 g of baking soda at 30°C and 1 atm, the model predicted approximately 135.5 ml of CO<sub>2</sub>, which demonstrated a

high degree of accuracy compared to the empirical result. Similarly, for an experiment involving 22 ml of vinegar and 3.2 g of baking soda at 20°C and 1 atm, the model predicted a CO<sub>2</sub> output of approximately 165.3 ml. These minor discrepancies confirmed that the model was effectively trained. The model's ability to make accurate predictions showed that it was not solely based on static data but also had the flexibility to adapt to changing experimental conditions. This confirms that artificial intelligence can serve as an effective tool for in-depth and multidimensional analysis of chemical reactions.

It is important to note that AI-based analysis not only automates the interpretation of experimental data but also helps students develop fundamental research skills such as data interpretation, identifying inter-variable relationships, and drawing scientific conclusions. Additionally, this methodology supports the implementation of modern pedagogical approaches in chemistry education. Students learn not only what reactions occur, but also why they occur and under which conditions. The use of artificial intelligence integrates both visual and analytical learning approaches, representing a practical manifestation of next-generation educational technologies in the classroom. In conclusion, the study confirmed that incorporating AI into chemistry education not only enriches the teaching process but also fosters the development of scientific reasoning and research competencies among students. This approach can be extended to other chemical reactions, laboratory experiments, and natural phenomena modeling, ultimately contributing to improved educational quality and functional efficiency.

## CONCLUSION

This study has explored the applicability of artificial intelligence – particularly tools such as ChatGPT and linear regression models – within the context of chemistry education, demonstrating the functional and pedagogical value of these technologies in the instructional process. The findings confirm that the integration of AI technologies into chemistry classes contributes not only to the acquisition of scientific knowledge but also significantly enhances critical thinking, analytical reasoning, and the ability to draw scientific conclusions. The AI model developed to analyze the reaction between vinegar and baking soda successfully predicted the amount of CO<sub>2</sub> gas produced and provided accurate estimations even under complex conditions by accounting for variables such as temperature and pressure. This illustrates that AI technologies are not only effective in analyzing laboratory-based phenomena but also serve as powerful tools in delivering personalized and adaptive learning within various teaching strategies. The study further emphasizes that the integration of AI into chemistry education is a key component of the broader digital transformation in education. Successful implementation requires teachers to possess adequate technological preparedness, the establishment of clear ethical frameworks, and the promotion of AI literacy among students. AI-based instructional approaches increase student engagement, allow for a deeper understanding of experimental outcomes, and improve learning efficiency through automated data analysis. Ultimately, the integration of AI technologies into chemistry education will play a pivotal role in shaping future teaching models. Research in this area lays the foundation for a more flexible, adaptive, and innovative educational system. Future studies should investigate the applicability of this approach across other disciplines, compare different AI models, and evaluate their effectiveness in large-scale learning environments.

## REFERENCES

- [1] Koubaa, A. GPT-4 vs. GPT-3.5: A concise showdown, *Preprints. Org.* 2023030422, **2023**, pp. 1-11, <https://www.preprints.org/manuscript/202303.0422/v1>
- [2] Rudolph, J. and Tan, S. ChatGPT: Bullshit spewer or the end of traditional assessments in higher education?, *Journal of applied learning and teaching*, 2023, v. 6(1), pp. 342-363, <https://doi.org/10.37074/jalt.2023.6.1.9>

- [3] Abuhassna, H.; Awae, F.; Adnan, M.; Daud, M. and Almheiri, A. The information age for education via artificial intelligence and machine learning: a bibliometric and systematic literature analysis, *International Journal of Information and Education Technology*, **2024**, v. 14(5), pp. 700-711, <https://doi.org/10.18178/ijiet.2024.14.5.2095>
- [4] Crompton, H. and Burke, D. Artificial intelligence in higher education: the state of the field, *International journal of educational technology in higher education*, 2023, v. 20(1), pp.1-22, <https://doi.org/10.1186/s41239-023-00392-8>
- [5] Marquez, R.; Barrios, N.; Vera, R.; Mendez, M.; Tolosa, L.; Zambrano, F. and Li, Y. A perspective on the synergistic potential of artificial intelligence and product-based learning strategies in biobased materials education, *Education for Chemical Engineers*, **2023**, v. 44, pp.164-180, <https://doi.org/10.21203/rs.3.rs-2711749/v1>
- [6]. Nagiyev, K.; Mirbagirova, G.; Mammadova, K. Enhancing experimental competencies in chemistry education through the use of virtual laboratories. *Baku State University Journal of Chemistry and Material Sciences*, **2025**, v. 2(1), pp.26–32. <https://doi.org/10.30546/209501.201.2025.1.02.069>
- [7] Maslej, N.; Fattorini, L.; Brynjolfsson, E.; Etchemendy, J.; Ligett, K.; Lyons, T. and Perrault, R. Artificial intelligence index report 2023, *arXiv preprint arXiv:2310.03715*, **2023**, pp.125-167, <https://doi.org/10.48550/arXiv.2310.03715>
- [8] Fuchs, K. Exploring the opportunities and challenges of NLP models in higher education: is Chat GPT a blessing or a curse?, In *Frontiers in education*, **2023**, v. 8, 1166682, pp.1-4, <https://doi.org/10.3389/feduc.2023.1166682>
- [9] Ray, P. ChatGPT: A comprehensive review on background, applications, key challenges, bias, ethics, limitations and future scope, *Internet of Things and Cyber-Physical Systems*, 2023, v. 3, pp. 121-154, <https://doi.org/10.1016/j.iotcps.2023.04.003>
- [10] Nazir, A. and Wang, Z. A comprehensive survey of ChatGPT: advancements, applications, prospects, and challenges, *Meta-radiology*, 2023, v. 1(2), pp.1-9, <https://doi.org/10.1016/j.metrad.2023.100022>
- [11] Asgarova, A.; Asadov, K.; Nagiyev, K. Formation of chemistry teachers' competencies for the organization of students' self-activities. *Baku State University Journal of Chemistry and Material Sciences*, **2025**, v. 2(1), pp.3–14. <https://doi.org/10.30546/209501.201.2025.1.02.079>
- [12] Chiu, W. Implications for the use of PowerPoint, classroom response systems, teams, and whiteboard to enhance online teaching of chemistry subjects in community college, *Journal of Chemical Education*, **2020**, v. 97(9), pp.3135-3139, <https://doi.org/10.1021/acs.jchemed.0c00830>