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INTEGRATION OF ARTIFICIAL INTELLIGENCE (AI) IN PROBLEM-BASED LEARNING (PBL) FOR CHEMISTRY EDUCATION

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Abstract: *This study used the Decision-Making Trial and Evaluation Laboratory (DEMATEL) method to examine the cause-and-effect relationships among key factors influencing the integration of Artificial Intelligence (AI) in Problem-Based Learning (PBL) for chemistry education. Four main factors were identified and analysed: AI guidance quality, AI adaptability to student mastery levels, AI support for scientific reasoning, and student engagement and motivation. Expert evaluation and cause-effect analysis revealed that AI guidance quality (D–R = 1.378) and AI adaptability to student levels (D–R = 0.348) are the main driving factors in this system. This means both factors exert strong influence on the other factors. In contrast, AI support for scientific reasoning (D–R = –0.477) and student engagement and motivation (D–R = –1.249) function primarily as effect factors—meaning they are influenced by other AI qualities and functions. Priority analysis based on D+R values showed that AI support for scientific reasoning is the most important factor in the overall system (6.227), followed by AI guidance quality (6.163) and AI adaptability (6.045). Overall, these findings emphasize that effective use of AI in chemistry PBL depends more on pedagogy-based AI design rather than technological features alone. AI guidance quality and its ability to adapt to student levels serve as essential foundations for enhancing students' scientific thinking abilities while also increasing their engagement and motivation in learning.*

Keywords: *Artificial Intelligence; Problem-Based Learning; Chemistry Education; DEMATEL Analysis; AI Scaffolding; Scientific Reasoning*

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Introduction

The Artificial Intelligence (AI) has emerged as a transformative force in education, shifting learning from traditional teacher-centered approaches toward experiences that are more personalized, adaptive, and data-driven (Holme et al., 2015; Hwang & Tu, 2021). AI technologies—including machine learning, natural language processing, intelligent tutoring systems, and adaptive learning platforms—offer new opportunities to enhance teaching effectiveness and student learning outcomes. In chemistry education, the growing significance of AI is reflected in its recognition by the International Union of Pure and Applied Chemistry (IUPAC) as one of the "10 Most Important New Technologies in Chemistry 2023" (Gomollón-Bel, 2023). Educational applications of AI, such as automated assessment, personalized content delivery, and real-time feedback, further highlight its potential to improve the quality of chemistry teaching and learning (Yildirim & Akcan, 2024).

Alongside these developments, Problem-Based Learning (PBL) has been widely established as an effective student-centred pedagogical approach in chemistry education. By engaging students in solving complex, real-world problems, PBL supports conceptual understanding, critical thinking, self-directed learning, and long-term knowledge retention (Hmelo-Silver, 2004). Its inquiry-oriented nature aligns closely with the epistemic practices of chemistry, fostering hypothesis formulation, experimental design, data analysis, and evidence-based reasoning, while also developing students' problem-solving, collaboration, and metacognitive skills (Willemse et al., 2019). Despite the strong theoretical alignment between AI and PBL, significant challenges continue to limit the effective integration of AI within chemistry-based PBL environments. Many existing AI tools are designed for general educational use and lack the domain-specific chemical knowledge needed to support abstract reasoning, complex problem-solving, and theory–practice connections central to chemistry learning (Feldman-Maggor et al., 2025; Yildirim & Akcan, 2024).

Ethical and educational risks further complicate AI integration, including threats to academic integrity, student over-reliance on AI-generated outputs, reduced development of critical thinking, and the potential for biased or scientifically inaccurate feedback (GEM Report UNESCO, 2023; Watts et al., 2023). Studies have shown that generative AI tools may produce explanations that appear sophisticated yet contain conceptual or mechanistic errors inconsistent with accepted chemical principles (Talanquer, 2022; Yik & Dood, 2024). Moreover, the rapid content generation capabilities of AI challenge conventional assessment practices and raise equity concerns, as unequal access to AI resources may widen existing educational disparities (Clark et al., 2024; Guzmán et al., 2019). Addressing these challenges requires a coordinated and multi-dimensional approach, including the development of chemistry-specific AI tools aligned with PBL principles, targeted professional development for teachers, evidence-based ethical guidelines, and institutional strategies that promote equitable access. These efforts are essential to ensure that the integration of AI in PBL genuinely supports students' scientific thinking and meaningful learning in chemistry, rather than encouraging superficial learning or inequitable learning practices.

Literature Review

Effectiveness of AI in Chemistry Education: Empirical Evidence

The increasing body of research on the use of Artificial Intelligence (AI) in chemistry education shows encouraging results, but it also highlights several important issues that need to be carefully considered. In general, most studies report positive effects on learning outcomes,

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particularly in supporting the learning process. However, researchers continue to raise concerns related to ethical issues and academic integrity. Evidence from existing studies indicates that AI applications are most commonly used in higher education, with intelligent tutoring systems and conversational agents such as ChatGPT being the most frequently adopted tools. Research has also shown that AI-based tutoring systems used for solving stoichiometry problems, including highly scaffolded systems (e.g., Stoich Tutor) and dynamically scaffolded systems (e.g., ORCCA), are effective in improving students' procedural learning. Systems that provide more structured and detailed scaffolding tend to produce better gains in conceptual understanding, as they offer more opportunities for students to practice unit analysis and chemical operations (Borchers et al., 2025; King et al., 2022). Interestingly, student preference data reveal a contrasting pattern, as learners often prefer systems that provide less guidance, even though these systems result in lower learning outcomes. This finding suggests that the relationship between student autonomy, level of scaffolding, and learning effectiveness is complex and requires careful consideration when integrating AI into PBL environments.

The impact of generative AI tools in chemistry education presents additional challenges that need to be addressed. A study by Watts et al., (2023), which compared student responses with multiple AI chatbot responses in organic chemistry writing tasks, found clear differences not only among chatbot outputs but also between the problem-solving approaches of chatbots and students. Their analysis showed that AI chatbots generally do not engage in mechanistic reasoning at the same level as students, raising concerns about the suitability of AI-generated content as a learning model. Similarly, Yik & Dood (2024) reported that although ChatGPT can produce explanations of organic reaction mechanisms that appear detailed and convincing, these explanations often contain subtle but scientifically significant inaccuracies. This is concerning because students may accept incorrect information without critically evaluating it. Overall, these findings highlight the importance of developing students' critical evaluation skills alongside the use of AI in learning. Students should be guided to use AI as a learning support tool while also being trained to question, verify, and correct AI-generated information rather than accepting it uncritically.

Problem-Based Learning in Chemistry: Foundations and Outcomes

Numerous meta-analyses and systematic reviews consistently report the positive effects of Problem-Based Learning (PBL) on various aspects of student development. Schmidt-McCormack et al., (2019) found that PBL increases students' motivation and interest by making learning more engaging and personally meaningful. Similarly, Dochy et al. (2003) reported that PBL has a positive impact on students' self-regulation and confidence in their ability to learn independently, which are important affective factors for sustained academic engagement. From a cognitive perspective, many studies show that PBL improves chemistry students' conceptual understanding, critical thinking skills, and problem-solving abilities more effectively than traditional teaching methods (Gürses et al., 2007; Hmelo-Silver, 2004). More recent studies have expanded understanding of PBL effectiveness across different chemistry topics and educational levels. Research on the use of PBL in electrochemistry has shown significantly higher achievement among students exposed to PBL compared to those taught using traditional expository instruction (Bilgin et al., 2017). Studies at the lower secondary level also indicate that PBL not only improves academic achievement but also enhances students' attitudes toward chemistry (Charif et al., 2017). However, the existing literature also highlights important research gaps and implementation challenges. Research on PBL in secondary school chemistry remains limited, as most studies focus on university or lower secondary contexts (Yildirim & Akcan, 2024). In addition, effective PBL implementation requires adequate teacher training,

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sufficient resources, substantial time investment, and careful problem design. These factors are often underreported in previous studies despite their strong influence on PBL effectiveness (Hung, 2025; Koh et al., 2025). Another ongoing challenge discussed in the literature is the difficulty of implementing PBL in large classes while maintaining intensive facilitator support and meaningful small-group collaboration, which are essential features of effective PBL.

Synergies Between AI and PBL: Theoretical Frameworks

The integration of Artificial Intelligence (AI) with Problem-Based Learning (PBL) is supported by several key educational theoretical frameworks, including social constructivism, cognitive load theory, and intelligent tutoring systems (ITS). From a social constructivist perspective, AI technologies can support collaborative knowledge construction by promoting active student engagement and peer interaction, which are central elements of PBL (Vygotsky, 1978; Graesser et al., 2018). AI-based learning scaffolding can also be understood as operating within students' zones of proximal development, by providing adaptive support that helps learners progress from their current level of competence toward higher levels of achievement (Belland, 2017; Plass & Pawar, 2020). According to cognitive load theory, well-designed AI systems are able to reduce extraneous cognitive load by handling routine calculations, presenting problems in a more structured manner, and providing timely access to relevant information. This allows students' working memory to be used more efficiently for developing deeper understanding of chemistry concepts, which is essential for problem-solving within PBL environments (Sweller et al., 1998; Mousavinasab et al., 2021). Research on intelligent tutoring systems (ITS) further provides specific frameworks for understanding how AI can enhance the implementation of PBL in chemistry education. VanLehn's (2006) taxonomy of tutoring behaviors identifies several key functions that AI systems can perform in PBL contexts, including problem selection, instructional scaffolding, learning assessment, and metacognitive support. Recent advances in adaptive learning technologies demonstrate that AI can personalize PBL experiences by analyzing student performance data, identifying knowledge gaps, adjusting problem difficulty, and delivering targeted feedback without requiring continuous teacher intervention (Kulik & Fletcher, 2016; Graesser et al., 2018). In addition, the Technological Pedagogical Content Knowledge (TPACK) framework has been applied to examine chemistry teachers' competencies in implementing AI-enhanced PBL. This highlights that effective AI integration requires not only strong understanding of chemistry content and PBL pedagogy, but also informed awareness of AI capabilities, limitations, and ethical implications (Mishra et al., 2023; Celik, 2023; Lorenz & Romeike, 2023).

Critical Debates: Challenges and Ethical Considerations

Although the integration of Artificial Intelligence (AI) with Problem-Based Learning (PBL) offers strong potential, several key issues require careful attention. One major concern is that many existing AI systems still rely on fixed algorithms that do not fully reflect the contextual, open-ended, and collaborative nature of PBL (Luckin et al., 2016; Castaneda & Selwyn, 2018). Research has also shown that excessive reliance on AI-based scaffolding may weaken core PBL goals, such as reducing productive learning challenges, limiting exploration of multiple problem-solving strategies, and decreasing opportunities for students to develop self-directed learning skills (Belland, 2017; Loyens et al., 2023). In addition, ethical issues related to the use of AI in chemistry education have been widely discussed. Studies have identified risks such as bias, inaccurate information, and AI hallucinations, which may negatively affect learning if students accept AI-generated content without critical evaluation (Talanquer, 2023; Yik & Dood, 2024). UNESCO's framework on generative AI in education highlights eight critical concerns, including human agency, equity, cultural diversity, data privacy, consent in content use, model

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transparency, digital information pollution caused by AI-generated content, and the risk of marginalizing diverse perspectives (Miao & Holmes, 2023). Recent studies emphasize that responsible AI integration requires explicit attention to these ethical dimensions. This includes transparent communication about the limitations of AI systems, the development of students' critical AI literacy, and the design of assessment methods that can distinguish genuine student learning from task completion that relies heavily on AI support (Feldman-Maggor et al., 2024; Susnjak & McIntosh, 2024).

Overall, the literature review reveals several important research gaps that need to be addressed in studies on AI-integrated PBL in chemistry education. Most existing studies are short-term in nature and place limited emphasis on long-term learning outcomes. In addition, understanding of how different types and levels of AI scaffolding influence various aspects of chemistry learning—such as conceptual understanding, procedural skills, scientific reasoning, and collaborative learning—remains limited. Teacher perspectives, professional development needs, and practical challenges of classroom implementation have also received insufficient attention, despite their critical importance for successful adoption. Given the rapid advancement of AI technologies, these gaps highlight the need for a systematic and evidence-based research approach to identify and prioritize the key factors that influence the effectiveness of AI integration in chemistry PBL. Therefore, this study employs a structured analytical method to examine the cause–effect relationships among the main factors affecting the implementation of AI-supported PBL in chemistry education.

Methodology

This study employed the Decision-Making Trial and Evaluation Laboratory (DEMATEL) method. DEMATEL is a structural modeling technique developed by the Science and Human Affairs Program of the Battelle Memorial Institute in Geneva between 1972 and 1976 to analyze complex real-world problems (Fontela & Gabus, 1976). Over time, DEMATEL has evolved into an effective multi-criteria decision-making tool that allows researchers to visualize cause–effect relationships among factors within complex systems through the construction of structural models and impact–relation maps (Si et al., 2018). The key strength of the DEMATEL method lies in its ability to convert qualitative judgments into quantitative indicators, thereby revealing interdependencies and feedback relationships among system elements (Wu & Lee, 2007). Unlike traditional analytical approaches that assume criteria are independent, DEMATEL explicitly considers the mutual influence and complex relationships that exist in real decision-making situations. As a result, this method is particularly useful for identifying critical factors and for understanding both the direct and indirect effects of one factor on others within a system (Tzeng et al., 2007).

DEMATEL Procedural Framework

The implementation of the DEMATEL method involves a systematic five-step procedure designed to transform expert judgments into a structural model that reveals cause–effect relationships among the factors under study. The first step is the construction of the direct-relation matrix, in which experts evaluate the degree of direct influence between each pair of factors using a predefined scale, typically ranging from 0 (no influence) to 4 (very high influence) (Seyed-Hosseini et al., 2006). The second step involves normalizing the direct-relation matrix by dividing each value by the maximum row sum. This process ensures that all values fall within a standardized and comparable range (Lin & Wu, 2008). In the third step, the total-relation matrix is calculated to capture both direct and indirect influences among the factors. This matrix is obtained using the formula $T = X(I - X)^{-1}$, where X represents the

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normalized direct-relation matrix and I denotes the identity matrix (Tseng, 2009). The fourth step calculates the prominence and relationship indices by summing the rows (D) and columns (R) of the total-relation matrix. The value D + R indicates the overall importance of each factor within the system, while D − R distinguishes between cause factors (positive values) and effect factors (negative values) (Liou et al., 2007). The final step is the construction of a cause–effect diagram, where these indices are plotted on a two-dimensional graph. The horizontal axis represents factor importance (D + R), and the vertical axis represents causal relationships (D − R). This visual representation clearly illustrates the structural relationships among factors and supports informed decision-making and strategic planning (Hsu et al., 2013; Yang & Tzeng, 2011).

Table 1: Step in DEMATEL

Step 1	**Generate the Direct-Relation Matrix** Purpose: To identify the relationships among n criteria/factors within the system Procedure: • Construct an n × n matrix, where *n* represents the number of factors • Each expert is asked to complete the matrix independently • Values in each row represent the influence of one factor on other factors • Values in each column represent the influence received by that factor from other factors • When multiple experts are involved, calculate the average (mean) of all expert evaluations to obtain a single direct-relation matrix Formula: $$\mathbf{X} = \begin{bmatrix} \mathbf{0} & \cdots & \boldsymbol{x_{n1}} \\ \vdots & \ddots & \vdots \\ \boldsymbol{x_{1n}} & \cdots & \mathbf{0} \end{bmatrix}$$ Note: The diagonal values of the matrix (where row = column) are set to 0, as a factor does not influence itself
Step 2	**Compute the normalized direct-relation matrix** Purpose: To standardize all values within a common range so that they can be easily compared Procedure: • Calculate the sum of each row and each column in matrix X • Identify the maximum value among all row and column sums (denoted as k) • Divide each element in matrix X by the value k Formula: $$k = max\left\{max \sum_{j=1}^{n} x_{ij}, \sum_{i=1}^{n} x_{ij}\right\}$$ $$N = \frac{1}{k} * X$$ Output: A normalized matrix (N), where all values range between 0 and 1
Step 3	Compute the total relation matrix Purpose: To capture both direct and indirect influences among all factors in the system Procedure: • Generate an n × n identity matrix (I), where diagonal elements are 1 and all other elements are 0 • Subtract the normalized matrix N from the identity matrix to obtain (I − N) • Compute the inverse of the matrix (I − N), denoted as $(I - N)^{-1}$ • Multiply the normalized matrix N by $(I - N)^{-1}$ to obtain the total-relation matrix

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	Formula: $$T = \lim_{k \to +\infty} (N^1 + N^2 + \cdots + N^k)$$ Equivalent to: $T = N \times (I - N)^{-1}$ Output: The total-relation matrix (T), which represents the overall influence (direct and indirect) among all factors.
Step 4	**Setting the Threshold Value** Purpose: • To identify significant causal relationships among factors • To eliminate weak or negligible relationships when constructing the Network Relationship Map (NRM) Procedure: • Calculate the average value of all elements in the total-relation matrix T • Use this average value as the threshold value • Compare each element in matrix T with the threshold value • Set all values below the threshold to zero, as these relationships are considered insignificant • Retain only values greater than the threshold for further analysis and visualization Application in NRM: • Only relationships with values greater than the threshold are displayed in the Network Relationship Map (NRM) • Partial or weak relationships are excluded to produce a clearer and more meaningful causal structure Threshold Value Used in This Study: • Threshold value = 0.811 Output: • A filtered internal relations matrix used to construct the NRM, showing only meaningful causal links among factors
Step 5	**Final output and create a causal diagram** Purpose: To determine the importance and causal role of each factor in the system Procedure: Calculate the sum of each row in matrix T to obtain D $D = \sum_{j=1}^{n} T_{ij}$ Calculate the sum of each column in matrix T to obtain R $R = \sum_{i=1}^{n} T_{ij}$ Compute D + R and D − R for each factor Interpretation: • D + R → Indicates the overall importance (prominence) of a factor in the system • D − R → Indicates the net effect of a factor: Positive value → Cause factor Negative value → Effect factor Output: A causal diagram, where: Horizontal axis = D + R (importance) Vertical axis = D − R (cause–effect)

Sampling Technique for DEMATEL Application

Selecting an appropriate sampling technique is a critical part of implementing the DEMATEL method, as the quality and representativeness of expert judgments directly affect the validity and reliability of the resulting structural model. Purposive sampling, also known as judgmental or expert sampling, is the most commonly used approach in DEMATEL studies. In this method, participants are deliberately selected based on their specialized knowledge, relevant experience, and deep understanding of the problem being studied (Patton, 2002; Etikan et al., 2016). The

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appropriate sample size for DEMATEL studies is still debated among researchers. However, most studies recommend involving between 5 and 15 experts, as this range provides a balance between obtaining diverse perspectives and managing practical constraints such as data collection and consensus building (Chen & Hung, 2010; Li & Tzeng, 2009). Experts are usually selected based on several criteria, including more than five years of professional experience in the relevant field, at least a master's degree, current involvement in related decision-making processes, and demonstrated expertise through publications or practical achievements (Dalalah et al., 2011; Shieh et al., 2010). In this study, five experts were selected as the main participants to provide expert judgments for the implementation of the DEMATEL method.

DEMATEL Questionnaire Scale Explanation

This study employs the DEMATEL (Decision Making Trial and Evaluation Laboratory) method to analyze the cause–effect relationships among the identified factors. Respondents were asked to evaluate the degree of direct influence of each factor on other factors using a five-point scale. The definition of each score in this five-point scale is presented in Table 2.

Table 2: DEMATEL Influence Scale Used in the Study

Score	Level of Influence	Description
0	No influence	The factor has no direct influence on another factor
1	Low influence	The factor has a very minimal effect on another factor
2	Moderate influence	The factor has a reasonable level of effect on another factor
3	High influence	The factor has a significant effect on another factor
4	Very high influence	The factor has a very strong cause–effect relationship with another factor

Findings

Table 3.1: Direct Relation Matrix

	Quality of AI Scaffolding	AI Adaptivity to Student Proficiency Levels	AI Support for Scientific Reasoning	Student Engagement & Motivation
Quality of AI Scaffolding	0	3.6	3.6	3.6
AI Adaptivity to Student Proficiency Levels	2.6	0	3.2	3
AI Support for Scientific Reasoning	2.4	2.2	0	3.2
Student Engagement & Motivation	1.2	2	2.6	0

Table 3.2: The Normalized Direct-Relation Matrix

	Quality of AI Scaffolding	AI Adaptivity to Student Proficiency Levels	AI Support for Scientific Reasoning	Student Engagement & Motivation
Quality of AI Scaffolding	0	0.333	0.333	0.333
AI Adaptivity to Student Proficiency Levels	0.241	0	0.296	0.278
AI Support for Scientific Reasoning	0.222	0.204	0	0.296
Student Engagement & Motivation	0.111	0.185	0.241	0

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Table 3.3: The Total Relation Matrix

	Quality of AI Scaffolding	AI Adaptivity to Student Proficiency Levels	AI Support for Scientific Reasoning	Student Engagement & Motivation
Quality of AI Scaffolding	0.598	0.962	1.088	1.122
AI Adaptivity to Student Proficiency Levels	0.7	0.602	0.938	0.956
AI Support for Scientific Reasoning	0.634	0.71	0.637	0.894
Student Engagement & Motivation	0.46	0.575	0.689	0.517

Table 3.4: The Total Relationships Matrix by Considering the Threshold Value

	Quality of AI Scaffolding	AI Adaptivity to Student Proficiency Levels	AI Support for Scientific Reasoning	Student Engagement & Motivation
Quality of AI Scaffolding	0	0.962	1.088	1.122
AI Adaptivity to Student Proficiency Levels	0	0	0.938	0.956
AI Support for Scientific Reasoning	0	0	0	0.894

Table 3.5: The Final Output

	R	**D**	**D+R**	**D-R**
Quality of AI Scaffolding	2.392	3.771	6.163	1.378
AI Adaptivity to Student Proficiency Levels	2.849	3.197	6.045	0.348
AI Support for Scientific Reasoning	3.352	2.875	6.227	-0.477
Student Engagement & Motivation	3.489	2.24	5.729	-1.249

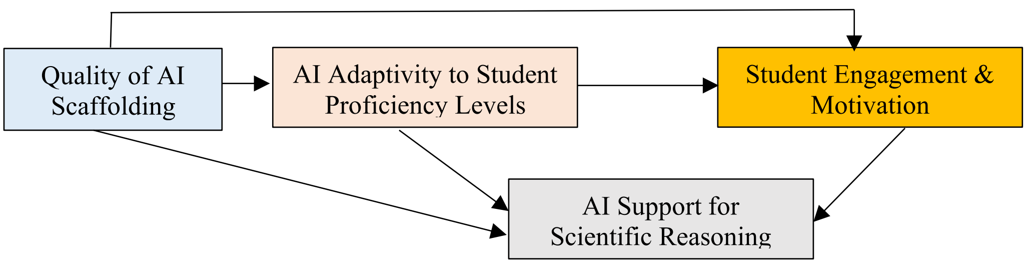

Figure 1: DEMATEL Based Structural Model of AI Integration Factors in Chemistry Problem-Based Learning

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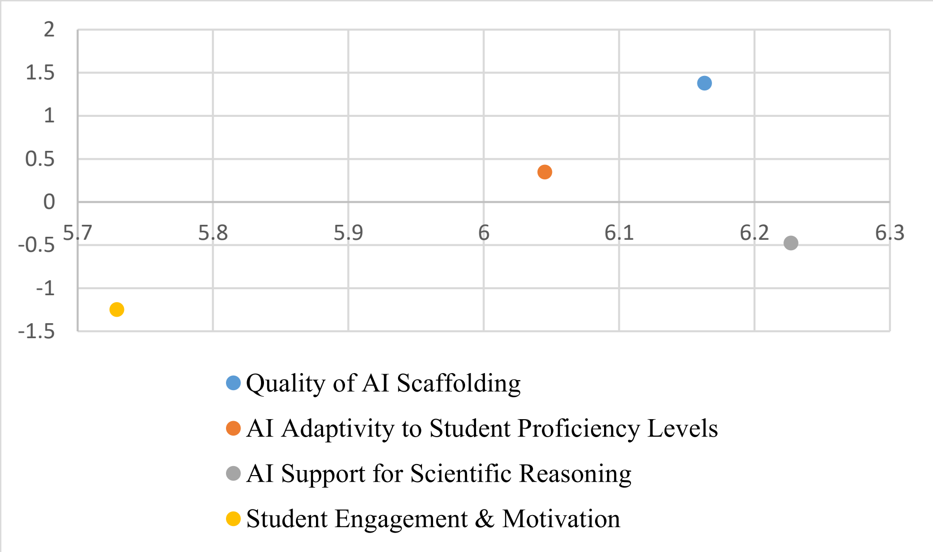

Figure 2: Cause–Effect Diagram

Discussion

The cause–effect diagram produced from the DEMATEL analysis provides a clear understanding of the structural relationships among the key factors influencing the integration of Artificial Intelligence (AI) in Problem-Based Learning (PBL) for chemistry education. Based on the positions of the factors along the importance (D + R) and cause–effect (D − R) axes, the results distinguish between driving factors and outcome factors within the system. The findings show that Quality of AI Scaffolding is the most influential driving factor, with high importance and a positive net effect, highlighting its foundational role in supporting students as they solve complex chemistry problems through structured guidance and step-by-step reasoning support. AI Adaptivity to Student Proficiency Levels also functions as a driving factor, indicating that AI systems capable of adjusting feedback and task difficulty based on students' learning levels are important for effective PBL implementation. In contrast, AI Support for Scientific Reasoning and Student Engagement and Motivation emerge as outcome factors that are mainly influenced by the quality and adaptivity of AI support rather than acting as direct drivers themselves. This suggests that improvements in reasoning and motivation do not occur automatically through AI use, but instead result from well-designed, pedagogically aligned AI scaffolding. Overall, the findings emphasize that successful AI integration in chemistry PBL depends more on strong instructional design and adaptive support than on surface-level outcomes alone.

Conclusion

The DEMATEL analysis in this study establishes a clear cause–effect hierarchy among the factors influencing the integration of Artificial Intelligence (AI) in Problem-Based Learning (PBL) for chemistry education. The findings show that quality of AI scaffolding and AI adaptivity to students' proficiency levels act as the main driving factors, which in turn influence AI support for scientific reasoning as well as student engagement and motivation. These results clarify that AI does not automatically improve learning outcomes; rather, its effectiveness in PBL depends on how well AI is designed to guide students and adapt support to their learning levels. For chemistry teachers and educational technologists, these findings offer practical guidance by highlighting the need to prioritize the development of chemistry-specific AI scaffolding grounded in domain expertise, adaptive algorithms that respond to individual learning progress, and professional development programs that equip teachers with the skills to

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integrate AI strategically within PBL contexts. As the use of AI in education continues to grow globally, this study provides empirical evidence that technological sophistication must be balanced with pedagogical sophistication to fully realize the potential of AI in chemistry education. Future research is recommended to validate these cause–effect relationships through longitudinal studies, explore contextual variations across different student populations and chemistry topics, and develop evidence-based frameworks that support the co-design of AI systems by chemistry educators, students, and technology developers to ensure alignment with authentic learning needs in scientific problem-solving.

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